X-RAY CRYSTALLOGRAPHIC STUDIES OF FOUR PHOTOREACTIVE TETRAHYDRONAPHTHOQUINOL DERIVATIVES AND FIVE RELATED COMPOUNDS

by

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ABSTRACT

The structures of four 4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4-ol derivatives have been studied and related to their observed photochemical reactivity. H-abstractions are dominant in the solid state photolyses of these compounds because of their conformations and the topochemical control by the lattice. All structures have been solved by direct methods and refined by least squares procedures. The 2,3,6,7-tetramethyl-4α-ol derivative, $C_{14}H_{20}O_2$, is monoclinic, space group $C2/c$, a = 13.898(3), b = 5.228(1), c = 17.316(3) Å, β = 97.442(7)° and Z = 4. This structure was refined to R = 0.058 for 888 reflections. The 2,3- and 6,7-dimethyl-4α-ol compounds $C_{12}H_{16}O_2$, are orthorhombic, space group $P2_12_12_1$, and monoclinic, space group $P2_1/c$, respectively. For the 2,3-derivative, a = 5.148(1), b = 12.269(2), c = 16.478(3) Å, Z = 4 and the refinement of 671 data led to an R of 0.031. The 6,7-compound, a = 9.242(3), b = 22.724(3), c = 5.139(2) Å, β = 102.7(1)°, Z = 4, was refined to R = 0.032 for 626 data. 2,3,4α,4aβ,6,7,8aβ-heptamethyl-4β-ol, $C_{17}H_{26}O_2$, is monoclinic, space group $P2_1/c$, a = 7.497(2), b = 16.792(3), c = 12.687(3) Å, β = 105.30(1)° and Z = 4. An R-value of 0.041 was obtained from the refinement of 1934 reflections. The above compounds have similar conformations which are favorable to H-abstraction reactions.

The 6,7-dimethyl-1α,4α-diol $C_{12}H_{18}O_2$, crystallizes in the monoclinic system, space group $P2_1/c$, a = 13.870(2),

$\underline{b}$ = 18.025(4), $\underline{c}$ = 9.236(1) Å, β = 108.098(6)° , $\underline{Z}$ = 8 and was refined to R = 0.032 for 1461 reflections. The diol compound adopts the same conformation as those above but is not photoreactive. The following four compounds were derived from either tetrahydronaphthoquinol progenitors or their oxidized forms, tetrahydronaphthoquinones. A twistane-like structure, twistenone $C_{10}H_{10}O_2$, was found to crystallize in the monoclinic system, space group $\underline{P}2_1/\underline{n}$, $\underline{a}$ = 6.381(2), $\underline{b}$ = 19.454(2), $\underline{c}$ = 6.708(2) Å, β = 106.24(1)° and $\underline{Z}$ = 4. Refinement of 930 reflections converged at R = 0.037. 5-(2,3-dimethylphenyl)-γ-butyrolactone crystals, $C_{12}H_{14}O_2$, are monoclinic, space group $\underline{P}2_1/\underline{n}$, $\underline{a}$ = 10.847(3), $\underline{b}$ = 6.924(1), $\underline{c}$ = 13.654(4) Å, β = 95.22(1)° and $\underline{Z}$ = 4. The structure was refined to R = 0.057 for 569 reflections. It was hoped that elucidation of this structure would aid in determining the intermediate compound from which it was formed. The methylene ketone $C_{17}H_{24}O$, derived from the acetylation product of the previously described heptamethyl-4β-ol, is monoclinic, space group $\underline{P}2_1/\underline{a}$, $\underline{a}$ = 12.374(2), $\underline{b}$ = 8.771(1), $\underline{c}$ = 13.743(2) Å, β = 104.027(6)° , $\underline{Z}$ = 4 and refined to R = 0.037 for 1369 data. A reaction designed to pinacolize a diketone cage compound resulted in a different product from which the hydroxy mesylate derivative $C_{17}H_{28}O_4S$, was formed. The crystals are monoclinic, space group $\underline{P}2_1/\underline{c}$, $\underline{a}$ = 9.246(2), $\underline{b}$ = 10.938(1), $\underline{c}$ = 17.335(4) Å, β = 102.11(1)° and $\underline{Z}$ = 4. Refinement converged at R = 0.042 for 2995 reflections.

TABLE OF CONTENTS

Title Page i

Abstract ii

Table Of Contents iv

List Of Tables vii

List Of Figures x

Acknowledgement xii

GENERAL INTRODUCTION 1

Crystallographic Introduction 2

Data Collection 2

Determination Of Cell Constants 5

Data Reduction 5

Solution By Direct Methods 6

Refinement 11

Chemical Introduction 12

Photochemistry: Structure-Reactivity Relationships .. 12

Thesis Outline 19

Schematic Of The Thesis Layout 21

PART I 22

CHAPTER I: 2,3,6,7-TETRAMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-NAPHTHOQUIN-4α-OL 23

Introduction 24

Experimental 24

Solution And Refinement 27

Discussion 30

CHAPTER II: 2,3-DIMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-

NAPHTHOQUIN-4α-OL

AND 6,7-DIMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-NAPHTHOQUIN-4α

-OL 42

Introduction 43

Experimental 43

Solution And Refinement 46

2,3-Dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-

ol 46

6,7-Dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-

ol 47

Discussion 48

CHAPTER III: 2,3,4α,4aβ,6,7,8aβ-HEPTAMETHYL-4aβ,5,8,8aβ-

TETRAHYDRO-1-NAPHTHOQUIN-4β-OL 65

Introduction 66

Experimental 66

Solution And Refinement 68

Discussion 69

Comparison Of Compounds (III)-(VII) 75

CHAPTER IV: 6,7-DIMETHYL-4aβ,5,8,8aβ-TETRAHYDRONAPHTHOQUIN-

1α,4α-DIOL 94

Introduction 95

Experimental 96

Solution And Refinement 98

Discussion 103

Comparison With Tetrahydronaphthoquin-4α-ols 112

Asymmetric Unit Size - Structure Comparison 118

PART II 120

CHAPTER V: A TWISTANE DERIVATIVE (TWISTENONE) 121

Introduction 122

Experimental 124

Solution And Refinement 125

Discussion 126

CHAPTER VI: 5-(2,3-DIMETHYLPHENYL)-γ-BUTYROLACTONE 137

Introduction 138

Experimental 139

Solution And Refinement 140

Discussion 143

CHAPTER VII: 1,3,4,5,6,9-HEXAMETHYL-8-EXO-METHYLENETRICYCLO [4.4.0.$0^{3,9}$]DEC-4-ENE-2-ONE 154

Introduction 155

Experimental 155

Solution And Refinement 157

Discussion 161

CHAPTER VIII: 1,2,3,5,6,8-HEXAMETHYL-4-MESYL-7-HYDROXY-TETRACYCLO[4.2.1.$1^{2,5}$.$0^{3,7}$]DECANE 172

Introduction 173

Experimental 173

Solution And Refinement 176

Discussion 181

SUMMARY 190

References 193

SUPPLEMENTARY MATERIAL 198

LIST OF TABLES

GENERAL INTRODUCTION 1

PART I 22

CHAPTER I 23

I. Positional and isotropic thermal parameters ... 31

II. Anisotropic thermal parameters 32

III. Bond lengths and angles 36

IV. Bond lengths and angles involving hydrogen atoms 37

V. Torsion angles 39

CHAPTER II 42

VI. Positional and isotropic thermal parameters ... 48

VII. Anisotropic thermal parameters 50

VIII. Torsion angles 51

IX. Geometrical parameters in the β-enone abstraction reaction 57

X. Bond lengths and angles 61

CHAPTER III 65

XI. Positional and isotropic thermal parameters ... 70

XII. Anisotropic thermal parameters 72

XIII. Parameters relevant to photochemical activity in the derivatives 77

XIV. Bond lengths in the derivatives 82

XV. Bond angles in the derivatives 83

XVI. Torsion angles in the derivatives 86

XVII. Supplementary bond lengths and angles in (VI) . 88

XVIII. Bond lengths involving hydrogen atoms in (VI) . 89
XIX. Bond angles involving hydrogen atoms in (VI) .. 90
XX. Supplementary torsion angles in (VI) 91
CHAPTER IV 94
XXI. Positional and isotropic thermal parameters ... 100
XXII. Anisotropic thermal parameters 102
XXIII. Bond lengths 106
XXIV. Bond angles 107
XXV. Bond lengths involving hydrogen atoms 108
XXVI. Bond angles involving hydrogen atoms 109
XXVII. Hydrogen bonding geometries 111
XXVIII. Torsion angles 113
PART II 120
CHAPTER V 121
XXIX. Positional and isotropic thermal parameters ... 127
XXX. Anisotropic thermal parameters 128
XXXI. Bond lengths 129
XXXII. Least squares planes 130
XXXIII. Bond angles 135
CHAPTER VI 137
XXXIV. Positional and isotropic thermal parameters ... 144
XXXV. Anisotropic thermal parameters 145
XXXVI. Bond lengths and angles 148
XXXVII. Bond lengths and angles involving hydrogen atoms 149
XXXVIII. Torsion angles 150
CHAPTER VII 154
XXXIX. Positional and isotropic thermal parameters ... 159

XL. Anisotropic thermal parameters 160

XLI. Bond angles 162

XLII. Bond angles involving hydrogen atoms 164

XLIII. Torsion angles 165

XLIV. Bond lengths 168

XLV. Bond lengths involving hydrogen atoms 169

CHAPTER VIII 172

XLVI. Positional and isotropic thermal parameters ... 178

XLVII. Anisotropic thermal parameters 180

XLVIII. Torsion angles 183

XLIX. Bond lengths 185

L. Bond angles 186

LIST OF FIGURES

GENERAL INTRODUCTION 1

1. Definitions of τ_o and Δ_o 15
2. Production of 4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4-ols 16
3. Conformations in naphthoquinols 18
4. Definitions of τ_c and Δ_c 18
5. Relationship of the diol to naphthoquinones and naphthoquinols 20

PART I 22

CHAPTER I 23

6. Preparative reaction scheme 25
7. E-map; projection onto least squares plane through electron density peaks 29
8. Stereo diagram of the molecular packing of type A molecules 34
9. Stereo diagram of the molecule 35

CHAPTER II 42

10. Stereo diagrams of the molecules 56
11. Stereo packing diagrams 59

CHAPTER III 65

12. Stereo diagram of the molecule 73
13. Stereo packing diagram 75

CHAPTER IV 94

14. Stereo diagram of a type A molecule 103
15. Stereo packing diagram 104

PART II 120

CHAPTER V 121

16. Results of different methods of irradiation 123

17. Torsion angles 131

18. Torsion angles in twistane and the idealized twist-boat conformation 133

19. Stereo diagram of the molecule 134

20. Stereo packing diagram 136

CHAPTER VI 137

21. Reaction scheme leading to the lactone 139

22. Stereo diagram of the molecule 146

23. Stereo packing diagram 147

CHAPTER VII 154

24. Reaction scheme leading to the methylene ketone .. 156

25. Stereo diagrams of the molecule and the contents of the unit cell 171

CHAPTER VIII 172

26. Reaction scheme leading to the hydroxy mesylate derivative 174

27. Stereo packing diagram 181

28. Stereo diagram of the molecule 188

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GENERAL INTRODUCTION

Crystallographic Introduction

The fundamental principles and techniques of X-ray diffraction in crystal structure analysis are given in several texts (1-6). In addition, the various methods of obtaining a structural solution and refining that solution given a reliable data set have been well-developed and elegantly communicated by a number of authors (7-15). Throughout the text that follows, references will be made to these invaluable contributors in conjunction with their contributions to the art of crystallography.

The general procedures of data collection and structural solution and refinement are common to all structures presented in this work. It is hoped that an outline of these procedures will enable the reader to appreciate better the ensuing experimental sections.

Data collection

Data for all structures were measured on an Enraf-Nonius CAD4 automatic diffractometer. Usually, a crystal is mounted on the goniometer in a general orientation. An automatic search routine is then invoked to explore reciprocal space in a methodical manner in an effort to find up to a maximum of 25 reflections. Accurate positioning of these reflections is effected by a centering procedure in which different types of scans and apertures are employed in locating the reflection peak-centers. The resulting setting angles are used in composing

a collection of vectors which includes the scattering vector for each reflection and the sum and difference vectors for each combination of two scattering vectors. From this vector set a primitive cell and orientation matrix are determined, and the reflections' indices are calculated. Refinement of the orientation matrix, effected by further centering of the reflections and followed by a least squares fitting procedure, is continued until the angular deviation between the real scattering vector (based on integral h,k,l values) and the scattering vector calculated from the most recent orientation matrix is less than 0.05° for all measured reflections. Once a suitable orientation matrix is obtained, the parameters to be employed in data collection are chosen. A brief description of the collection procedure with the most commonly adjusted parameters underlined is included in the following paragraphs.

The region of reciprocal space to be explored is restricted to a range of theta values which, for practical purposes, is limited by the crystal's general scattering ability. An omega scan angle is derived from the expression (DOMA + DOMB*tanθ) for each reflection within the theta limits. Whereas DOMB is a constant (0.347 for Mo radiation) required in calculating the widening of the reflection due to the $K\alpha_1$-$K\alpha_2$ split at high θ-angles, DOMA varies from sample to sample and depends mainly on the mosaic spread in the crystal. The actual scan is extended 25% on each side to include background measurement. The horizontal aperture width at the detector is also controlled as a function of theta through the relationship (APTA + tanθ), APTA being an adjustable parameter usually assuming a value of 1.5-

2.5 mm. The vertical aperture is selected prior to data collection and consists of a manually insertable slit (4 mm has been found to be appropriate for most crystals). The type of scan to be employed throughout the data collection is determined from an analysis of the peak profiles of several reflections. Scan types range from pure ω-scans to ω-$2(n/6)\theta$ scans, where n is some integer between 1 and 6.

Reflections are generally collected in a zigzag mode in which the indices are stepped through, one by one, from their minimum to maximum values thereby exhausting the data points in that region of reciprocal space. Initially each reflection is scanned at the maximum speed, and from the peak intensity and accompanying background counts $\sigma(M)/M$ is calculated (M = scan count - B; $\sigma(M)$ = (scan count + 2B)$^{1/2}$ where M is the measured intensity and B is the time-averaged background). If this value is greater than the prescan acceptance ratio R, the reflection is classified as weak, otherwise the $\sigma(M)/M$ is compared to the ratio R' required from the final scan data; $\sigma(M)/M \geq R'$ forces a final scan to be carried out at a speed proportional to the square of the ratio $[\sigma(M)/M]/R'$; a less-than condition indicates that the preliminary scan data are good and no additional scan is required.

Orientation control reflections are checked periodically during data collection to ensure proper crystal orientation. Each reflection is scanned to determine the peak center. The bisecting vector for the reflection is compared with the scattering vector calculated from the current orientation matrix. An angular difference of more than a maximum allowable

deviation forces reorientation and recalculation of the orientation matrix.

Intensity standards (usually three reflections) are monitored hourly throughout data collection and are compared to the intensities of the same standards collected at the beginning of the data set. A decrease of more than a specified percentage (most often 25%) in any one of the standard reflections' intensity halts the data collection.

Determination of cell constants

Upon completion of the data collection, 25 reflections with relatively high intensities and high theta values are chosen from the data as the new set of reference reflections. These are centered and used in determining a more accurate orientation matrix. Theta angles are determined independent of the zero error of the detector by employing an omega scan at negative theta-negative hkl. The difference in the omega values for the positive and negative reflections yields an accurate value for 2θ when ω and θ are coupled in a 1:2 angular ratio. Final cell constants are then determined by constrained least squares fit to the $\sin\theta$ values for the centered reference reflections.

Data reduction

The data is processed with a locally written data reduction program (16); Lorentz and polarization corrections are applied; scaling of the reflections sometimes finds application such as in the case of intensity decay over the duration of data

collection; and the determination of observed reflections is carried out based on the criterion of $I/\sigma(I)$ being greater than or equal to n, where n = any positive real number; $I = c(S - B)$, where c is a scale factor accounting for the above corrections, varying scan speeds and the attenuator if used, S is the scan count and B is the time-averaged background; $\sigma^2(I) = S + 2B + (z(S - B))^2$, z being an additional factor which allows for instrumental instability. The output from the data reduction consists of the reflections' indices, the theta values, and the corrected intensities along with their standard deviations. At this point, the data are ready for use in the structure solving process and subsequent refinement of the solution.

Solution by direct methods

The procedures and techniques employed in determining the unobservable phases directly from the data are known collectively as 'direct methods'. A brief account of these methods is deemed necessary for they were used exclusively in obtaining the solutions to the structures presented in this thesis.

The approach taken in direct methods is largely statistical in nature making frequent use of probabilities and probability distributions. For the statistics to be valid it is necessary to reduce all relative quantities to an absolute scale since the *a priori* probability distributions are based on assumptions, and calculations using these assumptions. It is therefore, convenient in the initial stages of solving any structure to

remove the dependence of the observed structure factors $Fo(\vec{h})$, on atomic scattering factors (which in turn depend on the scattering angle and are affected by thermal vibration). This is done by defining normalized structure factors $E(\vec{h})$, where $|E(\vec{h})|^2 = k^2|Fo(\vec{h})|^2/\{\epsilon\Sigma f_j^2\}$; k is a scaling factor required to convert the relative $Fo(\vec{h})$ values, derived from the intensities, to absolute quantities based on the scattering material in the unit cell, and ϵ is an integer inserted to account for symmetry inherent in particular zones depending on the space group. These E-values, having no θ-dependence nor vibrational component, correspond to structures derived from a stationary-point-atom model. One of the main advantages of using E's rather than F's is that probability expressions are simplified. This arises from the consideration that if the atoms are randomly arranged in the cell the probability distribution of E is normal with a variance of unity.

The statistical properties of the E's are independent of the chemical composition and are useful in distinguishing between centrosymmetric and non-centrosymmetric space groups. The expectation value for $|E(\vec{h})|^2$ is 1.000 by definition, regardless of the space group symmetry. However, $\langle|E(\vec{h})|\rangle$ is 0.798 for centric intensity distributions which usually are characteristic of centrosymmetric space groups, whereas, an acentric distribution of intensities, characteristic of non-centrosymmetric space groups yields a $\langle|E(\vec{h})|\rangle$ value of 0.886. If the E-statistics obtained from a structure are such that space group assignment (with respect to centrosymmetry) is ambiguous, a further, more powerful statistical test is

available in the form of the N(z), or zero moment test (10). In this test N(z) is plotted against z, where N(z) is the fraction of reflections whose intensities, $|E(\vec{h})|^2$, are less than or equal to a specified fraction, z, of the average intensity $\overline{|E(\vec{h})|^2}$. A comparison of the experimental distribution over incremental values of z with the theoretical N(z) cumulative probability distribution curves usually provides the necessary information needed to distinguish centric from acentric distributions. It is, however, important to remember that pseudo-symmetry in the cell and point-group symmetry of projections can have noticeable effects on the above distributions and it is imperative, therefore, to consider any known molecular symmetry and probable molecular orientation in the unit cell (possibly based on crystal habit and/or cell parameters) before deciding whether or not the space group has centrosymmetry.

The next step toward solving the structure by direct methods is to obtain a listing of all reflection triples satisfying the Sayre relationship $\vec{h} = \vec{k} + \vec{h}-\vec{k}$ (12). Such triples, also known as Σ_2-relationships, are paramount in determining the phases of a large number of reflections knowing relatively few phases initially. The relationship among the phases of the Σ_2's , $\phi(\vec{h}) \sim \langle\phi(\vec{k}) + \phi(\vec{h}-\vec{k})\rangle$ is derived from Sayre's equation (12), which expressed in terms of normalized structure factors is $E(\vec{h}) = N^{1/2}\langle E(\vec{k})E(\vec{h}-\vec{k})\rangle$, where $\langle\ \rangle$ means the average over all values of $\vec{k}$ and N is the number of atoms in the cell. The symbol $\sim$ in the expression involving the phases within each Σ_2, means 'probably equal to'.

In the case of centrosymmetric structures the phase of each reflection is either 0 or π and corresponds to the assignment of a (+) or (-) sign, respectively to the magnitude $|E(\vec{h})|$. The probability that the sign of $E(\vec{h})$ will be +ve is given by, $P_+ = 1/2 + 1/2\tanh\{N^{-1/2}|E(\vec{h})|\Sigma E(\vec{k})E(\vec{h}-\vec{k})\}$ and the probability of $E(\vec{h})$ being -ve is just $P_- = 1 - P_+$. Sign indicators of greater than a probability of 0.95 are usually taken as correct.

As suggested above, a few phases must be known in advance regardless of the space group in order to initiate the phase determining operation. Three and sometimes fewer reflections are assigned arbitrary phases at the start. These reflections are chosen according to specific rules (which are space group dependent) to be origin determining (17). An obvious requirement in choosing these reflections is that they enter into as many Σ_2-combinations as possible. Other phases may have been determined (prior to this point) with a high degree of probability by so called Σ_1-relationships, which are special cases of the more general Σ_2-formula and depend only the magnitude of the normalized structures factors involved. In the case of non-centrosymmetric space groups an additional phase must be specified in order to define the positive sense of the coordinate system. The phasing of the remaining bulk of reflections begins.

Once the Σ_2 listing is exhausted using known and probability determined phases there will most likely remain some reflections which are as yet phaseless. Some of these reflections are assigned symbols (letters) for the phases, and

through the Σ_2's in which these reflections are involved simple mathematical relationships among the symbols can arise. Because symbols are used for phases the method is known as the 'Symbolic Addition' method (14). At the end of this phase determining process the reflections which remain with symbol phases are permuted with values of 0 and π in the centrosymmetric case, and $\pm\pi/4$ and $\pm 3\pi/4$ in the non-centrosymmetric case thereby generating sets of phases corresponding to each permutation.

The method described above for the direct determination of phases from the magnitudes of the structure factors has been implemented in many forms and one of the most widely used is the FORTRAN IV written computer program MULTAN (18). The program differs basically in one respect from the Symbolic Addition method; MULTAN assigns explicit values to the phases of the base reflections which by the Symbolic Addition method would have been represented by symbols. The advantage gained by employing phase values at the outset is evident in the solving of non-centrosymmetric structures whereby the initial phases (and subsequently determined approximate phases) are refined in an iterative manner by the tangent formula, $\tan\phi(\vec{h}) = \{\Sigma G[\sin(\phi(\vec{h}-\vec{k}) + \phi(\vec{k}))]\}/\{\Sigma G[\cos(\phi(\vec{h}-\vec{k}) + \phi(\vec{k}))]\}$, where G is a function of the E-values of the reflections $\vec{k}$ and $\vec{h}-\vec{k}$. Each set of phases determined for a given permutation of the variable base phases is assessed according to its internal consistency and the structural model it represents. These assessments are quantified and displayed as 'figures of merit'. Generally, but not always, the set of phases yielding the best figures of merit constitutes the solution, and these phases in combination with the

magnitudes of the normalized structure factors act as coefficients in a Fourier synthesis in producing a three-dimensional electron density map referred to as an E-map. An interpretable E-map which makes chemical sense is obviously the true test of the correctness of a set of phases.

Refinement

The refinement of the parameters for all structures following was accomplished by utilizing full matrix least squares procedures. The function minimized throughout refinement was $\Sigma w(|Fo| - k|Fc|)^2$, where Fo and Fc are the observed and calculated structure factors, k a scaling factor (where k is now the reciprocal of the k given on page 7), and w a weight associated with each reflection. A useful indicator of the general progress of a particular structural refinement is found in the R-value, or the residual value which is defined as $R = \Sigma||Fo| - k|Fc||/\Sigma|Fo|$. The weighted residual is given by $Rw = [\Sigma w(|Fo| - k|Fc|)^2/\Sigma w|Fo|^2]^{1/2}$ and is more closely related to the function minimized $\Sigma w\Delta^2$ (where $\Delta = |Fo| - k|Fc|$).

There is a variety of weighting schemes available for use in the refinement. In the initial stages, unit weights may be chosen to accelerate convergence; however, in the final stages of the refinement the weights should reflect the accuracy of the data. Weights may be absolute , derived from the errors in the intensities, or they may be relative, calculated such that uniform averages over $w\Delta^2$ are achieved for ranges of Fo values. For this work absolute weights were given by $1/\sigma^2(Fo)$, where

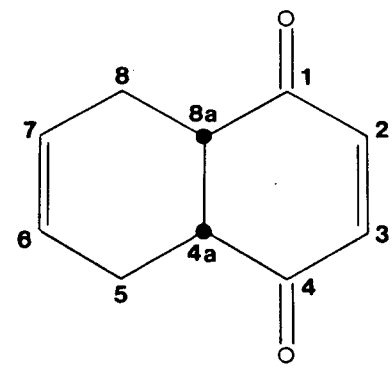
$\sigma^2(Fo) = \sigma^2(I)/(4I)$, whereas, relative weights were calculated from the polynomial $(A + BFo + CFo^2 + DFo^3)^{-1}$ (19).

Scattering factors (f^0) for all non-hydrogen atoms were taken from Cromer and Mann (20) while those for hydrogen atoms were from reference 21. The form of the scattering factors in the refinement of atoms assumed to vibrate isotropically is $f = f^0\exp[-8\pi^2\overline{u^2}(\sin\theta/\lambda)^2]$, where $\overline{u^2}$ is the mean-square displacement of the atom from its average position. For atoms with anisotropic thermal vibrations $f = f^0\exp[-2\pi^2\Sigma\Sigma U_{ij}h_i a_i^* h_j a_j^*]$. In the Tables that follow, Uiso = $\overline{u^2}$, and Ueq is one third the trace of the diagonalized temperature factor matrix.

Chemical Introduction

Photochemistry: structure-reactivity relationships

Research into the solution photochemistry of the 4aβ,5,8,8aβ-tetrahydro-1,4-naphthoquinones was initiated in an effort to determine their reactivities and to compare them with



4aβ,5,8,8aβ-tetrahydro-1,4-naphthoquinone

similar, known systems containing a -(CH_2)n- bridge across C(5) and C(8) (22,23). Whereas the latter systems were found to react via [2+2] intramolecular cycloaddition forming a cyclobutane ring with carbons 2, 3, 6 and 7, the tetrahydronaphthoquinones reacted by various hydrogen abstraction processes (24,25). The observed photoproducts from abstraction reactions resulted from molecules and intermediates which were conformationally labile in solution. Little control over the photoreactions could be exercised in a medium affording such freedom of motion, and therefore the restrictions offered by a crystal lattice seemed appealing; thus, entry was made into the realm of solid state photochemistry.

Interestingly, a variety of photoproducts resulted from the irradiation of various naphthoquinone derivatives in the solid state (26). Although photoproducts from the solid state reactions were invariably observed in solution, the converse was not true, for some of the solution products required extensive conformational rearrangements which were not possible in the confines of the crystal lattice. In the solid state, the main reaction routes identified were initiated by one of four steps: i) intermolecular [2+2] dimerization involving C(2)=C(3) bonds, ii) β-H abstraction by oxygen[1], iii) γ-H abstraction by carbon, or iv) intramolecular [2+2] cycloaddition involving C(1)=O(1) and C(6)=C(7) bonds. It was observed that a hierarchy existed

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[1] The symbol β has two different meanings in the text: i) it may refer to the configuration, as in 4aβ,5,8,8aβ-tetrahydro..., or ii) it may refer to the position of attachment of one atom relative to another, as in β-H abstraction. The context of the sentence should remove any ambiguity.

among the initiating steps in which [2+2] intermolecular photodimerization was the preferred reaction if the surroundings permitted it; the remainder of the above list is in the order of the next most likely to least likely process.

Solid state/solution photoproduct differences hinged on the method of biradical collapse following β-H or γ-H abstraction; conformational changes of the biradicals in solution allowed for a greater variety of products.

From the crystal structure analysis, the pertinent geometric parameters involved in each of the solid state reactions were derived for comparison with ideal situations. For abstraction reactions, the ideal geometry is achieved when the abstracting orbital is directed at the abstractable atom and the distance over which abstraction is to take place does not exceed the van der Waals radii sum for the atoms involved. For β-H abstraction by oxygen the orbital responsible for the abstraction is the non-bonding, p-like orbital on the oxygen which lies in the plane of the carbonyl and is directed normal to the C=O bond. The radii sum limit for this process is 2.72 Å (27). For convenience of calculation and comparison with other derivatives, the position of the β-H with respect to the n-orbital can be characterized by three values (Fig. 1): τ_o, the angular deviation between the O(1)...H_{abs} vector and the mean plane through the carbonyl group; Δ_o, the C(1)=O(1)...H_{abs} angle; and the O(1)...H_{abs} distance. Optimum values for τ_o and Δ_o are 0° and 90°, respectively (as alluded to above).

Similar definitions are used to characterize the γ-H abstraction-by-carbon process in which the C(2) 2p-orbital does

the abstracting. In this case, the mean plane considered is the C(1), C(2), C(3), C(4) plane to which the 2p-orbital is perpendicular in the ground state. Assuming that the reactive excited state has the same shape as the ground state, ideal conditions for this abstraction process are: $\tau_c = 90°$, which is the angle between the C(2)...H_{abs} vector and its projection onto the mean plane C(1),...,C(4); $\Delta_c = 90°$, which is the C(3)=C(2)...H_{abs} angle; and the abstraction distance being less than 2.90 Å (27), the van der Waals radii sum limit for C and H.

The [2+2] cycloaddition reactions involve 2p-orbitals. Schmidt (28) has suggested that for such a reaction to occur, the reacting double bonds must be parallel and separated by less than 4.1 Å. Indeed, for naphthoquinones undergoing this reaction, and those undergoing the abstraction processes, all satisfied the respective requisite geometries.

Having studied the effects of substituents and conformational changes on the photoreactivity in the

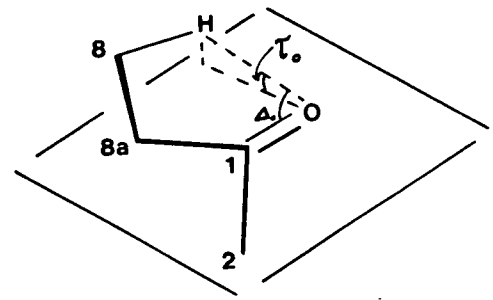


Figure 1

Definitions of τ_o and Δ_o.

naphthoquinone system, it was of interest next, to compare the effect of altering the active chromophore. What effect, if any, would a reduction to an enone from an ene-dione chromophore have on the observed photoreactions?

A study was initiated into the 4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4-ol system (29) (Fig. 2). Members of this series were readily afforded by sodium borohydride reduction of the corresponding naphthoquinones. Both isomers are formed on reduction, but not necessarily in equal amounts since the reactions are governed chiefly by steric approach and not by product development control. One isomer has the hydroxyl group 'anti', the other 'syn' to the bridgehead substituents[2] and are

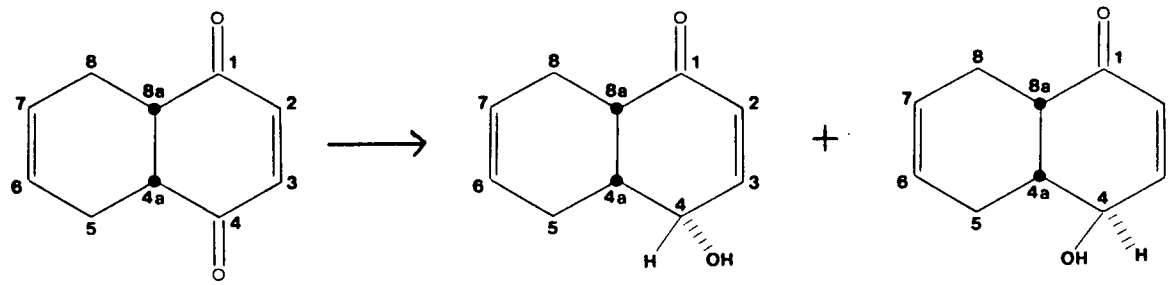


Figure 2

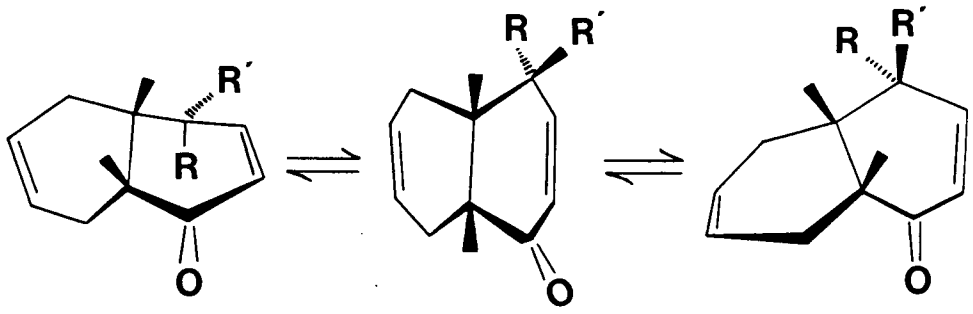
Production of 4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4-ols.

referred to as α- and β-hydroxy compounds, respectively. The two isomers crystallize in distinct conformations in which the bulkier OH group occupies the less sterically hindered pseudo-

[2] The terms 'anti' and 'syn' were deliberately chosen to describe the configuration of the hydroxyl group relative to the bridgehead substituents to avoid confusion with the 'cis'-fused ring junction.

equatorial position. These conformations may interconvert by twisting about the C(4a)-C(8a) bridge resulting in a ring-flip (Fig. 3). Both conformations can be described as a half-chair cyclohexene ring cis-fused to a half-chair cyclohexenone moiety. The solid state photoproducts result mainly from H(8) abstraction by C(3) in the 4β-ol derivatives and from H(5) abstraction by C(3) in the 4α-ol derivatives. In solution, however, a cage compound is the major photoproduct (29,30) and results from a high energy conformer (Fig. 3), intermediate between the 4α-ol and 4β-ol conformations (and not available in the crystal lattice) which reacts via intramolecular [2+2] cycloaddition across the C(2)=C(3) and C(6)=C(7) double bonds.

Definitions relevant to abstraction geometries (Fig. 4) are similar to those in the naphthoquinone system; τ_c is the angle between the C(3)...H_{abs} vector and its projection onto the mean plane of the C(2)=C(3) double bond (C(1), C(2), C(3), C(4)); Δ_c is the H_{abs}...C(3)=C(2) angle. In this case, ideal τ_c and Δ_c values should be 90° if the reactive excited state has the same shape as the ground state. Several of the naphthoquinols displayed geometry resembling the above in the solid state, and most of these derivatives reacted via H-abstraction by carbon; the hexamethyl-4β-ol derivative, however, showed no reactivity in the solid state (30). Although this was attributed to the long C(3)...H_{abs} distance of 2.92 Å which is greater than the van der Waals radii sum of 2.90 Å for C and H, it was felt that so sharp a cut-off was not highly probable and that there must be an additional factor preventing reaction. Almost all of the 4α-ols displayed the additional geometry suitable for oxygen



conformation typical of 4β-ols; R = H, R' = OH

conformation typical of 4α-ols; R = OH, R' = H

Figure 3

Conformations in naphthoquinols.

abstraction of a β-H, but this reaction was not observed.

Despite the wealth of information gained from the study of the parent naphthoquinol and five of its derivatives, some puzzling features still remained. Were there, indeed, well-defined limits for the abstraction processes? What were the effects of substituents on molecular conformations and ultimately on reactivity? Did the change of chromophore prohibit β-H abstraction by oxygen in the naphthoquinols? Was hydrogen bonding a factor in reactivity?

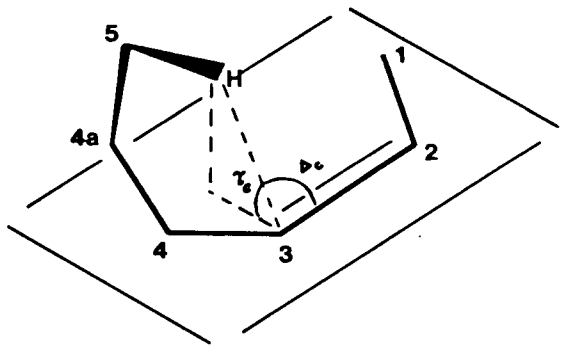


Figure 4

Definitions of τ_C and Δ_C.

Thesis outline

The present work[3] described in Part I of this thesis was undertaken in an attempt to clarify the roles of substituents and conformations in the solid state photoreactions. To determine the extent in which topochemistry controls the solid state reactions, comparisons are made with photoreactions in solution.

The first two chapters deal with methyl-substituted 4α-ols and their photoreactions in the solid state. At the end of the second chapter a conclusion is reached regarding oxygen abstraction reactions in naphthoquinols. The following chapter illustrates the building of a specific molecule into a predicted conformation based on the structural foundation laid by previously determined naphthoquinol structures. In addition to this example of 'crystal engineering', a structural comparison is made with the derivatives in the first two chapters and with the parent naphthoquinol from which they were derived. Chapter IV includes a description of the fully reduced naphthoquinone, namely the 1α,4α-diol (Fig. 5). Though photochemically inert (at the wavelength of interest for naphthoquinols) it is very closely related in structure to the other derivatives in Part I. Some structural comparisons are made illustrating this point.

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[3] The preparative work (including crystallizations) and photochemistry of all compounds discussed in this thesis, unless otherwise stated, were carried out by W. K. Appel, D. Herbert, Z. Q. Jiang, J. R. Scheffer, L. Walsh and Y. F. Wong.

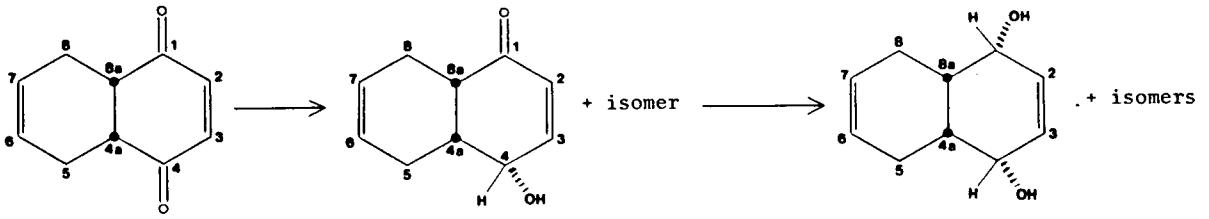


Figure 5

Relationship of the diol to naphthoquinones and naphthoquinols.

The initial interest in the structure, however, arose from an unsuccessful attempt to characterize the structure in the solid state by ^{13}C-NMR.

The second Part of this thesis is devoted to unusual products whose precursors are either naphthoquinones, naphthoquinols or derivatives thereof. Chapter V highlights a twistane-like (31) structure (later referred to as a 'twistenone') which was produced in an appreciable quantity following a minor modification in the method of photolysis of unsubstituted naphthoquinone in solution.

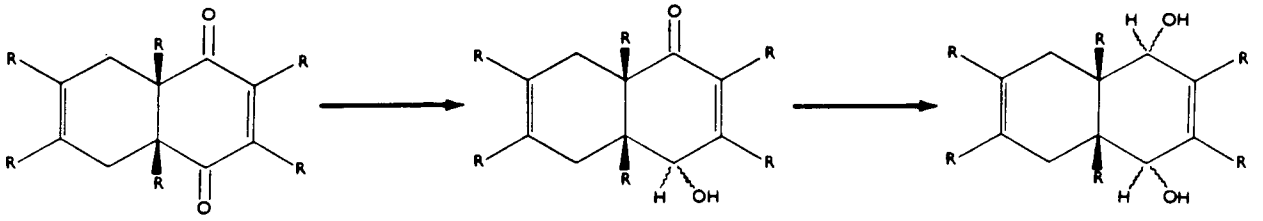
Irradiation of the 6,7-dimethyl-naphthoquinone by the same method that produced the twistenone yielded a new product which will be called X, unseen in previous studies and as yet uncharacterized. Chapter VI goes on to discuss the structure determination of the γ-lactone resulting from the thermolysis of X. Unfortunately, this structure did not provide as many clues to the identity of X as was hoped it would.

Treatment of the heptamethyl-4β-ol (whose structure is described in Chapter III, Part I) with acetic anhydride and zinc chloride results in a tricyclic methylene ketone which upon irradiation undergoes a rearrangement yielding the structure

discussed in Chapter VII.

Finally, Chapter VIII describes the structure of a derivative of the cage compound produced in solution by photolysis of the hexamethyl-4α-ol (30). The derivative discussed resulted from unsuccessful efforts to perform an intramolecular pinacolization of the oxidized cage compound.

Schematic of the Thesis Layout



Chapters I, II, III

Chapter IV

Unusual reaction products

Chapters V, VI

Chapters VII, VIII

PART I

CHAPTER I

2,3,6,7-TETRAMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-NAPHTHOQUIN-4α-OL

Introduction

The tetramethyl derivative discussed in this chapter is the first of four tetrahydronaphthoquinol derivatives, with various methyl substitution patterns, presented in Part I. The structure is described with respect to its conformation and the geometrical parameters important in the solid state photochemical process.

Experimental

The 2,3,6,7-tetramethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol[1] was prepared by the same general reaction scheme used in obtaining similar naphthoquinols (29), namely by reducing the appropriate Diels-Alder adduct with sodium borohydride. In the present case the thermal reaction between 2,3-dimethyl-p-benzoquinone and 2,3-dimethyl-1,3-butadiene yielded the required adduct (I) (Figure 6). The reduced adducts, (II) and (III), were separated. Various attempts were made at recrystallizing (III) by slow evaporation and, although most of the solvent systems afforded crystals, none were suitable for structural analysis. For example, benzene solutions gave tiny diamond shaped plates with the longest dimension being only 0.1 mm; crystals from ethanol/acetone solutions were fairly large but upon inspection under a polarizing microscope they were found to be twinned – a condition wherein two crystals are

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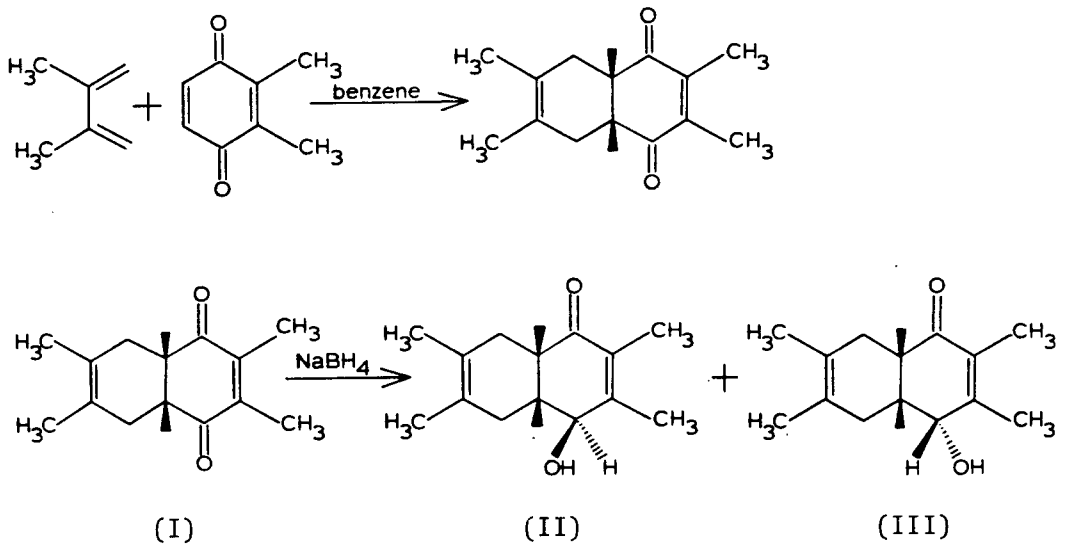
[1] IUPAC name: 4α-hydroxy-2,3,6,7-tetramethyl-4aβ,5,8,8aβ-tetrahydro-1(4H)-naphthalenone

intergrown in such a way that the crystallographic directions of one are related to the corresponding directions of the second by either two-fold or mirror symmetry (and less frequently by a 3-, 4- or 6-fold axis, or center of symmetry). Other systems involving hexane and acetone were tried, but to no avail. However, crystals grown from ethanol/petroleum ether solutions appeared suitable for diffraction study and hence one of these was mounted for photographs and subsequent data collection. The crystal employed measured 0.3 x 0.6 x 0.4 mm^3 and was tabular in habit.



(I) (II) (III)

Figure 6

Preparative reaction scheme leading to 2,3,6,7-tetramethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4β-ol (II) and the isomeric 4α-ol (III).

Preliminary Weissenberg and precession photographs were taken in an attempt to ascertain the space group. The films revealed the absence conditions $\underline{h}0\underline{l}$, $\underline{l} = 2\underline{n} + 1$ and $\underline{hkl}$, $\underline{h} + \underline{k} = 2\underline{n} + 1$ which are characteristic of the two space groups $\underline{C}2/\underline{c}$ and

Cc. A density calculation based on a unit cell volume of approximately 1250 Å^3 (from the axial measurements on the photographs) indicated that four molecules were present in the unit cell.

Crystal data: $C_{14}H_{20}O_2$, MW = 220.31, monoclinic a = 13.898(3), b = 5.228(1), c = 17.316(3) Å, β = 97.442(7)°, V = 1247.7(5) Å^3, Z = 4, D_c = 1.1728 g cm^{-3}, D_o = 1.174 g cm^{-3}, μ(MoKα) = 0.714 cm^{-1}, λ = 0.71073 Å, space group C2/c, from absences and structure analysis.

The crystal was mounted in a general orientation on an Enraf-Nonius CAD4 diffractometer. Cell constants and an orientation matrix were determined from the setting angles for 25 centered reflections. A Delaunay reduction program provided the transformation matrix required to convert the primitive cell found by the CAD4 to the corresponding C-centered cell indicated on the photographs.

Data were collected in the theta range 0.0-27.5 degrees (minimum interplanar spacing of 0.77 Å) using graphite monochromatized Mo radiation with omega scan speeds of 2.01-10.06 deg min^{-1}. From an analysis of various peak profiles, the best scan type was determined to be an ω-2(1/6)θ scan with an ω-scan angle of (1.30 + 0.35tanθ) degrees (each scan being extended by 25% on both sides for background measurement). A variable horizontal aperture width of (2.00 + 1.00tanθ) mm was employed and the vertical aperture was fixed at 4 mm.

Crystal orientation checks were performed on three

reference reflections after every 100 reflections collected. The intensities of three check reflections, which were monitored hourly throughout data collection, were found to decay by not more than 0.3%. Lorentz and polarization corrections were applied in the usual manner to the 1435 reflections collected, of which 61.9% (888) had $I \geq 3\sigma(I)$ (where $\sigma^2(I) = S + 2B + (0.04(S - B))^2$, S = scan count and B = time-averaged background).

Solution and Refinement

A comparison of the average E-values with their expectation values indicated a centric distribution of intensities. Furthermore, the zero moment test (10) showed a curve (for all data) very closely resembling the theoretical centric distribution plot. Despite this strong suggestion of a centrosymmetric structure the fact remained that the molecule was asymmetric and there were only four such molecules in the unit cell (based on density). However, the approximate two-fold molecular symmetry may have been the cause of the centric distribution and on this basis an attempt was made to solve the structure in the non-centrosymmetric space group, Cc.

One hundred sixty-four E's with magnitudes greater than 1.6 were input to MULTAN. The only phase determined by the Σ_1-relationship had an indicated probability of 1.00 with 30 contributors. Origin determining reflections and one required to define the positive sense of the b-axis were chosen according to the rules governed by the space group symmetry. The result of

the phase determining process yielded 16 sets of phases of which only 4 were independent. Although there was no outstanding solution, the set with the highest figure of merit gave an interpretable E-map (presented in Figure 7) which showed two fused six-membered rings with substituents at all but the bridgehead carbons. Peaks 10, 15 16 and 17 were all located in positions, relative to the ring, which were possible oxygen locations. However, mass spectral and IR data indicated only two oxygens in the molecule (Fig. 6) and their positions were para- to each other. A further disturbing aspect, evident on the E-map, was the relatively low height of the those peaks which were possibly due to oxygens. Peak heights which are directly proportional to the electron density at the peak positions are presumed a priori to be slightly higher for oxygen than carbon atoms. The presence of four small peaks at positions 10, 15, 16 and 17 instead of two relatively large peaks at 10 and 17, or 15 and 16 warned of the possibility of partial occupation of these sites by oxygen atoms, i.e. a disordered structure.

Based on the asymmetry of the molecule, full matrix least squares refinement of the structural parameters was initiated in the non-centrosymmetric space group Cc with oxygens given the coordinates of peaks 10 and 17 from the E-map. Six cycles of refinement of 14 carbon and 2 oxygen atoms with anisotropic thermal parameters led to the residual index R, of 0.17. Further cycling produced no significant changes in the parameters. The large degree of correlation between parameters of the cyclohexenone moiety and those of the cyclohexene part of the molecule suggested that the asymmetric unit consisted of less

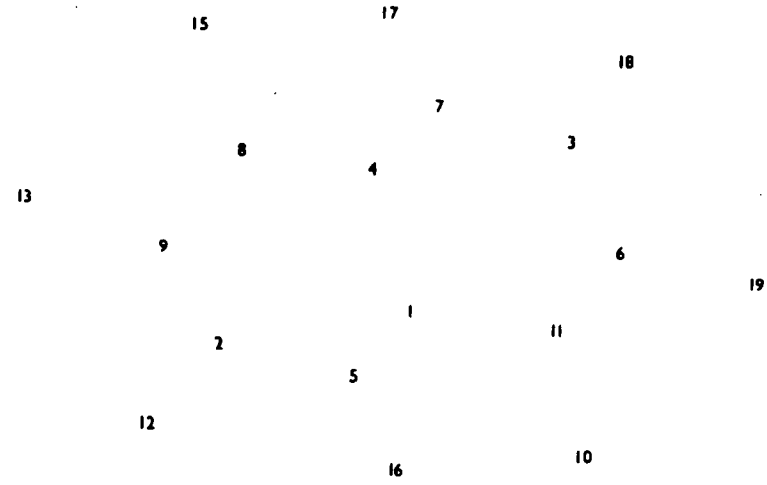


Figure 7

E-map; projection onto least squares plane through electron density peaks. Lowest number corresponds to position of highest density.

than one molecule. A difference-Fourier map indicated excess density peaks of 2-3 e/Å^3 within bonding distances of C(5) and C(8). Combined with the large magnitude of the temperature factors of the two oxygens, these excess density peaks suggested a disordered structure whereby the molecule appears as two, fused cyclohexenone moieties. Refinement proceeded in the centrosymmetric space group C2/c with the molecule lying on the two-fold rotation axis. Oxygen atoms were included initially with isotropic thermal parameters and at 50% occupancy, thus allowing for the rotational disorder.

Ten hydrogens were located from a difference-Fourier map, while those on C(8) and O(4) were not found due to the nature of the disorder. In the latter stages, all non-hydrogen atoms were refined with anisotropic temperature factors whereas, the hydrogen atoms were included with isotropic thermal parameters. The oxygen atoms and the two hydrogen atoms attached to C(5)

were held at fifty per cent occupancy. The structure converged at R = 0.058 and Rw = 0.078 for the 888 reflections with $I \geq 3\sigma(I)$; for the complete data set R = 0.088 and Rw = 0.078. The final difference synthesis revealed two peaks (0.208,0.231,0.245) and (0.179,0.131,0.271) of magnitudes 0.479 and 0.508 e/Å^3, respectively, in the region of O(4). However, neither of these can be directly attributed to the missing hydrogen, H(O4), in view of the poor bonding geometry they require at O(4) and the spatial proximity to that atom. The largest peak on the difference map had coordinates (0.030,0.248,0.534) and a magnitude of 0.516 e/Å^3. The mean and maximum parameter shifts on the final cycle were 0.037 and 0.203σ, respectively. The standard deviation of an observation of unit weight was 1.0017.

Reflections for which $I < 3\sigma(I)$ were classified as unobserved and not used in the refinement. Observed reflections were assigned weights calculated from the polynomial, $w = (A + BFo + CFo^2 + DFo^3)^{-1}$, where A = 0.3385, B = 0.02351, C = 0.002002 and D = 0.000097. This gave uniform averages of $w(|Fo| - k|Fc|)^2$ over ranges of Fo. Final positional and thermal parameters are presented in Table I and anisotropic temperature factors for the non-hydrogen atoms are given in Table II.

Discussion

The structure consists of molecules well-separated along the c-axis with the closest non-hydrogen approach being greater than 3.5 Å in that direction. There are two possible

Table I

Final positional (fractional x 10^5, C(31) and O(1)' x 10^4, H x 10^3)

and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)

with estimated standard deviations in parentheses

Atom[2]	x	y	z	Ueq/Uiso
C(1)	-4646(16)	-1559(41)	32373(12)	52
C(2)	4666(16)	-7399(37)	37272(11)	52
C(21)	3947(27)	-26259(60)	43749(16)	73
C(3)	12901(16)	3987(45)	35893(12)	57
C(31)	2248(3)	-95(10)	4084(2)	96
C(4)	13402(16)	22347(47)	29261(13)	58
C(8a)	-4660(14)	21141(37)	26932(11)	48
O(1)'	-1157(3)	-1380(11)	3362(3)	93
O(4)'	21719(22)	20315(60)	25989(20)	64
H1(21)	56(3)	-196(7)	482(2)	103(11)
H2(21)	1(3)	-402(8)	421(3)	138(15)
H3(21)	98(4)	-362(9)	449(3)	160(18)
H1(31)	218(3)	-15(9)	458(3)	129(14)
H2(31)	262(4)	-176(11)	409(3)	181(22)
H3(31)	266(4)	110(10)	399(3)	163(20)
H(4)	142(2)	392(6)	314(2)	88(9)
H1(5)'	68(4)	-182(9)	211(3)	58(12)
H2(5)'	99(4)	5(11)	148(3)	59(16)
H(8a)	-45(2)	363(5)	302(1)	56(6)

[2] Primed (') atoms are at positions of 50% occupancy

Table II

Final anisotropic thermal parameters ($\underline{U}ij$ X 10^4 Å^2)

and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
C(1)	521(12)	536(12)	532(11)	-37(9)	141(9)	14(10)
C(2)	642(13)	487(11)	445(10)	2(9)	77(9)	17(9)
C(21)	993(22)	718(17)	479(13)	-10(16)	109(12)	97(13)
C(3)	563(13)	641(13)	494(11)	-6(10)	-8(9)	-3(10)
C(31)	678(19)	1407(34)	720(19)	-70(21)	-148(14)	218(20)
C(4)	526(13)	591(13)	611(12)	-123(9)	63(10)	11(11)
C(8a)	516(12)	411(10)	509(10)	39(8)	71(8)	-77(9)
O(1)'	619(24)	1138(36)	1027(32)	-313(23)	105(21)	232(28)
O(4)'	530(18)	701(19)	719(19)	-39(14)	184(14)	-39(16)

intermolecular O...O contact distances less than 3 Å. These contacts can occur between the hydroxyl oxygen atom of one molecule and that of the carbonyl in the adjacent molecule, related by the centering condition, or between the same hydroxyl oxygen and the two-fold symmetry related oxygen in the neighboring centered molecule. The O(4)(x,y,z)...O(1)(1/2+x,1/2-y,z) distance of 2.652(5) Å suggests that hydrogen bonds link molecules in the [110] and [1$\bar{1}$0] directions. However, the O(4)(x,y,z)...O(4)(1/2-x,1/2+y,1/2-z) distance of 2.804(4) Å suggests hydrogen bonding takes place between disordered molecules. The above intermolecular distances are consistent with the observation that the crystal cleaves easily parallel to the (001) face.

Disorder in the structure, assumed to be 50:50, results in an apparent two-fold symmetry axis through the molecule. This disorder may be rationalized on the basis that there appears to be little stereochemical hindrance preventing the two molecular orientations from co-existing in the same crystal, provided that alignment for hydrogen bonding is maintained.

The disorder arises from packing arrangements in which slabs parallel to (001) contain molecules of two types, A and B (where A and B are related by 180 degrees rotation about b). Two kinds of hydrogen bonding are possible within the slabs. They join molecules in the sequence A...A (or B...B) and A...B (or B...A). The bonds linking molecules of similar type are O(4)(x,y,z)-H...O(1)(1/2+x,1/2-y,z) interactions whereas molecules of different types are joined by O(4)(x,y,z)-H...O(4)(1/2-x,1/2+y,1/2-z) hydrogen bonds. There are several

packing arrangements consistent with the dual composition and available hydrogen bonding within each slab, and since packing forces are a major influence on the crystal energy, the arrangements leading to hydrogen bonding networks linking the maximum number of molecules within the slabs yield the most probable structure.

Figure 8 shows a stereoscopic drawing of the contents of the unit cell with C(4) labelled by its adjoining hydrogen. The molecules adopt a conformation which consists of a half-chair cyclohexene ring cis-fused to a second half-chair cyclohexenone

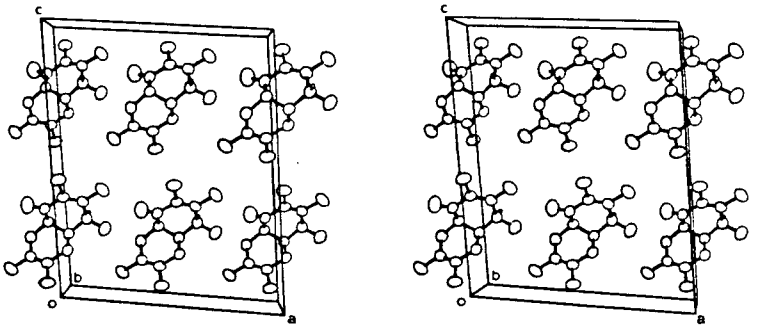


Figure 8

Stereo diagram of the molecular packing of type A molecules viewed approximately down b.

moiety (Fig. 9) similar to previously studied naphthoquinols (32).

In comparison with accepted values (33), the mean bond lengths are found to be slightly smaller, with distances of

1.524 Å for $C(sp^3)$-$C(sp^3)$ and 1.504 Å for $C(sp^3)$-$C(sp^2)$. Carbon to hydrogen bond lengths generally do not deviate significantly from the accepted values. Bond angles are normal and are given in Tables III and IV along with bond lengths. Some ring strain, indicated by a C(4)-C(3)-C(2)-C(1) torsion angle of -2.3° (Table

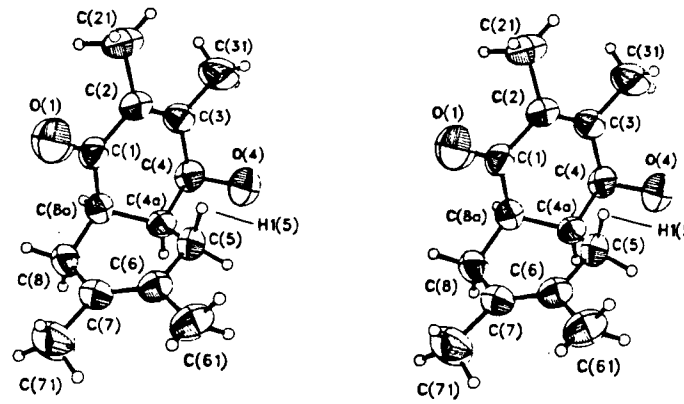


Figure 9

Stereo diagram of 2,3,6,7-tetramethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

V) and compounded by an O(1)-C(1)-C(2)-C(3) torsion angle of 175.0°, results in the carbonyl oxygen lying 0.1 Å above the mean plane through the former four atoms and C(1) lying 0.005 Å below the same mean plane.

The molecule, exhibiting the same conformation as other naphthoquin-4α-ol derivatives in the series is geometrically suited to H(5) abstraction by the β-carbon, C(3), upon photochemical excitation. The C(3)...H1(5) distance of 2.84(5) Å is less than the van der Waals contact distance of 2.90 Å. Other

Table III

Bond lengths[3] (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1) -C(2)	1.484(3)	C(3) -C(31)	1.510(4)
C(1) -C(8a)	1.515(3)	C(3) -C(4)	1.505(3)
C(1) -O(1)	1.199(4)	C(4) -O(4)	1.356(4)
C(2) -C(21)	1.506(3)	C(4) -C(8a)"	1.514(3)
C(2) -C(3)	1.339(3)	C(8a) -C(8a)"	1.533(4)

Bond angles (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(1) -C(8a)	116.6(2)	C(31) -C(3) -C(4)	114.7(2)
C(2) -C(1) -O(1)	116.6(3)	C(3) -C(4) -O(4)	113.3(2)
C(8a) -C(1) -O(1)	126.5(3)	C(3) -C(4) -C(8a)"	113.7(2)
C(1) -C(2) -C(21)	115.0(2)	O(4) -C(4) -C(8a)"	110.5(2)
C(1) -C(2) -C(3)	120.6(2)	C(1) -C(8a) -C(8a)"	109.8(1)
C(21) -C(2) -C(3)	124.4(2)	C(1) -C(8a) -C(4)"	114.2(2)
C(2) -C(3) -C(31)	122.3(3)	C(8a)"-C(8a) -C(4)"	109.7(2)
C(2) -C(3) -C(4)	123.0(2)		

[3] Double primes (") denote symmetry related atoms.

Table IV

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(21) -H1(21)	0.86(4)	C(31) -H3(31)	0.88(5)
C(21) -H2(21)	0.93(4)	C(4) -H(4)	0.96(3)
C(21) -H3(21)	0.96(5)	C(8a) -H(8a)	0.98(2)
C(31) -H1(31)	0.88(5)	C(1)" -H1(5)	1.08(5)
C(31) -H2(31)	1.01(6)	C(1)" -H2(5)	0.93(6)

Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(21) -H1(21)	112(2)	C(3) -C(4) -H(4)	108(2)
C(2) -C(21) -H2(21)	112(3)	O(4) -C(4) -H(4)	99(2)
C(2) -C(21) -H3(21)	112(3)	H(4) -C(4) -C(8a)"	111(2)
H1(21)-C(21) -H2(21)	133(4)	C(1) -C(8a) -H(8a)	106(1)
H1(21)-C(21) -H3(21)	84(3)	C(8a)"-C(8a) -H(8a)	107(1)
H2(21)-C(21) -H3(21)	94(3)	C(4)" -C(8a) -H(8a)	109(1)
C(3) -C(31) -H1(31)	111(3)	C(2)" -C(1)" -H1(5)	108(2)
C(3) -C(31) -H2(31)	124(3)	C(2)" -C(1)" -H2(5)	114(3)
C(3) -C(31) -H3(31)	109(3)	C(8a)"-C(1)" -H1(5)	108(3)
H1(31)-C(31) -H2(31)	95(4)	C(8a)"-C(1)" -H2(5)	107(4)
H1(31)-C(31) -H3(31)	112(4)	H1(5) -C(1)" -H2(5)	102(4)
H2(31)-C(31) -H3(31)	106(4)		

pertinent geometric factors considered in the abstraction process include the angle C(2)-C(3)...H1(5), Δ_c, and the angle subtended by the C(3) to H1(5) vector and its projection on the plane of the carbon-carbon double bond, τ_c; these angles were found to be 79.5 and 53.5 degrees, respectively. These values are comparable to those found in similar substituted naphthoquinols that were shown to undergo H-abstraction by the β-enone carbon (30,32).

Photochemical results of the present compound indicate clearly that H1(5)-abstraction by C(3) is the major process taking place. Whereas the molecular geometry is also favorable to H(8) abstraction by O(1) as in naphthoquinone derivatives (26,34), this reaction was not observed in the present compound.

Table V

Torsion angles (deg) with estimated standard deviations in parentheses

Atoms				Value
C(8a)	-C(1)	-C(2)	-C(21)	167.6(2)
C(8a)	-C(1)	-C(2)	-C(3)	-11.5(3)
O(1)	-C(1)	-C(2)	-C(21)	-5.9(5)
O(1)	-C(1)	-C(2)	-C(3)	175.0(4)
C(2)	-C(1)	-C(8a)	-C(8a)"	42.0(3)
C(2)	-C(1)	-C(8a)	-C(4)"	165.6(2)
O(1)	-C(1)	-C(8a)	-C(8a)"	-145.2(5)
O(1)	-C(1)	-C(8a)	-C(4)"	-21.6(5)
C(1)	-C(2)	-C(3)	-C(31)	178.6(3)
C(1)	-C(2)	-C(3)	-C(4)	-2.3(3)
C(21)	-C(2)	-C(3)	-C(31)	0.4(4)
C(21)	-C(2)	-C(3)	-C(4)	178.7(2)
C(2)	-C(3)	-C(4)	-O(4)	-143.5(3)
C(2)	-C(3)	-C(4)	-C(8a)"	-16.3(3)
C(31)	-C(3)	-C(4)	-O(4)	35.7(4)
C(31)	-C(3)	-C(4)	-C(8a)"	162.9(3)
C(3)	-C(4)	-C(8a)"	-C(8a)	46.5(2)
C(3)	-C(4)	-C(8a)"	-C(1)"	-77.1(2)
O(4)	-C(4)	-C(8a)"	-C(8a)	175.2(2)
O(4)	-C(4)	-C(8a)"	-C(1)"	51.5(3)
C(1)	-C(8a)	-C(8a)"	-C(4)	-58.9(2)
C(1)	-C(8a)	-C(8a)"	-C(1)"	67.3(3)

Table V (continued)

C(4)"	-C(8a)	-C(8a)"	-C(4)	174.9(2)
C(4)"	-C(8a)	-C(8a)"	-C(1)"	-58.9(2)
C(2)	-C(1)	-C(8a)	-H(8a)	-73.8(13)
O(1)	-C(1)	-C(8a)	-H(8a)	99.0(14)
C(1)	-C(2)	-C(21)	-H1(21)	-118(3)
C(1)	-C(2)	-C(21)	-H2(21)	44(3)
C(1)	-C(2)	-C(21)	-H3(21)	149(3)
C(3)	-C(2)	-C(21)	-H1(21)	61(3)
C(3)	-C(2)	-C(21)	-H2(21)	-136(3)
C(3)	-C(2)	-C(21)	-H3(21)	-32(3)
C(2)	-C(3)	-C(31)	-H1(31)	-42(3)
C(2)	-C(3)	-C(31)	-H2(31)	70(4)
C(2)	-C(3)	-C(31)	-H3(31)	-165(4)
C(4)	-C(3)	-C(31)	-H1(31)	139(3)
C(4)	-C(3)	-C(31)	-H2(31)	-109(4)
C(4)	-C(3)	-C(31)	-H3(31)	16(4)
C(2)	-C(3)	-C(4)	-H(4)	107(2)
C(31)	-C(3)	-C(4)	-H(4)	-74(2)
C(3)	-C(4)	-C(8a)"	-H(8a)"	164.2(13)
O(4)	-C(4)	-C(8a)"	-H(8a)"	-67.1(14)
H(4)	-C(4)	-C(8a)"	-C(8a)	-76(2)
H(4)	-C(4)	-C(8a)"	-H(8a)"	42(2)
H(4)	-C(4)	-C(8a)"	-C(1)"	161(2)
C(1)	-C(8a)	-C(8a)"	-H(8a)"	-177.8(13)

Table V (continued)

C(4)" -C(8a) -C(8a)"-H(8a)"	56.0(13)
H(8a)"-C(8a) -C(8a)"-C(4)	56.0(13)
H(8a)"-C(8a) -C(8a)"-H(8a)"	-63(3)
H(8a)"-C(8a) -C(8a)"-C(1)"	-177.8(13)
H1(5) -C(1)" -C(2)" -C(21)"	-71(3)
H1(5) -C(1)" -C(2)" -C(3)"	110(3)
H2(5) -C(1)" -C(2)" -C(21)"	42(4)
H2(5) -C(1)" -C(2)" -C(3)"	-137(4)
H1(5) -C(1)" -C(8a)"-C(4)	44(3)
H1(5) -C(1)" -C(8a)"-C(8a)	-80(3)
H1(5) -C(1)" -C(8a)"-H(8a)"	164(3)
H2(5) -C(1)" -C(8a)"-C(4)	-65(4)
H2(5) -C(1)" -C(8a)"-C(8a)	171(4)
H2(5) -C(1)" -C(8a)"-H(8a)"	55(4)

CHAPTER II

2,3-DIMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-NAPHTHOQUIN-4α-OL AND 6,7-DIMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-NAPHTHOQUIN-4α-OL

Introduction

The structures of the title compounds were investigated and further confirmation of the geometric requirements leading to the established naphthoquinol reaction patterns was sought from the structural data.

Experimental

Preparation of the title compounds involved sodium borohydride reduction of the appropriate Diels-Alder adducts resulting from the thermal reactions between butadiene and 2,3-dimethyl-benzoquinone, and between 2,3-dimethylbutadiene and benzoquinone which yielded the 2,3- (IV) and 6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ols[1] (V), respectively. Crystals of the individual compounds were afforded by slow evaporation of petroleum ether/ethanol solutions and were shown to be better than 98 per cent pure by GC analysis. Mass spectral data confirmed the assigned chemical formulae $C_{12}H_{16}O_2$. All crystals exhibited acicular habits and those chosen for data collection were cut from larger crystals to measure 0.1 x 0.3 x 0.5mm^3 and 0.4 x 0.2 x 0.1mm^3 for the 2,3- and 6,7-dimethyl compounds, respectively.

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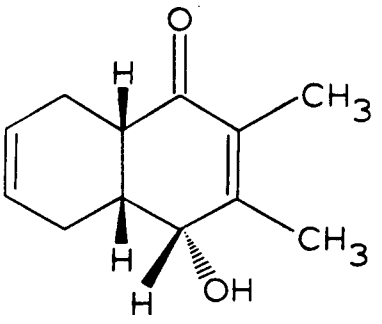
[1] IUPAC names: 4α-hydroxy-2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1(4H)-naphthalenone and 4α-hydroxy-6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1(4H)-naphthalenone

2,3-Dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (IV)

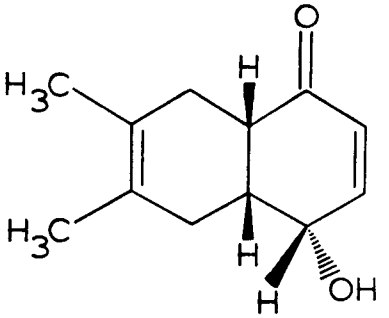
Crystal data: $C_{12}H_{16}O_2$, MW = 192.3, orthorhombic $\underline{a}$ = 5.148(1), $\underline{b}$ = 12.269(2), $\underline{c}$ = 16.478(3) Å, $\underline{V}$ = 1040.8(4) Å^3, $\underline{Z}$ = 4, $\underline{D}_c$ = 1.226 g cm^{-3}, μ(MoKα) = 0.764 cm^{-1}, λ = 0.71073 Å, space group $\underline{P}2_12_12_1$; $\underline{h}00$, $\underline{h}$ = 2$\underline{n}$ + 1, 0$\underline{k}$0, $\underline{k}$ = 2$\underline{n}$ + 1, 00$\underline{l}$, $\underline{l}$ = 2$\underline{n}$ + 1 absent.

6,7-Dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (V)

Crystal data: $C_{12}H_{16}O_2$, MW = 192.3, monoclinic $\underline{a}$ = 9.242(3), $\underline{b}$ = 22.724(3), $\underline{c}$ = 5.139(2) Å, β = 102.7(1)°, $\underline{V}$ = 1052.8(5) Å^3, $\underline{Z}$ = 4, $\underline{D}_c$ = 1.213 g cm^{-3}, μ(MoKα) = 0.756 cm^{-1}, λ = 0.71073 Å, space group $\underline{P}2_1/\underline{c}$; $\underline{h}0\underline{l}$, $\underline{l}$ = 2$\underline{n}$ + 1, 0$\underline{k}$0, $\underline{k}$ = 2$\underline{n}$ + 1 absent.



(IV)



(V)

Final cell constants for both structures were obtained by least squares fit to the sinθ values for 25 centered reflections.

In the remaining 'Experimental' text, quantities in brackets refer to the 6,7-dimethyl compound. Parameters after which no brackets follow are to be regarded as the same for both title compounds.

Data collection proceeded in the theta range 0.0-27.5° [0.0-25.0°] using graphite monochromatized MoKα radiation. An ω -2(4/6)θ [ω-2θ] scan was employed with an ω-scan angle of (0.75 + 0.35tanθ) [(0.55 + 0.35tanθ)] degrees. Each scan was extended 25% on both sides of the peak to allow for background measurement. The horizontal slit width was varied according to the θ-dependent relationship (2.00 + 1.00tanθ) mm [(2.50 + 1.00tanθ) mm] while the vertical slit remained open at a constant 4 mm. The setting angles of three reference reflections were checked periodically to ensure proper crystal orientation throughout data collection. Three other reflections were chosen as intensity controls and monitored every 3600 s of X-ray exposure time. Processing of the data which included application of Lorentz and polarization corrections, showed little or no decay in the check reflections' intensities. Of the 1413 [1834] reflections collected, 671 [626], or 47.5% [34.1% (55% for $0°<\theta\leq20°$)] were classified as observed having $I \geq 3\sigma(I)$, where $\sigma^2(I)$ is defined as $S + 2B + (0.04(S - B))^2$; S is the scan count and B the time-averaged background. The linear absorption coefficients indicated that absorption corrections

were not warranted.

Solution and Refinement

2,3-Dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

The structure was solved by direct methods using the largest 156 E-values. The acentric E-distribution was consistent with the previously assigned non-centrosymmetric space group. The E-map obtained from the solution with the highest figure of merit in MULTAN clearly indicated the positions of the 14 non-hydrogen atoms. After two cycles of full matrix least squares refinement of non-hydrogen atoms with anisotropic thermal parameters, a difference-Fourier map revealed the positions of the 16 hydrogens. Convergence was reached at $R = 0.031$ and $Rw = 0.036$ for the observed data ($I \geq 3\sigma(I)$), whereas, for the complete data set $R = 0.103$ and $Rw = 0.036$. The weighting scheme $w = 1/\sigma^2(F)$ was employed[2], where $\sigma^2(F)$ is derived from the previously defined $\sigma^2(I)$. A weighting analysis confirmed the suitability of the chosen weights by showing uniform average values of $w(|Fo| - k|Fc|)^2$ over ranges of $|Fo|$. A difference synthesis, following refinement, showed random fluctuations with the highest peak corresponding to 0.15 e/Å^3. In the final cycle of refinement 191 parameters were varied using 671 observed data and no parameter shift exceeded 0.39σ. The standard deviation in an observation of unit weight was 1.210.

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[2] The F in $\sigma^2(F)$ and all subsequent occurrences of F, not followed by the modifiers 'o' or 'c', are synonymous with Fo.

6,7-Dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

MULTAN yielded the positional parameters for the 14 non-hydrogen atoms. Following full matrix least squares refinement of the non-hydrogen atoms, the coordinates of the 16 hydrogen atoms were obtained from a difference-Fourier map. Refinement proceeded with anisotropic thermal parameters for carbons and oxygens and isotropic thermal parameters for the hydrogens until the refinement converged. The difference-Fourier, calculated after convergence, indicated that the largest peak, corresponding to excess density of 0.12 e/Å^3, was in the immediate vicinity of O(1). The mean and maximum parameter shifts on the final cycle of refinement were 0.020 and 0.20σ, respectively. The weights used in the refinement, $w = 1/\sigma^2(F)$ gave uniform average values of $w(|Fo| - k|Fc|)^2$ over ranges of $|Fo|$. The final R-value was 0.032 and Rw = 0.037 for the 191 parameters and 626 observations, whereas for the complete data set R = 0.167 and Rw = 0.037. The standard deviation in an observation of unit weight was 1.193. Final atomic coordinates and temperature factors for (IV) and (V) are given in Table VI. Anisotropic thermal parameters for non-hydrogen atoms are presented in Table VII.

Discussion

Molecules of (IV) and (V) assume a conformation which is similar to that found in other tetrahydronaphthoquinols (Chapter I and reference 32). The torsion angles, C(5)-C(4a)-C(8a)-C(1), of 66.6(3)° for (IV) and 67.3(4)° for (V) (Table VIII), indicate the degree of twist in this conformation, which consists of a

Table VI

Final positional (fractional x 10^4, H x 10^3)

and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)

with estimated standard deviations in parentheses

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Atom	x	y	z	Ueq/Uiso
C(1)	3659(8)	31(3)	1937(2)	41
C(2)	3612(7)	-161(3)	1055(2)	41
C(21)	1863(11)	-1062(4)	770(4)	63
C(3)	5099(7)	441(3)	550(2)	40
C(31)	5222(12)	238(5)	-351(3)	67
C(4)	6849(7)	1340(3)	862(2)	38
C(4a)	6156(7)	1739(3)	1706(2)	34
C(5)	3753(9)	2472(3)	1728(2)	40
C(6)	2729(7)	2621(3)	2571(2)	44
C(7)	3430(9)	2024(3)	3193(2)	49
C(8)	5332(10)	1113(4)	3142(2)	52
C(8a)	5790(7)	754(3)	2268(2)	39
O(1)	2076(5)	-400(2)	2386(2)	59
O(4)	7017(6)	2225(2)	292(2)	47
H1(21)	279(14)	-166(5)	65(3)	130(25)
H2(21)	45(18)	-129(7)	108(5)	205(41)
H3(21)	102(16)	-93(6)	21(4)	165(29)
H1(31)	499(11)	-46(4)	-48(3)	103(20)
H2(31)	432(11)	77(4)	-67(3)	106(22)
H3(31)	712(14)	43(5)	-54(4)	139(24)
H(4)	866(7)	103(2)	86(2)	30(8)
H(4a)	765(7)	218(3)	190(2)	40(10)
H1(5)	229(8)	212(3)	135(2)	67(12)
H2(5)	422(7)	318(3)	150(2)	38(10)
H(6)	155(8)	323(3)	262(2)	47(10)
H(7)	287(8)	216(3)	377(2)	58(11)
H1(8)	479(9)	46(4)	346(3)	78(15)
H2(8)	694(9)	129(3)	340(2)	68(13)
H(8a)	727(7)	39(2)	221(2)	24(9)
H(O4)	570(12)	245(5)	19(3)	98(22)

Table VI (continued)

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Atom	x	y	z	Ueq/Uiso
C(1)	-877(4)	-560(2)	1056(9)	40
C(2)	502(5)	-805(2)	2635(10)	43
C(3)	1047(5)	-1307(2)	1972(9)	43
C(4)	357(4)	-1651(2)	-443(9)	41
C(4a)	-1283(4)	-1513(2)	-1388(9)	36
C(5)	-2240(5)	-1767(2)	396(11)	42
C(6)	-3800(5)	-1515(2)	-116(9)	46
C(61)	-4832(8)	-1847(3)	1252(18)	72
C(7)	-4182(4)	-1036(2)	-1589(9)	49
C(71)	-5736(7)	-785(4)	-2182(21)	84
C(8)	-3103(5)	-689(2)	-2774(11)	50
C(8a)	-1501(4)	-848(2)	-1613(9)	37
O(1)	-1460(3)	-136(1)	1858(6)	58
O(4)	627(3)	-2265(1)	149(8)	53
H(2)	94(4)	-58(2)	423(9)	60(14)
H(3)	196(4)	-146(1)	281(7)	31(10)
H(4)	91(4)	-154(1)	-191(7)	42(11)
H(4a)	-159(3)	-167(1)	-318(8)	31(10)
H1(5)	-178(4)	-170(1)	240(9)	49(13)
H2(5)	-233(4)	-221(2)	18(7)	48(12)
H1(61)	-583(8)	-170(3)	75(13)	139(26)
H2(61)	-462(6)	-224(3)	120(12)	119(25)
H3(61)	-467(8)	-181(3)	304(17)	163(40)
H1(71)	-593(7)	-65(3)	-398(15)	126(31)
H2(71)	-579(8)	-43(3)	-152(16)	158(34)
H3(71)	-650(7)	-105(3)	-191(13)	143(28)
H1(8)	-333(4)	-76(2)	-474(10)	64(14)
H2(8)	-320(4)	-26(2)	-255(8)	60(13)
H(8a)	-87(4)	-69(1)	-261(7)	31(11)
H(O4)	-941(5)	-243(2)	-121(10)	57(18)

Table VII

Final anisotropic thermal parameters (U_{ij} x 10^3 Å^2)

and their estimated standard deviations

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	30(2)	33(2)	58(3)	6(2)	4(2)	10(2)
C(2)	35(2)	38(2)	49(2)	2(2)	0(2)	1(2)
C(21)	55(3)	48(3)	86(4)	-11(3)	-2(3)	-7(3)
C(3)	33(2)	40(2)	46(2)	5(2)	4(2)	-5(2)
C(31)	81(4)	64(3)	54(3)	-6(3)	10(3)	-15(3)
C(4)	27(2)	42(2)	45(2)	1(2)	1(2)	7(2)
C(5)	36(2)	38(2)	46(2)	4(2)	-3(2)	6(2)
C(6)	41(2)	42(2)	50(3)	2(2)	4(2)	-8(2)
C(7)	49(3)	57(2)	39(2)	-2(2)	2(2)	-2(2)
C(8)	50(3)	64(3)	41(3)	-2(3)	-7(2)	12(2)
C(8a)	25(2)	48(2)	46(2)	9(2)	-2(2)	9(2)
C(4a)	23(2)	40(2)	40(2)	-4(2)	-2(2)	6(2)
O(1)	52(2)	58(2)	67(2)	-17(2)	15(2)	8(1)
O(4)	38(2)	57(2)	47(2)	-5(1)	6(1)	15(1)

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	44(3)	35(2)	41(3)	-3(2)	13(2)	-1(2)
C(2)	47(3)	42(3)	39(3)	-6(2)	6(2)	-7(2)
C(3)	34(3)	52(3)	44(3)	-1(2)	7(2)	1(2)
C(4)	52(3)	34(3)	40(3)	3(2)	19(3)	0(2)
C(4a)	46(3)	39(2)	25(3)	-2(2)	10(2)	-3(2)
C(5)	46(3)	44(3)	38(3)	-7(2)	9(2)	3(2)
C(6)	44(3)	52(3)	42(3)	-9(2)	11(2)	-10(2)
C(61)	62(4)	77(5)	87(6)	-6(3)	38(4)	-1(4)
C(7)	39(3)	57(3)	46(3)	4(2)	-1(2)	-5(2)
C(71)	49(4)	85(5)	110(7)	8(4)	2(4)	-3(5)
C(8)	56(3)	49(3)	40(3)	4(2)	1(2)	5(2)
C(8a)	42(3)	39(3)	33(3)	-3(2)	12(2)	3(2)
O(1)	61(2)	50(2)	60(2)	4(2)	11(2)	-13(2)
O(4)	75(2)	40(2)	45(2)	9(2)	18(2)	-1(2)

Table VIII

Torsion angles (deg) with estimated standard deviations in parentheses

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Atoms				Value
C(8a)	-C(1)	-C(2)	-C(21)	167.2(4)
C(8a)	-C(1)	-C(2)	-C(3)	-12.0(5)
O(1)	-C(1)	-C(2)	-C(21)	-11.0(5)
O(1)	-C(1)	-C(2)	-C(3)	169.8(3)
C(2)	-C(1)	-C(8a)	-C(8)	166.9(3)
C(2)	-C(1)	-C(8a)	-C(4a)	42.0(4)
O(1)	-C(1)	-C(8a)	-C(8)	-15.0(5)
O(1)	-C(1)	-C(8a)	-C(4a)	-139.8(3)
C(1)	-C(2)	-C(3)	-C(31)	176.8(4)
C(1)	-C(2)	-C(3)	-C(4)	0.5(5)
C(21)	-C(2)	-C(3)	-C(31)	-2.4(6)
C(21)	-C(2)	-C(3)	-C(4)	-179.7(4)
C(2)	-C(3)	-C(4)	-C(4a)	-18.8(5)
C(2)	-C(3)	-C(4)	-O(4)	-146.2(3)
C(31)	-C(3)	-C(4)	-C(4a)	163.8(4)
C(31)	-C(3)	-C(4)	-O(4)	36.4(5)
C(3)	-C(4)	-C(4a)	-C(5)	-75.6(4)
C(3)	-C(4)	-C(4a)	-C(8a)	48.2(4)
O(4)	-C(4)	-C(4a)	-C(5)	51.6(4)
O(4)	-C(4)	-C(4a)	-C(8a)	175.4(3)
C(4a)	-C(5)	-C(6)	-C(7)	-13.7(5)
C(6)	-C(5)	-C(4a)	-C(4)	165.6(3)
C(6)	-C(5)	-C(4a)	-C(8a)	42.6(4)
C(5)	-C(6)	-C(7)	-C(8)	0.3(6)
C(6)	-C(7)	-C(8)	-C(8a)	-15.7(6)
C(7)	-C(8)	-C(8a)	-C(1)	-78.9(5)
C(7)	-C(8)	-C(8a)	-C(4a)	45.0(5)
C(1)	-C(8a)	-C(4a)	-C(4)	-59.0(4)
C(1)	-C(8a)	-C(4a)	-C(5)	66.6(4)
C(8)	-C(8a)	-C(4a)	-C(4)	174.8(3)
C(8)	-C(8a)	-C(4a)	-C(5)	-59.5(4)
C(2)	-C(1)	-C(8a)	-H(8a)	-69(2)
O(1)	-C(1)	-C(8a)	-H(8a)	110(2)
C(1)	-C(2)	-C(21)	-H1(21)	-102(4)
C(1)	-C(2)	-C(21)	-H2(21)	23(6)
C(1)	-C(2)	-C(21)	-H3(21)	147(5)
C(3)	-C(2)	-C(21)	-H1(21)	77(4)
C(3)	-C(2)	-C(21)	-H2(21)	-157(6)
C(3)	-C(2)	-C(21)	-H3(21)	-34(5)

Table VIII (continued)

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

C(2)	-C(3)	-C(31)	-H1(31)	-31(4)
C(2)	-C(3)	-C(31)	-H2(31)	106(4)
C(2)	-C(3)	-C(31)	-H3(31)	-147(3)
C(4)	-C(3)	-C(31)	-H1(31)	147(4)
C(4)	-C(3)	-C(31)	-H2(31)	-76(4)
C(4)	-C(3)	-C(31)	-H3(31)	31(4)
C(2)	-C(3)	-C(4)	-H(4)	102(2)
C(31)	-C(3)	-C(4)	-H(4)	-75(2)
C(3)	-C(4)	-C(4a)	-H(4a)	167(2)
O(4)	-C(4)	-C(4a)	-H(4a)	-66(2)
H(4)	-C(4)	-C(4a)	-C(5)	166(2)
H(4)	-C(4)	-C(4a)	-C(8a)	-70(2)
H(4)	-C(4)	-C(4a)	-H(4a)	48(3)
C(3)	-C(4)	-O(4)	-H(O4)	57(5)
C(4a)	-C(4)	-O(4)	-H(O4)	-72(5)
H(4)	-C(4)	-O(4)	-H(O4)	170(5)
C(4a)	-C(5)	-C(6)	-H(6)	164(2)
H1(5)	-C(5)	-C(6)	-C(7)	107(2)
H1(5)	-C(5)	-C(6)	-H(6)	-75(3)
H2(5)	-C(5)	-C(6)	-C(7)	-134(2)
H2(5)	-C(5)	-C(6)	-H(6)	43(3)
C(6)	-C(5)	-C(4a)	-H(4a)	-77(2)
H1(5)	-C(5)	-C(4a)	-C(4)	44(2)
H1(5)	-C(5)	-C(4a)	-C(8a)	-79(2)
H1(5)	-C(5)	-C(4a)	-H(4a)	161(3)
H2(5)	-C(5)	-C(4a)	-C(4)	-73(2)
H2(5)	-C(5)	-C(4a)	-C(8a)	163(2)
H2(5)	-C(5)	-C(4a)	-H(4a)	44(3)
C(5)	-C(6)	-C(7)	-H(7)	174(3)
H(6)	-C(6)	-C(7)	-C(8)	-177(2)
H(6)	-C(6)	-C(7)	-H(7)	-3(4)
C(6)	-C(7)	-C(8)	-H1(8)	-138(3)
C(6)	-C(7)	-C(8)	-H2(8)	109(3)
H(7)	-C(7)	-C(8)	-C(8a)	169(2)
H(7)	-C(7)	-C(8)	-H1(8)	47(4)
H(7)	-C(7)	-C(8)	-H2(8)	-66(4)
C(7)	-C(8)	-C(8a)	-H(8a)	160(2)
H1(8)	-C(8)	-C(8a)	-C(1)	46(3)
H1(8)	-C(8)	-C(8a)	-C(4a)	170(3)
H1(8)	-C(8)	-C(8a)	-H(8a)	-75(3)
H2(8)	-C(8)	-C(8a)	-C(1)	156(3)
H2(8)	-C(8)	-C(8a)	-C(4a)	-80(3)
H2(8)	-C(8)	-C(8a)	-H(8a)	35(3)
C(1)	-C(8a)	-C(4a)	-H(4a)	-175(2)
C(8)	-C(8a)	-C(4a)	-H(4a)	59(2)
H(8a)	-C(8a)	-C(4a)	-C(4)	54(2)
H(8a)	-C(8a)	-C(4a)	-C(5)	180(2)
H(8a)	-C(8a)	-C(4a)	-H(4a)	-62(3)

Table VIII (continued)

Torsion angles (deg) with estimated standard deviations in parentheses

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Atoms				Value
C(8a)	-C(1)	-C(2)	-C(3)	-10.4(6)
O(1)	-C(1)	-C(2)	-C(3)	171.2(4)
C(2)	-C(1)	-C(8a)	-C(4a)	38.5(5)
C(2)	-C(1)	-C(8a)	-C(8)	164.2(4)
O(1)	-C(1)	-C(8a)	-C(4a)	-143.2(4)
O(1)	-C(1)	-C(8a)	-C(8)	-17.4(6)
C(1)	-C(2)	-C(3)	-C(4)	2.3(6)
C(2)	-C(3)	-C(4)	-C(4a)	-23.1(6)
C(2)	-C(3)	-C(4)	-O(4)	-147.6(4)
C(3)	-C(4)	-C(4a)	-C(5)	-72.7(5)
C(3)	-C(4)	-C(4a)	-C(8a)	50.4(5)
O(4)	-C(4)	-C(4a)	-C(5)	49.3(5)
O(4)	-C(4)	-C(4a)	-C(8a)	172.4(4)
C(4)	-C(4a)	-C(5)	-C(6)	166.0(4)
C(8a)	-C(4a)	-C(5)	-C(6)	43.0(5)
C(4)	-C(4a)	-C(8a)	-C(1)	-58.0(5)
C(4)	-C(4a)	-C(8a)	-C(8)	175.1(4)
C(5)	-C(4a)	-C(8a)	-C(1)	67.3(5)
C(5)	-C(4a)	-C(8a)	-C(8)	-59.5(5)
C(4a)	-C(5)	-C(6)	-C(61)	168.6(5)
C(4a)	-C(5)	-C(6)	-C(7)	-12.9(6)
C(5)	-C(6)	-C(7)	-C(71)	178.5(6)
C(5)	-C(6)	-C(7)	-C(8)	-2.7(7)
C(61)	-C(6)	-C(7)	-C(71)	-3.1(9)
C(61)	-C(6)	-C(7)	-C(8)	175.6(6)
C(6)	-C(7)	-C(8)	-C(8a)	-13.6(7)
C(71)	-C(7)	-C(8)	-C(8a)	165.3(5)
C(7)	-C(8)	-C(8a)	-C(1)	-80.2(5)
C(7)	-C(8)	-C(8a)	-C(4a)	44.7(6)
C(8a)	-C(1)	-C(2)	-H(2)	173(3)
O(1)	-C(1)	-C(2)	-H(2)	-6(3)
C(2)	-C(1)	-C(8a)	-H(8a)	-77(2)
O(1)	-C(1)	-C(8a)	-H(8a)	102(2)
C(1)	-C(2)	-C(3)	-H(3)	174(3)
H(2)	-C(2)	-C(3)	-C(4)	179(3)
H(2)	-C(2)	-C(3)	-H(3)	-10(4)
C(2)	-C(3)	-C(4)	-H(4)	97(2)
H(3)	-C(3)	-C(4)	-C(4a)	164(2)
H(3)	-C(3)	-C(4)	-O(4)	40(2)

Table VIII (continued)

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

H(3)	-C(3)	-C(4)	-H(4)	-75(3)
C(3)	-C(4)	-C(4a)	-H(4a)	165(2)
O(4)	-C(4)	-C(4a)	-H(4a)	-73(2)
H(4)	-C(4)	-C(4a)	-C(5)	168(2)
H(4)	-C(4)	-C(4a)	-C(8a)	-69(2)
H(4)	-C(4)	-C(4a)	-H(4a)	47(3)
C(3)	-C(4)	-O(4)	-H(O4)	112.3(5)
C(4a)	-C(4)	-O(4)	-H(O4)	-11.8(4)
H(4)	-C(4)	-O(4)	-H(O4)	-132(2)
C(4)	-C(4a)	-C(5)	-H1(5)	45(2)
C(4)	-C(4a)	-C(5)	-H2(5)	-72(2)
C(8a)	-C(4a)	-C(5)	-H1(5)	-78(2)
C(8a)	-C(4a)	-C(5)	-H2(5)	165(2)
H(4a)	-C(4a)	-C(5)	-C(6)	-74(2)
H(4a)	-C(4a)	-C(5)	-H1(5)	165(3)
H(4a)	-C(4a)	-C(5)	-H2(5)	48(3)
C(4)	-C(4a)	-C(8a)	-H(8a)	51(2)
C(5)	-C(4a)	-C(8a)	-H(8a)	176(2)
H(4a)	-C(4a)	-C(8a)	-C(1)	-173(2)
H(4a)	-C(4a)	-C(8a)	-C(8)	60(2)
H(4a)	-C(4a)	-C(8a)	-H(8a)	-65(3)
H1(5)	-C(5)	-C(6)	-C(61)	-67(2)
H1(5)	-C(5)	-C(6)	-C(7)	112(2)
H2(5)	-C(5)	-C(6)	-C(61)	45(2)
H2(5)	-C(5)	-C(6)	-C(7)	-136(2)
C(5)	-C(6)	-C(61)	-H1(61)	-174(4)
C(5)	-C(6)	-C(61)	-H2(61)	-37(4)
C(5)	-C(6)	-C(61)	-H3(61)	71(5)
C(7)	-C(6)	-C(61)	-H1(61)	7(4)
C(7)	-C(6)	-C(61)	-H2(61)	144(4)
C(7)	-C(6)	-C(61)	-H3(61)	-107(5)
C(6)	-C(7)	-C(71)	-H1(71)	-142(4)
C(6)	-C(7)	-C(71)	-H2(71)	116(6)
C(6)	-C(7)	-C(71)	-H3(71)	-18(5)
C(8)	-C(7)	-C(71)	-H1(71)	39(4)
C(8)	-C(7)	-C(71)	-H2(71)	-63(6)
C(8)	-C(7)	-C(71)	-H3(71)	163(4)
C(6)	-C(7)	-C(8)	-H1(8)	108(2)
C(6)	-C(7)	-C(8)	-H2(8)	-136(2)
C(71)	-C(7)	-C(8)	-H1(8)	-73(2)
C(71)	-C(7)	-C(8)	-H2(8)	43(2)
C(7)	-C(8)	-C(8a)	-H(8a)	168(2)
H1(8)	-C(8)	-C(8a)	-C(1)	159(2)
H1(8)	-C(8)	-C(8a)	-C(4a)	-76(3)
H1(8)	-C(8)	-C(8a)	-H(8a)	47(3)
H2(8)	-C(8)	-C(8a)	-C(1)	45(3)
H2(8)	-C(8)	-C(8a)	-C(4a)	169(3)
H2(8)	-C(8)	-C(8a)	-H(8a)	-68(4)

half-chair cyclohexene ring cis-fused to a second half-chair cyclohexenone moiety (Fig. 10). The hydroxyl group in both structures occupies the less stereochemically hindered pseudo-equatorial position in the cyclohexenone ring. Relatively short distances between the β-enone carbon C(3), and H1(5), and between the α-enone carbon C(2), and C(5) are a result of this conformation. Such molecular geometry makes H1(5)-abstraction by C(3) and subsequent collapse of the ensuing biradical, (C(2)...C(5)), highly favorable upon ultraviolet irradiation. This sequence is observed for both the 2,3- and 6,7-dimethyl compounds in which the C(3) to H1(5) distances are 2.84(4) and 2.82(3) Å, respectively. Both these values are less than the suggested (26) van der Waals radii sum limit of 2.90 Å for hydrogen abstraction by carbon. A list of other parameters involved in the abstraction reaction is given in Table IX.

A further consequence of this twisted conformation in the solid state, exhibited by naphthoquinols in which the hydroxyl group is <u>anti</u> to the bridgehead substituents, is the geometrically suitable position of the β-hydrogen, H(8), to oxygen abstraction. Although this reaction is observed in substituted naphthoquinones (26), its absence in the photoreactivity of naphthoquinols has been rationalized on the basis of the following two points (29). Firstly, in the quinone systems, the carbonyl group aids in stabilizing the biradical resulting from intramolecular β-H abstraction, whereas, the quinols lack this possibility of π-electron delocalization. Secondly, any charge transfer interaction (which may be required for β-H abstraction) between the cyclohexene double bond and the

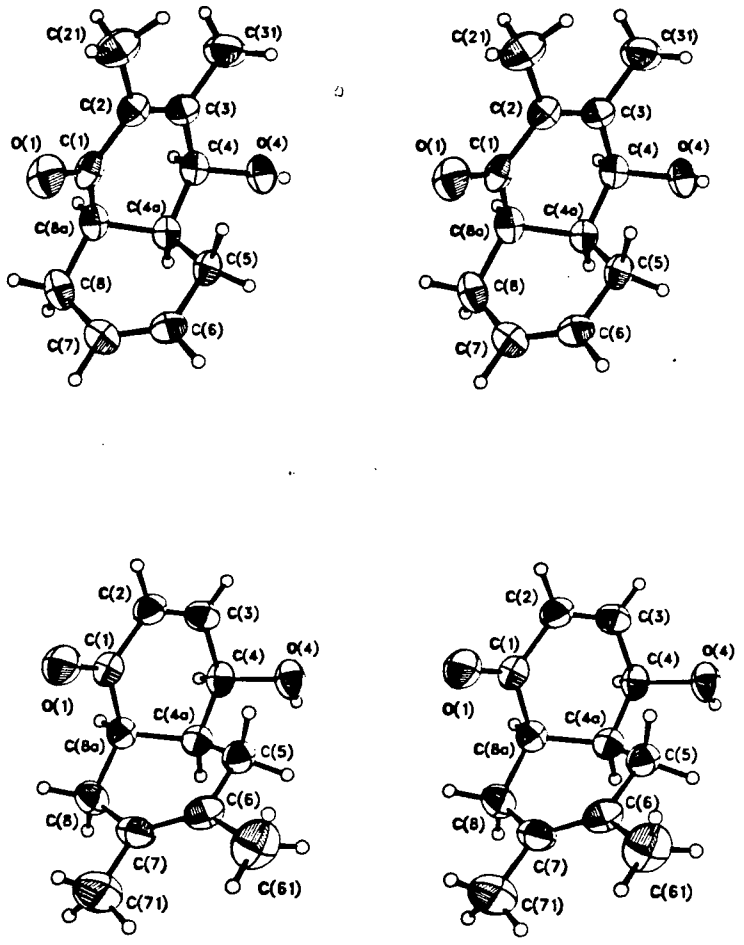

Figure 10

Stereo diagrams of 2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (top), and 6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (bottom).

excited ene-one chromophore is facilitated by the 2-ene-1,4-dione moiety which is a better electron acceptor than the 2-ene-1-one chromophore.

While the 2,3-dimethyl-naphthoquinol (IV) exhibits no oxygen abstraction photoreactivity, the 6,7-dimethyl compound yields a second solid state photoproduct which results from the unprecedented tetrahydronaphthoquinol reaction, oxygen

Table IX

Geometrical parameters in the β-enone abstraction reaction

τ_C = angle between C(3)...H1(5) vector and the plane of the C(2)=C(3) double bond

Δ_C = H1(5)...C(3)=C(2) angle.

	Δ_C(°)	τ_C(°)	C(3)...H1(5) (Å)	C(2)...C(5) (Å)
(IV)	79.7(8)	54.1	2.84(4)	3.416(5)
(V)	80.9(7)	56.7	2.82(3)	3.353(6)

abstraction of a β-hydrogen. The pertinent geometrical factors in the abstraction process are τ_O, the angle subtended by the oxygen to β-H vector and its projection onto the plane of the carbonyl group, and Δ_O, the C(1)=O(1)...β-H angle. These angles are 1 and 81(1) degrees, respectively which are close to the ideal abstraction angles of $\tau_O = 0°$ and $\Delta_O = 90°$.

Further investigation of the unsubstituted and other substituted tetrahydronaphthoquinols reveals that the oxygen

abstraction photoprocess occurs only in the systems in which the 2 and 3 positions on the cyclohexenone moiety are unsubstituted (35). This suggests that once conformational control is established, methyl substitution (or lack thereof) on the enone double bond plays a critical role in determining the photochemical reaction pathway in the solid state. In view of these recent findings, the previous rationale (page 55) used in explaining the lack of oxygen abstraction in tetrahydronaphthoquinols becomes less general.

Irradiation in solution, where conformational equilibration is facile affords mainly intramolecular [2+2] cycloadducts (35) owing to the presence of higher energy conformers which place the two intramolecular double bonds parallel to each other and within reacting distance. The absence of [2+2] intramolecular cycloaddition products in the solid state photolysis of (IV) and (V) is due mainly to the inability of the reactant molecules to undergo the extensive conformational rearrangement required to attain the reacting geometry. In the ground state, the C=C double bonds are non-parallel with C(2)...C(7) and C(3)...C(6) separations of 4.427(5) and 4.442(5) Å, respectively for (IV), and 4.427(6) and 4.397(6) Å for (V).

Generally, bond lengths and angles (Table X) correspond to accepted values (33). However, angles involving the methyl groups deviate slightly from the normal values, reflecting the steric interaction between adjacent substituents.

Molecules of (IV) are linked in the crystal (Fig. 11) by O(4)-H...O(4) hydrogen bonds to form chains running along a. The O(4)-H...O(4) angle is 166(6)° with an H...O(4) distance of

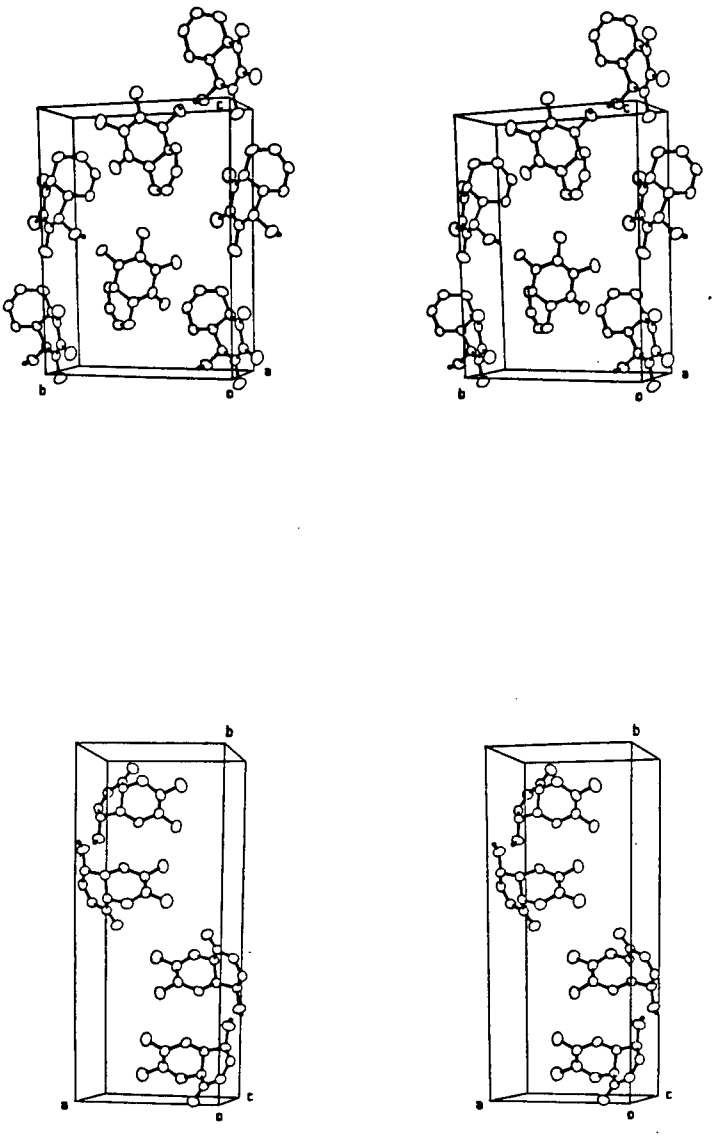

Figure 11

Stereo packing diagram of 2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (top), and 6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (bottom).

2.09(6) Å; the O(4)...O(4) separation is 2.830(2) Å. Similarly, O(4)-H...O(4) interactions join molecules of (V) in the crystal forming a linkage along the c-axis. The hydrogen bond angle and distance are 171(5)° and 2.00(5) Å, respectively, and the O(4)...O(4) distance is 2.783(2) Å. All other intermolecular contacts correspond to normal van der Waals distances.

Table X

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Bond lengths (Å) with estimated standard deviations in parentheses

Bond		Length	Bond		Length
C(1)	-C(2)	1.471(5)	C(4)	-O(4)	1.438(4)
C(1)	-C(8a)	1.512(5)	C(5)	-C(6)	1.497(5)
C(1)	-O(1)	1.221(4)	C(5)	-C(4a)	1.530(5)
C(2)	-C(21)	1.502(6)	C(6)	-C(7)	1.310(5)
C(2)	-C(3)	1.351(5)	C(7)	-C(8)	1.489(6)
C(3)	-C(31)	1.506(7)	C(8)	-C(8a)	1.525(6)
C(3)	-C(4)	1.514(5)	C(8a)	-C(4a)	1.533(5)
C(4)	-C(4a)	1.518(5)			

Bond angles (deg) with estimated standard deviations in parentheses

Bonds			Angle	Bonds			Angle
C(2)	-C(1)	-C(8a)	117.5(3)	C(4a)	-C(4)	-O(4)	111.7(3)
C(2)	-C(1)	-O(1)	121.2(4)	C(6)	-C(5)	-C(4a)	112.2(3)
C(8a)	-C(1)	-O(1)	121.3(3)	C(5)	-C(6)	-C(7)	124.1(3)
C(1)	-C(2)	-C(21)	115.9(4)	C(6)	-C(7)	-C(8)	123.9(4)
C(1)	-C(2)	-C(3)	120.8(3)	C(7)	-C(8)	-C(8a)	111.8(4)
C(21)	-C(2)	-C(3)	123.3(4)	C(1)	-C(8a)	-C(8)	113.4(3)
C(2)	-C(3)	-C(31)	122.7(4)	C(1)	-C(8a)	-C(4a)	109.5(3)
C(2)	-C(3)	-C(4)	121.8(3)	C(8)	-C(8a)	-C(4a)	111.2(3)
C(31)	-C(3)	-C(4)	115.5(4)	C(4)	-C(4a)	-C(5)	113.6(3)
C(3)	-C(4)	-C(4a)	113.9(3)	C(4)	-C(4a)	-C(8a)	109.2(3)
C(3)	-C(4)	-O(4)	111.3(3)	C(5)	-C(4a)	-C(8a)	110.5(3)

Table X (continued)

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(21) -H1(21)	0.90(6)	C(5) -H2(5)	0.98(3)
C(21) -H2(21)	0.93(9)	C(6) -H(6)	0.96(4)
C(21) -H3(21)	1.04(8)	C(7) -H(7)	1.00(3)
C(31) -H1(31)	0.89(5)	C(8) -H1(8)	0.99(4)
C(31) -H2(31)	0.96(5)	C(8) -H2(8)	0.96(5)
C(31) -H3(31)	1.05(7)	C(8a) -H(8a)	0.89(3)
C(4) -H(4)	1.01(3)	C(4a) -H(4a)	0.99(4)
C(5) -H1(5)	1.07(4)	O(4) -H(O4)	0.75(6)

Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(21) -H1(21)	110(4)	C(4a) -C(5) -H2(5)	108(2)
C(2) -C(21) -H2(21)	121(5)	H1(5) -C(5) -H2(5)	108(3)
C(2) -C(21) -H3(21)	115(4)	C(5) -C(6) -H(6)	114(2)
H1(21)-C(21) -H2(21)	107(5)	C(7) -C(6) -H(6)	122(2)
H1(21)-C(21) -H3(21)	99(5)	C(6) -C(7) -H(7)	124(2)
H2(21)-C(21) -H3(21)	102(6)	C(8) -C(7) -H(7)	112(2)
C(3) -C(31) -H1(31)	113(4)	C(7) -C(8) -H1(8)	113(3)
C(3) -C(31) -H2(31)	114(3)	C(7) -C(8) -H2(8)	112(3)
C(3) -C(31) -H3(31)	107(3)	C(8a) -C(8) -H1(8)	108(3)
H1(31)-C(31) -H2(31)	117(5)	C(8a) -C(8) -H2(8)	111(3)
H1(31)-C(31) -H3(31)	106(5)	H1(8) -C(8) -H2(8)	101(4)
H2(31)-C(31) -H3(31)	98(4)	C(1) -C(8a) -H(8a)	106(2)
C(3) -C(4) -H(4)	106(2)	C(8) -C(8a) -H(8a)	113(2)
C(4a) -C(4) -H(4)	110(2)	C(4a) -C(8a) -H(8a)	103(2)
O(4) -C(4) -H(4)	104(2)	C(4) -C(4a) -H(4a)	106(2)
C(6) -C(5) -H1(5)	110(2)	C(5) -C(4a) -H(4a)	107(2)
C(6) -C(5) -H2(5)	109(2)	C(8a) -C(4a) -H(4a)	110(2)
C(4a) -C(5) -H1(5)	108(2)	C(4) -O(4) -H(O4)	111(5)

Table X (continued)

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Bond lengths (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1) -C(2)	1.463(6)	C(4a) -C(8a)	1.525(5)
C(1) -C(8a)	1.514(6)	C(5) -C(6)	1.520(6)
C(1) -O(1)	1.219(4)	C(6) -C(61)	1.506(7)
C(2) -C(3)	1.321(5)	C(6) -C(7)	1.327(5)
C(3) -C(4)	1.487(6)	C(7) -C(71)	1.514(7)
C(4) -C(4a)	1.519(5)	C(7) -C(8)	1.501(6)
C(4) -O(4)	1.437(5)	C(8) -C(8a)	1.514(5)
C(4a) -C(5)	1.521(5)		

Bond angles (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(1) -C(8a)	116.7(4)	C(4a) -C(5) -C(6)	114.1(4)
C(2) -C(1) -O(1)	120.6(4)	C(5) -C(6) -C(61)	113.8(5)
C(8a) -C(1) -O(1)	122.6(4)	C(5) -C(6) -C(7)	122.0(4)
C(1) -C(2) -C(3)	121.4(5)	C(61) -C(6) -C(7)	124.1(5)
C(2) -C(3) -C(4)	123.5(4)	C(6) -C(7) -C(71)	123.1(5)
C(3) -C(4) -C(4a)	111.9(4)	C(6) -C(7) -C(8)	123.0(4)
C(3) -C(4) -O(4)	108.1(4)	C(71) -C(7) -C(8)	113.9(5)
C(4a) -C(4) -O(4)	112.5(3)	C(7) -C(8) -C(8a)	113.2(4)
C(4) -C(4a) -C(5)	113.6(4)	C(1) -C(8a) -C(4a)	110.0(3)
C(4) -C(4a) -C(8a)	109.6(3)	C(1) -C(8a) -C(8)	113.5(4)
C(5) -C(4a) -C(8a)	109.7(4)	C(4a) -C(8a) -C(8)	111.6(4)

Table X (continued)

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(2) -H(2)	0.98(4)	C(61) -H3(61)	0.90(8)
C(3) -H(3)	0.93(3)	C(71) -H1(71)	0.95(7)
C(4) -H(4)	1.03(4)	C(71) -H2(71)	0.88(8)
C(4a) -H(4a)	0.97(4)	C(71) -H3(71)	0.96(6)
C(5) -H1(5)	1.04(4)	C(8) -H1(8)	1.00(5)
C(5) -H2(5)	1.01(4)	C(8) -H2(8)	0.98(4)
C(61) -H1(61)	0.96(7)	C(8a) -H(8a)	0.93(3)
C(61) -H2(61)	0.91(6)	O(4) -H(O4)	0.79(5)

Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(1) -C(2) -H(2)	115(2)	H1(61)-C(61) -H2(61)	122(5)
C(3) -C(2) -H(2)	124(2)	H1(61)-C(61) -H3(61)	100(6)
C(2) -C(3) -H(3)	125(2)	H2(61)-C(61) -H3(61)	97(6)
C(4) -C(3) -H(3)	111(2)	C(7) -C(71) -H1(71)	106(4)
C(3) -C(4) -H(4)	107(2)	C(7) -C(71) -H2(71)	114(5)
C(4a) -C(4) -H(4)	110(2)	C(7) -C(71) -H3(71)	115(4)
O(4) -C(4) -H(4)	107(2)	H1(71)-C(71) -H2(71)	94(6)
C(4) -C(4a) -H(4a)	107(2)	H1(71)-C(71) -H3(71)	111(5)
C(5) -C(4a) -H(4a)	110(2)	H2(71)-C(71) -H3(71)	114(6)
C(8a) -C(4a) -H(4a)	107(2)	C(7) -C(8) -H1(8)	108(2)
C(4a) -C(5) -H1(5)	112(2)	C(7) -C(8) -H2(8)	112(2)
C(4a) -C(5) -H2(5)	111(2)	C(8a) -C(8) -H1(8)	109(2)
C(6) -C(5) -H1(5)	107(2)	C(8a) -C(8) -H2(8)	107(2)
C(6) -C(5) -H2(5)	107(2)	H1(8) -C(8) -H2(8)	106(4)
H1(5) -C(5) -H2(5)	105(3)	C(1) -C(8a) -H(8a)	100(2)
C(6) -C(61) -H1(61)	112(4)	C(4a) -C(8a) -H(8a)	109(2)
C(6) -C(61) -H2(61)	108(4)	C(8) -C(8a) -H(8a)	112(2)
C(6) -C(61) -H3(61)	117(5)	C(4) -O(4) -H(O4)	108(3)

CHAPTER III

2,3,4α,4aβ,6,7,8aβ-HEPTAMETHYL-4aβ,5,8,8aβ-TETRAHYDRO-1-NAPHTHOQUIN-4β-OL

Introduction

Solid state/solution photoreactivity differences have been observed in various substituted tetrahydronaphthoquinols (29,30,32,35). The divergence in reactivity patterns has been rationalized mainly by considering the fundamental distinction between the two phases, namely rigidity in the lattice versus mobility in solution. Reactions in solution, where molecular conformational equilibration is facile, are governed chiefly by kinetics, whereas, the solid state reactions are topochemically controlled. This lattice control can be exploited by designing a molecule so that its lowest energy conformation (in which it is most likely to crystallize) is one which predisposes the molecule to a specific reaction.

In an effort to test this conformational argument the title compound[1] was synthesized. This structural study was undertaken to verify the predicted conformation and to elucidate the geometric parameters involved in the observed photochemical reaction. A comparison of this compound and four other tetrahydronaphthoquinol derivatives (III)-(VII) is made in an attempt to ascertain substituent effects on the various structures and their reactivities.

Experimental

The title compound was prepared by methyllithium treatment

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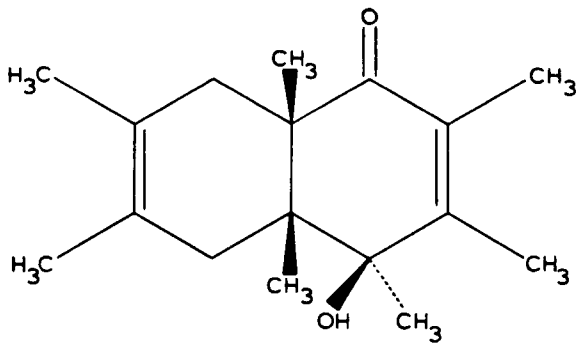
[1] IUPAC name: 4β-hydroxy-2,3,4α,4aβ,6,7,8aβ-heptamethyl-4aβ,5,8,8aβ-tetrahydro-1(4H)-naphthalenone

of the ene-dione, 2,3,4aβ,6,7,8aβ-hexamethyl-1,4-naphthoquinone. The two isomers formed were separated by fractional crystallization from cyclohexane/ethyl acetate which yielded acicular crystals of (VI).

Crystal data: $C_{17}H_{26}O_2$, MW = 262.4, monoclinic $\underline{a}$ = 7.497(2), $\underline{b}$ = 16.792(3), $\underline{c}$ = 12.687(3) Å, β = 105.30(1)°, $\underline{V}$ = 1540.4(6) Å^3, $\underline{Z}$ = 4, $\underline{D}_c$ = 1.141 g cm^{-3}, $\underline{D}_o$ = 1.140 g cm^{-3}, μ(MoKα) = 0.675 cm^{-1}, λ = 0.71073 Å, space group $\underline{P}2_1/\underline{c}$.

On the basis of the absences, $\underline{h}0\underline{l}$, $\underline{l}$ = 2$\underline{n}$ + 1 and 0$\underline{k}$0, $\underline{k}$ = 2$\underline{n}$ + 1 from precession and Weissenberg photographs, the space group was uniquely determined as $\underline{P}2_1/\underline{c}$. Data were collected with a crystal of dimensions 0.1 x 0.2 x 0.4 mm^3 and graphite monochromatized MoKα radiation. In the theta range 0.0-27.5°, 3516 reflections were collected with an ω–θ scan type. The omega scan width was calculated from the expression (0.80 + 0.35tanθ)° and extended 25% on each side of the peak for background measurement. The vertical aperture was constant at 4



(VI)

mm and the horizontal width was varied with theta according to the relationship (2.00 + 1.00tanθ) mm. In an attempt to improve the accuracy of the data, a non-equal test, whereby two final scans are done in opposite directions, was applied to each reflection. The odd and even increments in the 96 step intensity profile were compared on a statistical basis and a difference between corresponding values in the two scans of more than one standard deviation was the criterion for a repeat of measurement; failure a second time caused that reflection to be tagged making it readily identifiable after data processing.

Processing the data, which included Lorentz and polarization corrections applied in the usual manner, indicated that no reflection failed the non-equal test twice. Of the 3516 reflections collected, 1934 (55.0%) had $I \geq 3\sigma(I)$ where $\sigma^2(I) = S + 2B + (0.04(S - B))^2$, S being the scan count and B the time-averaged background.

Solution and Refinement

The positions of the 19 non-hydrogen atoms were located by MULTAN. Refinement of these atoms with isotropic temperature factors, followed by two cycles with anisotropic thermal parameters and a subsequent difference-Fourier yielded the coordinates for the 26 hydrogens. Refinement continued until convergence at R = 0.041 and Rw = 0.056. Towards the end of refinement the weighting scheme was changed from unit weights to $w = 1/\sigma^2(F)$, where $\sigma^2(F)$ is calculated from the $\sigma^2(I)$ defined above. A weighting analysis confirmed the suitability of the

chosen weights. Following convergence a final difference synthesis was calculated. The resulting map indicated residual density of 0.2 e/Å^3 in the region of O(4). This residue is possibly due to one of the oxygen lone pairs. The mean parameter shift on the final cycle of refinement was 0.198σ. The maximum shift of 1.290σ corresponded to the oscillating temperature factor of the methyl hydrogen, H1(21). The standard deviation in an observation of unit weight was 1.77. Final atomic coordinates and anisotropic thermal parameters are given in Tables XI and XII, respectively.

Discussion

Molecules of (VI) crystallize with the conformation common to all naphthoquinols studied in this series in which the bulkier substituent on C(4) assumes the pseudo-equatorial position. Although the 4-OH is <u>syn</u> to the bridgehead methyl groups, the conformation adopted (Fig. 12) is characteristic of the naphthoquinols which have the hydroxyl group <u>anti</u> to the bridgehead substituents, <u>i.e.</u> a half-chair cyclohexene ring cis-fused to a half-chair cyclohexenone moiety, with the bulkier 4-methyl substituent pseudo-equatorial. The degree of twist in the conformation can be described by the C(1)-C(8a)-C(4a)-C(5) torsion angle of 62.2(2)°. The spatial consequence of this arrangement is the proximity of the β-enone carbon C(3), to H1(5) (2.81(2) Å) (Table XIII). Furthermore, the angle between the C(3)...H1(5) vector and its projection onto the plane of the C(3)=C(2) double bond (C(1),...,C(4)), τ_C, and the angle

Table XI

Final positional (fractional x 10^5,H x 10^3)
and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)
with estimated standard deviations in parentheses

Atom	x	y	z	Ueq/Uiso
C(1)	85627(25)	11022(13)	72597(15)	41
C(2)	77531(27)	3371(13)	68018(15)	43
C(21)	89061(42)	-1482(23)	62201(27)	70
C(3)	60946(28)	1079(12)	68910(16)	42
C(31)	52062(46)	-6420(20)	63359(33)	72
C(4)	49635(25)	5859(12)	75154(15)	40
C(41)	41960(40)	191(19)	82425(24)	62
C(4a)	60761(24)	12836(12)	81957(15)	36
C(4a1)	47429(35)	18757(16)	85213(23)	54
C(5)	74006(29)	9490(13)	92495(16)	41
C(6)	89347(27)	14904(13)	98534(16)	44
C(61)	98744(50)	11991(23)	109961(21)	69
C(7)	93887(28)	21435(13)	94122(17)	47
C(71)	108809(50)	27135(23)	99922(30)	78
C(8)	84279(33)	23770(14)	82623(19)	49
C(8a)	72905(25)	17195(12)	75529(15)	37
C(8a1)	62208(36)	20932(18)	64595(20)	54
O(1)	101829(19)	12595(10)	73321(14)	64
O(4)	34349(19)	8803(10)	66657(12)	51

Table XI (continued)

H1(21)	818(6)	-26(2)	549(4)	145(14)
H2(21)	903(6)	-68(3)	646(4)	150(18)
H3(21)	989(8)	13(3)	612(4)	182(20)
H1(31)	384(5)	-65(2)	623(2)	93(10)
H2(31)	552(6)	-108(2)	680(3)	127(15)
H3(31)	545(5)	-71(2)	562(3)	110(12)
H1(41)	353(3)	33(1)	871(2)	64(7)
H2(41)	327(4)	-35(2)	777(2)	79(9)
H3(41)	523(4)	-32(2)	873(2)	73(8)
H1(O4)	246(4)	95(2)	690(2)	86(9)
H1(4a1)	380(4)	157(2)	884(2)	74(7)
H2(4a1)	539(4)	228(2)	900(2)	66(8)
H3(4a1)	398(4)	215(2)	788(2)	75(8)
H1(5)	795(3)	44(1)	908(2)	43(5)
H2(5)	668(3)	79(1)	975(2)	61(7)
H1(61)	1008(5)	61(2)	1103(3)	123(13)
H2(61)	1096(6)	137(2)	1122(4)	136(17)
H3(61)	918(7)	135(3)	1160(4)	161(18)
H1(71)	1179(6)	277(2)	960(4)	128(16)
H2(71)	1036(6)	329(3)	977(4)	166(19)
H3(71)	1139(6)	259(2)	1074(4)	137(15)
H1(8)	931(4)	254(1)	790(2)	63(7)
H2(8)	752(3)	284(1)	822(2)	66(7)
H1(8a1)	561(4)	171(2)	599(2)	69(9)
H2(8a1)	712(4)	233(2)	610(3)	99(10)
H3(8a1)	533(4)	251(1)	655(2)	71(8)

Table XII

Final anisotropic thermal parameters ($\underline{U}ij \times 10^4$ Å^2) and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
C(1)	297(10)	607(13)	337(10)	-11(9)	123(8)	26(9)
C(2)	342(10)	568(13)	379(10)	68(9)	97(8)	-54(10)
C(21)	543(16)	913(24)	657(17)	126(15)	205(14)	-268(17)
C(3)	385(11)	447(12)	408(11)	-1(9)	48(9)	-16(9)
C(31)	662(19)	640(19)	839(22)	-126(15)	149(16)	-205(17)
C(4)	270(9)	523(12)	403(10)	-29(9)	97(8)	46(9)
C(41)	534(15)	753(18)	609(15)	-232(14)	202(13)	52(15)
C(4a)	281(9)	459(11)	360(10)	11(8)	135(8)	-8(8)
C(4a1)	421(13)	659(17)	572(15)	93(12)	185(12)	-79(14)
C(5)	413(11)	491(13)	344(10)	8(10)	113(9)	33(9)
C(6)	378(11)	563(14)	371(10)	67(10)	88(9)	-47(10)
C(61)	673(19)	850(22)	432(14)	100(17)	-41(13)	8(14)
C(7)	392(11)	543(13)	454(12)	-18(10)	93(9)	-116(10)
C(71)	710(20)	879(24)	688(20)	-287(17)	62(17)	-196(18)
C(8)	477(13)	467(13)	550(13)	-84(11)	153(11)	17(11)
C(8a)	318(9)	434(11)	366(10)	-28(8)	99(8)	37(9)
C(8a1)	494(13)	627(17)	467(13)	-30(13)	83(11)	144(12)
O(1)	303(8)	922(13)	755(11)	-89(8)	246(8)	-131(9)
O(4)	254(7)	777(11)	498(8)	0(7)	78(6)	1(8)

between the C(3)...H1(5) and the C(3)=C(2) vectors, Δ_c, are 50° and 78.3(4)°, respectively. This geometry is highly favorable for hydrogen abstraction by the β-enone carbon and it is

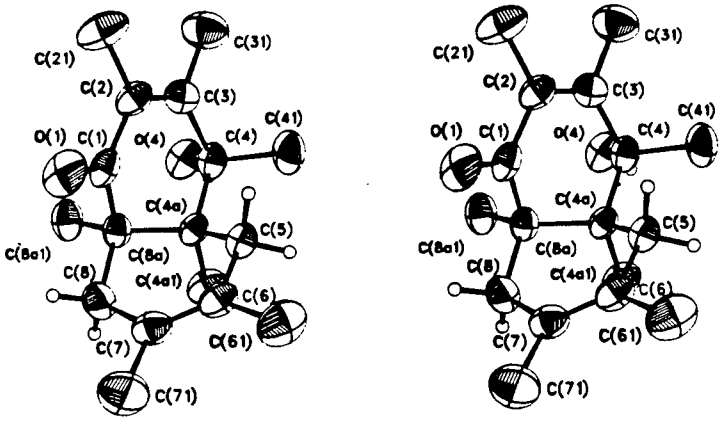


Figure 12

Stereo diagram of 2,3,4α,4aβ,6,8aβ-heptamethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4β-ol

therefore not surprising that this is the dominant reaction observed in the solid state photolysis (36). Irradiation in solution affords only the intramolecular [2+2] cycloaddition photoproduct, due to the presence of a high energy conformer not available in the crystal lattice.

It is interesting to note that oxygen abstraction of a β-

hydrogen does not occur despite molecular fulfillment of the geometric requirements. The β-H deviates only 1° from the plane of the carbonyl at a distance of 2.41(2) Å from O(1). The C=O...β-H angle of 82.7(6)° completes the almost perfect alignment of the β-H with the non-bonding orbital of O(1). However, it was argued in the previous chapter that substituents on the C(2) and C(3) positions of the cyclohexenone moiety play a critical role in determining the photochemical reaction pathway, possibly by lowering the energy of the (π,π^*) transition from which the carbon abstraction of H1(5) is considered to originate. The lack of β-H abstraction by oxygen in this system lends support to the above argument but does little to clarify the role(s) of the C(2) and C(3) substituents.

Bond distances, angles and torsion angles are presented in Tables XIV, XV, XVI, XVII, XVIII, XIX, and XX. The former two quantities generally do not deviate significantly from accepted values (33) with the exception of bonds C(3)-C(4) and C(4)-C(4a) whose lengths of 1.531(3) Å and 1.560(3) Å, respectively, are anomalously large compared to the same bonds in the closely related hexamethyl-4α-ol derivative (37). At present, no explanation is offered for these seemingly long bonds except to note the obvious difference between these two derivatives being the additional methyl group on C(4) in this structure. It is not expected that steric effects alone, due to the introduction of the C(41) methyl group would account for the increase in the length of the above bonds.

Hydrogen bonding, found in all the naphthoquinols studied in this series, is present in this structure as O(4)-H...O(1)

interactions linking molecules along the a-axis (Fig. 13), O...O = 2.855(2) Å, H...O = 1.99(3) Å, O-H...O = 172(3)°.

Comparison of Compounds (III)-(VII)

Comparisons of bond lengths and angles and torsion angles in analogous tetrahydronaphthoquinones (34) and more recently in tetrahydronaphthoquinols (32) have revealed the gross effects of

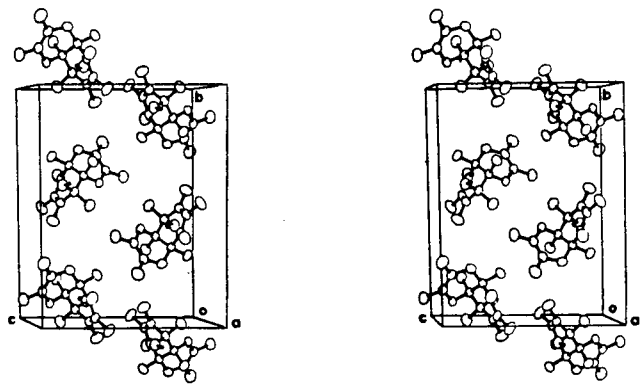


Figure 13

Stereo packing diagram of 2,3,4α,4aβ,6,8aβ-heptamethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4β-ol

substituents on the parent ring system. Many of the trends noted previously are corroborated in the present comparison of an additional four tetrahydronaphthoquinol derivatives. The

appropriate information regarding the parent, unsubstituted compound (32) has been reproduced (Tables XIII-XVI) to facilitate comparisons.

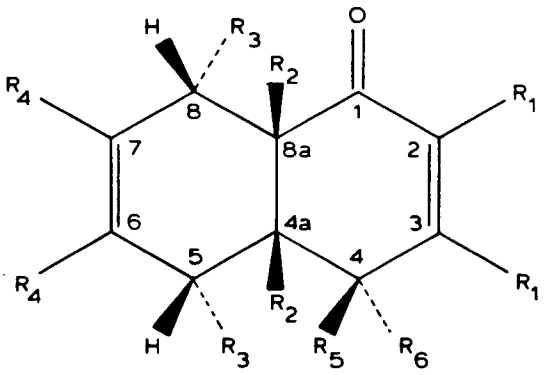
All six-membered rings adopt the half-chair conformation, predicted by Bucourt and Hainaut (38) as the most energetically stable conformation for both unsubstituted and substituted cyclohexenes. Although the tetrahydronaphthoquinols studied thus far include examples of OH-anti and OH-syn conformations, only the former are represented here for comparison with (VI) in which, despite the pseudo-axial syn position of the hydroxy group the conformation is similar to the OH-anti compounds. Compounds (III)-(VII) consist of two cis-fused cyclohexene rings, the carbon skeleton of which may be described by three approximate planes. Two planes containing atoms C(1) to C(4) and C(5) to C(8) make an angle of approximately 85° and subtend angles of close to 140° with respect to the third plane defined by atoms C(4), C(4a), C(8a) and C(8). The C(4)-C(4a)-C(8a)-C(8) torsion angles (Table XVI), averaging 175.7(5)°, indicate the extent to which these atoms approximate a plane. Torsion angles for the other planes range from -3.4(3)° to 2.3(5)°.

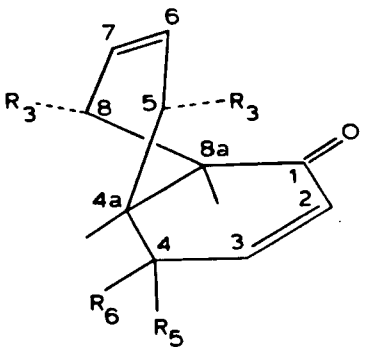
Substituents on carbons C(4a) and C(8a) appear to have little effect on the bridgehead torsion angle R_2-C(4a)-C(8a)-R_2 (Table XVI) which remains fairly constant, averaging -63° for compounds (III)-(VII). However, the internal twist angle, C(1)-C(8a)-C(4a)-C(5) decreases by ca. 5° upon methyl substitution at the bridgehead carbons (compound (VI)); similar results were observed in several naphthoquinone derivatives (34) and in other naphthoquinols (32). Whether this internal torsional decrease

Table XIII

Derivatives whose structures have been determined[2], with molecular conformations, parameters relevant to photochemical activity, and hydrogen bond distances (distances in Angstroms and angles in degrees).

Compound	(VII)	(IV)	(V)	(III)	(VI)
R_1	H	Me	H	Me	Me
R_2	H	H	H	H	Me
R_3	H	H	H	H	H
R_4	H	H	Me	Me	Me
R_5	H	H	H	H	OH
R_6	OH	OH	OH	OH	Me





Conformation common to all anti derivatives

(the bulkier group on C(4) is anti to bridgehead substituents)

[2] Information regarding (VII) has been obtained from reference 32.

Table XIII (continued)

Intramolecular geometries*

	(VII)	(IV)	(V)	(III)	(VI)
C(2)...H1(5)	2.94(2)	2.92(4)	2.92(3)	2.91(5)	2.86(2)
$\tau_{C(2)}$	52.1	52.0	53.8	51.7	48.9
$\Delta_{C(2)}$	71.3(3)	73.2(7)	72.5(7)	73(1)	74.5(4)
C(3)...H1(5)	2.81(2)	2.84(4)	2.82(3)	2.84(5)	2.81(2)
$\tau_{C(3)}$	55.7	54.1	56.7	53.5	50.0
$\Delta_{C(3)}$	82.2(4)	79.7(8)	80.9(7)	79(1)	78.3(4)
O...H1(8)	2.49(2)	2.49(4)	2.49(4)	2.58	2.41(2)
τ_O	0.6	1	4	3	1
Δ_O	81.8(5)	83(1)	81(1)	89	82.7(6)
C(3)...C(6)	4.381(2)	4.442(5)	4.397(6)	4.457(3)	4.453(3)
C(2)...C(7)	4.392(2)	4.427(5)	4.427(6)	4.457(3)	4.419(3)
d_1	4.35	4.40	4.37	4.42	4.40
C(1)...C(6)	3.404(2)	3.379(5)	3.414(5)	3.415(3)	3.293(3)
O(1)...C(7)	3.395(2)	3.332(4)	3.419(5)	3.487(5)	3.217(3)
θ	89	88	90	87	98
d_2	3.35	3.30	3.36	3.38	3.19
		Hydrogen bonding			
O(1)...O(4)	-	-	-	2.652(5)	2.855(2)
O(4)...O(4)	2.747(3)	2.830(2)	2.783(2)	2.804(2)	-
	2.833(3)				
		Primary photochemical reaction**			
Solution	(1)	(1)	(1)	(1)	(1)
Solid state	(2,3)	(2)	(2,3)	(2)	(2)

Table XIII (continued)

*For the C...H interactions Δ_C is the C=C...H angle and τ_C is the angle between the C...H vector and the enone plane defined by C(1)-C(2)=C(3)-C(4). For the O...H interactions Δ_O is the C=O...H angle and τ_O is the angle between the O...H vector and the carbonyl mean plane. d_1 is the C=C center-to-center distance and d_2 is the C=O, C(6)=C(7) center-to-center distance. θ is the angle between the normals to the carbonyl and the C(5)-C(6)=C(7)-C(8) mean planes.

**(1) Intramolecular [2+2] cycloaddition. (2) H-abstraction by the β-enone carbon C(3). (3) H-abstraction by the carbonyl oxygen O(1).

without a concomitant external increase is due to hybridization or steric effects is still not clear.

Generally, increased substitution in the naphthoquinols results in an enlarged ring size. This is evident in the increases in several bond lengths and angles (Tables XIV and XV). The C(2)=C(3) bond in compounds (III) and (IV) has a mean value of 1.345 Å which is 0.019 Å longer than the same but unsubstituted bond in the parent compound, (VII). The C(2)=C(3) bond in (VI) also appears to be lengthened, although the difference from (VII) is not definitely significant in this case (2.5σ). Substituents at positions C(2) and C(3) affect the C(2)-C(1)-C(8a) and C(3)-C(4)-C(4a) angles by enlarging them marginally ($<1.4^{\circ}$) with concomitant decreases in the internal C(2)=C(3) double bond angles. Similar substituent-associated effects are apparent at the C(6)=C(7) end of the ring. With methyl substituents at positions C(6) and C(7), the C(6)=C(7) double bond is lengthened by an average of 0.016 Å compared to the same bond in (VII) where hydrogens are the substituents. Compound (VI), whose C(6)=C(7) bond length is essentially the same as that in (VII) does not seem to follow this trend. The angles C(4a)-C(5)-C(6) and C(7)-C(8)-C(8a) show an increase of $1.4\text{-}4.6^{\circ}$ for R_4=Me, whereas the internal angles C(5)-C(6)=C(7) and C(6)=C(7)-C(8) generally decrease by $0.9\text{-}3.2^{\circ}$ for the same substitution. It is apparent from the above comparison that the increase in the internal angles involving the oxygen-bearing carbons as vertices is due mainly to substitution at the double-bonded carbons and not to the bridgehead substituents (32). It is not clear, however, why the double-bond distances in (VI) do

not follow the trend observed for the substituted double bonds of other derivatives (cf. 32).

It is observed in compounds (III)-(VI) that methyl substitution at the double bond tends to increase the single-bond lengths between the substituted double-bond carbons and the adjacent ring carbons. These bonds average 0.014 Å greater than the related bonds in the parent compound. The C(5)-C(6) distance of 1.484(3) Å in (III) seems anomalous with respect to the above trend; however, this may be a result of imperfections in the model owing to the disorder in that structure. Methyl substitution at C(2) and C(3) affects the external angles C(2)-C(1)-O(1) and C(3)-C(4)-O(4) by widening them 0.5-0.7° and 1.9-3.9°, respectively. This is attributed to steric effects between the oxygens and the bulky methyl groups. The tendency for the methyl groups to bend away from each other is limited by the opposing oxygen atoms which lie nearly in the same plane.

Molecules within crystals of each of the compounds (III)-(VII) are linked by hydrogen bonding. Molecules of (IV) and (V) are joined via O(4)...O(4) whereas (VI) is linked by O(4)-H...O(1) interactions. Due to the disorder in (III), it is difficult to discern the actual type of hydrogen bonding, but it has been suggested (see Chapter I, Discussion) that the two types, O(4)...O(4) and O(4)...O(1) are operative. The parent compound (VII) exhibits O(4)...O(4) intermolecular hydrogen bonding through disordered hydroxyl hydrogen atoms (32).

The photochemistry of these compounds in solution and the solid state has been discussed elsewhere (29,30,36,39). Compounds (III)-(VII) all react in the solid state. The

Table XIV. Bond distances (Å) with e.s.d.'s in parentheses for compounds (III)-(VII)

	(VII)	(IV)	(V)	(III)	(VI)
C(1) -C(2)	1.467(2)	1.471(5)	1.463(6)	1.484(3)	1.473(3)
C(2) -C(3)	1.326(2)	1.351(5)	1.321(5)	1.339(3)	1.335(3)
C(3) -C(4)	1.499(2)	1.514(5)	1.487(6)	1.505(3)	1.531(3)
C(4) -C(4a)	1.524(2)	1.518(5)	1.519(6)	1.514(3)	1.560(3)
C(4a)-C(5)	1.527(2)	1.530(5)	1.521(6)	1.515(3)	1.545(3)
C(5) -C(6)	1.497(2)	1.497(5)	1.520(6)	1.484(3)	1.507(3)
C(6) -C(7)	1.317(2)	1.310(5)	1.327(5)	1.339(3)	1.316(3)
C(7) -C(8)	1.490(2)	1.489(6)	1.501(6)	1.505(3)	1.499(3)
C(8) -C(8a)	1.518(2)	1.525(6)	1.514(5)	1.514(3)	1.533(3)
C(8a)-C(1)	1.516(2)	1.512(5)	1.514(6)	1.515(3)	1.520(3)
C(8a)-C(4a)	1.537(2)	1.533(5)	1.525(5)	1.533(4)	1.556(2)
C(1) -O(1)	1.216(2)	1.221(4)	1.219(4)	1.199(4)	1.223(2)
C(4) -O(4)	1.426(2)	1.438(4)	1.437(5)	1.356(4)	1.438(2)

Table XV. Bond angles (°) with e.s.d.'s in parentheses for compounds (III)-(VII)

	(VII)	(IV)	(V)	(III)	(VI)
C(2) -C(1) -C(8a)	116.7(1)	117.5(3)	116.7(4)	116.6(2)	118.1(2)
C(2) -C(1) -O(1)	120.5(1)	121.2(3)	120.6(4)	116.6(3)	121.0(2)
C(8a)-C(1) -O(1)	122.8(1)	121.3(3)	122.6(4)	126.5(3)	120.6(2)
C(1) -C(2) -C(3)	121.5(1)	120.8(3)	121.4(5)	120.6(2)	120.9(2)
C(2) -C(3) -C(4)	123.6(1)	121.8(3)	123.5(4)	123.0(2)	123.2(2)
C(3) -C(4) -C(4a)	112.0(1)	113.9(3)	111.9(4)	113.7(2)	113.1(1)
C(3) -C(4) -O(4)	109.4(1)	111.3(3)	108.1(4)	113.3(2)	103.5(1)
C(4a)-C(4) -O(4)	112.9(1)	111.7(3)	112.5(3)	110.5(2)	111.1(2)
C(4) -C(4a)-C(5)	113.0(1)	113.6(3)	113.6(4)	114.2(2)	109.5(1)
C(4) -C(4a)-C(8a)	109.6(1)	109.2(3)	109.6(4)	109.7(2)	111.4(1)
C(8a)-C(4a)-C(5)	111.1(1)	110.5(3)	109.7(4)	109.8(1)	107.0(1)
C(4a)-C(5) -C(6)	112.2(1)	112.2(3)	114.1(4)	116.6(2)	116.8(2)
C(5) -C(6) -C(7)	123.8(1)	124.1(3)	122.0(4)	120.6(2)	122.3(2)
C(6) -C(7) -C(8)	124.3(1)	123.9(4)	123.0(4)	123.0(2)	121.3(2)
C(7) -C(8) -C(8a)	111.8(1)	111.8(4)	113.2(4)	113.7(2)	115.7(2)
C(8) -C(8a)-C(1)	112.7(1)	113.4(3)	113.5(4)	114.2(2)	110.3(2)
C(8) -C(8a)-C(4a)	111.7(1)	111.2(3)	111.6(4)	109.7(2)	110.0(2)
C(4a)-C(8a)-C(1)	110.1(1)	109.5(3)	110.0(3)	109.8(1)	107.4(2)
C(1) -C(2) -C(21)	-	115.9(4)	-	115.0(2)	115.6(2)
C(21)-C(2) -C(3)	-	123.3(4)	-	124.4(2)	123.4(2)
C(2) -C(3) -C(31)	-	122.7(4)	-	122.3(2)	120.5(2)
C(31)-C(3) -C(4)	-	115.5(4)	-	114.7(2)	116.2(2)
C(5) -C(6) -C(61)	-	-	113.8(5)	115.0(2)	113.0(2)
C(61)-C(6) -C(7)	-	-	124.1(5)	124.4(2)	124.6(2)
C(6) -C(7) -C(71)	-	-	123.1(5)	122.3(2)	124.3(2)
C(71)-C(7) -C(8)	-	-	113.9(5)	114.7(2)	114.4(2)

pertinent geometrical parameters are given in Table XIII, page 77.

It has been suggested (26) that the intramolecular hydrogen abstraction by carbon or oxygen can occur over distances as great as the sum of the van der Waals radii of the two atoms involved. For carbon abstraction of hydrogen the suggested upper limit is 2.90 Å ($\bar{r}_w$(C) = 1.70 Å, $\bar{r}_w$(H) = 1.20 Å) whereas, for abstraction by oxygen the limit suggested is 2.72 Å ($\bar{r}_w$(O) = 1.52 Å, $\bar{r}_w$(H) = 1.20 Å). Table XIII shows C(2)...H distances all greater than the 2.90 Å limit while the C(3)...H distances range from 2.81 Å to 2.84 Å. Implicit in the above suggested limits is the requirement of otherwise favorable reacting geometry. This is indicated by the orientation of the orbital involved in the abstraction process relative to the position of the abstractable hydrogen. Although the exact orientation of the abstracting orbital with respect to the hydrogen atom to be abstracted is not directly observable, it can be inferred from the two angles τ and Δ. In the abstraction by carbon process τ_c is the angle between the $C_{abs}...H_{abs}$ vector and the plane of the C(2)=C(3) double bond (C(1), C(2), C(3), C(4)), and Δ_c is the angle between the $C_{abs}...H_{abs}$ and the C(2)=C(3) vectors. Angles of 90° for both τ_c and Δ_c imply the most favorable abstracting geometry with the abstracting C 2p-orbital collinear with the vulnerable hydrogen. All compounds, (III)-(VII) react via H1(5) abstraction by the β-enone carbon C(3), although the τ_c values in Table XIII appear much less than favorable. However, it is not unreasonable to expect 30-40° rotation around the C(2)=C(3) double bond upon

(π,π^*) excitation (26, and references therein). Rotation in a favorable sense yields a τ_c value of close to 90° for the molecule in the excited state.

The secondary solid state reaction observed in (V) and (VII) results in a dihydroxy 1,6-bonded product analogous to naphthoquinone products resulting from β-hydrogen abstraction reactions (35). Inspection of Table XIII reveals the favorable geometry of all compounds for the occurrence of carbonyl oxygen abstraction of β-hydrogen with O...H separations of less than 2.58 Å, and τ_o and Δ_o angles of 0° and 90°, respectively; τ_o being the angle subtended by the $O_{abs}...H_{abs}$ vector and the plane of the carbonyl (O(1), C(1), C(2), C(8a)), and Δ_o being the angle between the $O_{abs}...H_{abs}$ and the O=C vectors. The ideal geometry is based on the alignment of the abstractable hydrogen on C(8) and the n-orbital on the oxygen which lies in the plane of the carbonyl group and perpendicular to the double bond. However, only (V) and (VII) were observed to undergo this type of reaction. It was suggested in Chapter II that substituents on the enone double bond and their effects on the excited state of the molecule may be the critical feature in determining the probability of the above reaction.

No intramolecular [2+2] cycloaddition products are observed in the solid state, while in solution , where conformational equilibration is facile, all compounds undergo this reaction. The absence of [2+2] cycloaddition products in the solid state is rationalized on the basis of the remoteness of the double bonds and their askew orientations. For the above compounds, the angle between the vectors C(6)=C(7) and C(3)=C(2) is ca. 50° and

Table XVI. Torsion angles (°) with e.s.d.'s in parentheses for compounds (III)-(VII)

	(VII)[1]	(IV)	(V)	(III)	(VI)
C(1) -C(2) -C(3) -C(4)	-0.1(2)	-0.5(4)	2.3(5)	-2.3(3)	-3.4(3)
C(2) -C(3) -C(4) -C(4a)	-20.8(2)	-18.8(4)	-23.1(5)	-16.3(3)	-9.8(3)
C(3) -C(4) -C(4a)-C(8a)	49.1(1)	48.2(3)	50.4(4)	46.5(2)	40.9(2)
C(4) -C(4a)-C(8a)-C(1)	-58.1(1)	-59.0(3)	-58.0(4)	-58.9(2)	-57.4(2)
C(4a)-C(8a)-C(1) -C(2)	38.6(1)	42.0(4)	38.5(4)	42.0(3)	46.3(2)
C(8a)-C(1) -C(2) -C(3)	-9.4(2)	-12.0(4)	-10.4(5)	-11.5(3)	-16.5(3)
C(4a)-C(5) -C(6) -C(7)	-12.9(2)	-13.7(4)	-12.9(5)	-11.5(3)	-13.9(3)
C(5) -C(6) -C(7) -C(8)	-1.2(2)	-0.3(5)	-2.7(5)	-2.3(3)	-1.6(3)
C(6) -C(7) -C(8) -C(8a)	-14.6(2)	-15.7(5)	-13.6(5)	-16.3(3)	-15.6(3)
C(7) -C(8) -C(8a)-C(4a)	43.6(1)	45.0(4)	44.7(4)	46.5(2)	46.4(2)
C(8) -C(8a)-C(4a)-C(5)	-58.4(1)	-59.5(3)	-59.5(4)	-58.9(2)	-57.9(2)
C(8a)-C(4a)-C(5) -C(6)	41.6(1)	42.6(3)	43.0(4)	42.0(3)	43.1(2)
R_1 -C(4a)-C(8a)-R_2	-63(1)	-62(3)	-65(3)	-63(3)	-62.7(2)
C(4) -C(4a)-C(8a)-C(8)	176.0(1)	174.8(3)	175.1(3)	174.9(2)	-177.5(2)
C(1) -C(8a)-C(4a)-C(5)	67.5(1)	66.6(3)	67.3(4)	67.3(3)	62.2(2)
C(3) -C(4) -C(4a)-C(5)	-75.4(1)	-75.6(3)	-72.7(4)	-77.1(2)	-77.3(2)
C(8) -C(8a)-C(1) -C(2)	164.0(1)	166.9(3)	164.2(4)	165.6(2)	166.2(2)
O(1) -C(1) -C(8a)-C(4a)	-143.0(1)	-139.8(3)	-143.2(4)	-145.2(5)	-138.7(2)
O(1) -C(1) -C(8a)-C(8)	-17.6(2)	-15.0(4)	-17.4(5)	-21.6(5)	-18.8(3)
O(1) -C(1) -C(2) -C(3)	172.1(1)	169.8(4)	171.2(4)	175.0(4)	168.5(2)
O(4) -C(4) -C(3) -C(2)	-146.7(2)	-146.2(3)	-147.6(4)	-143.5(3)	110.6(2)
O(4) -C(4) -C(4a)-C(5)	48.6(1)	51.6(3)	49.3(4)	51.5(3)	166.8(1)
O(4) -C(4) -C(4a)-C(8a)	173.1(1)	175.4(3)	172.4(3)	175.2(2)	-75.0(2)
C(1) -C(8a)-C(8) -C(7)	-80.9(1)	-78.9(4)	-80.2(4)	-77.1(2)	-72.0(2)

[1] Torsion angles for (VII) refer to the enantiomer of the parent compound in Greenhough and Trotter, 1981 (32).

their double bond center-to-center separations are >4.3 Å. Similarly, unfavorable [2+2] intramolecular cycloaddition geometries exist for the C=O and C(6)=C(7) double bonds (Table XIII).

Table XVII

Supplementary bond lengths (Å) and angles (°) for compound (VI) with e.s.d.'s in parentheses

Bond	Length
C(2) -C(21)	1.514(3)
C(3) -C(31)	1.509(3)
C(4) -C(41)	1.539(3)
C(4a)-C(4a1)	1.541(3)
C(6) -C(61)	1.516(3)
C(7) -C(71)	1.508(3)
C(8a)-C(8a1)	1.541(3)

Bonds	Angle
C(3) -C(4) -C(41)	109.4(2)
C(41) -C(4) -C(4a)	111.3(2)
C(41) -C(4) -O(4)	108.2(2)
C(4) -C(4a)-C(4a1)	110.1(2)
C(4a1)-C(4a)-C(5)	108.5(2)
C(4a1)-C(4a)-C(8a)	110.3(2)
C(1) -C(8a)-C(8a1)	105.6(2)
C(4a) -C(8a)-C(8a1)	115.2(2)
C(8) -C(8a)-C(8a1)	108.2(2)

Table XVIII

Bond lengths involving hydrogen atoms (Å) in compound (VI) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(21) -H1(21)	0.95(4)	C(5) -H2(5)	0.97(2)
C(21) -H2(21)	0.94(4)	C(61) -H1(61)	1.00(4)
C(21) -H3(21)	0.91(5)	C(61) -H2(61)	0.84(4)
C(31) -H1(31)	0.99(3)	C(61) -H3(61)	1.06(5)
C(31) -H2(31)	0.93(4)	C(71) -H1(71)	0.95(4)
C(31) -H3(31)	0.98(4)	C(71) -H2(71)	1.05(5)
C(41) -H1(41)	1.02(2)	C(71) -H3(71)	0.95(5)
C(41) -H2(41)	1.00(3)	C(8) -H1(8)	0.94(3)
C(41) -H3(41)	1.03(3)	C(8) -H2(8)	1.02(2)
C(4a1)-H1(4a1)	1.03(3)	C(8a1)-H1(8a1)	0.92(3)
C(4a1)-H2(4a1)	0.96(3)	C(8a1)-H2(8a1)	0.99(3)
C(4a1)-H3(4a1)	0.98(3)	C(8a1)-H3(8a1)	1.00(3)
C(5) -H1(5)	1.01(2)	O(4) -H1(O4)	0.87(3)

Table XIX

Bond angles (deg) involving hydrogen atoms in compound (VI)

with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(21) -H1(21)	109(2)	C(6) -C(5) -H2(5)	108.0(13)
C(2) -C(21) -H2(21)	112(3)	H1(5) -C(5) -H2(5)	104(2)
C(2) -C(21) -H3(21)	112(3)	C(6) -C(61) -H1(61)	113(2)
H1(21)-C(21) -H2(21)	97(3)	C(6) -C(61) -H2(61)	112(3)
H1(21)-C(21) -H3(21)	104(4)	C(6) -C(61) -H3(61)	115(2)
H2(21)-C(21) -H3(21)	121(4)	H1(61)-C(61) -H2(61)	102(3)
C(3) -C(31) -H1(31)	113(2)	H1(61)-C(61) -H3(61)	108(3)
C(3) -C(31) -H2(31)	111(3)	H2(61)-C(61) -H3(61)	107(4)
C(3) -C(31) -H3(31)	111(2)	C(7) -C(71) -H1(71)	111(2)
H1(31)-C(31) -H2(31)	99(3)	C(7) -C(71) -H2(71)	106(2)
H1(31)-C(31) -H3(31)	108(3)	C(7) -C(71) -H3(71)	113(3)
H2(31)-C(31) -H3(31)	115(3)	H1(71)-C(71) -H2(71)	92(3)
C(4) -C(41) -H1(41)	110.4(14)	H1(71)-C(71) -H3(71)	113(3)
C(4) -C(41) -H2(41)	110(2)	H2(71)-C(71) -H3(71)	120(4)
C(4) -C(41) -H3(41)	111.1(14)	C(7) -C(8) -H1(8)	109.4(15)
H1(41)-C(41) -H2(41)	107(2)	C(7) -C(8) -H2(8)	113.2(14)
H1(41)-C(41) -H3(41)	110(2)	C(8a) -C(8) -H1(8)	106.0(15)
H2(41)-C(41) -H3(41)	108(2)	C(8a) -C(8) -H2(8)	104.6(13)
C(4a) -C(4a1)-H1(4a1)	110.4(14)	H1(8) -C(8) -H2(8)	107(2)
C(4a) -C(4a1)-H2(4a1)	111.8(15)	C(8a) -C(8a1)-H1(8a1)	111(2)
C(4a) -C(4a1)-H3(4a1)	110.7(15)	C(8a) -C(8a1)-H2(8a1)	109(2)
H1(4a1)-C(4a1)-H2(4a1)	113(2)	C(8a) -C(8a1)-H3(8a1)	112.8(15)
H1(4a1)-C(4a1)-H3(4a1)	104(2)	H1(8a1)-C(8a1)-H2(8a1)	105(2)
H2(4a1)-C(4a1)-H3(4a1)	107(2)	H1(8a1)-C(8a1)-H3(8a1)	109(2)
C(4a) -C(5) -H1(5)	109.3(11)	H2(8a1)-C(8a1)-H3(8a	109(2)
C(4a) -C(5) -H2(5)	108.9(13)	C(4) -O(4) -H1(O4)	112(2)
C(6) -C(5) -H1(5)	109.0(11)		

Table XX

Supplementary torsion angles (deg) for compound (VI)

with estimated standard deviations in parentheses

Atoms				Value
C(8a)	-C(1)	-C(2)	-C(21)	162.5(2)
O(1)	-C(1)	-C(2)	-C(21)	-12.5(3)
C(2)	-C(1)	-C(8a)	-C(8a1)	-77.2(2)
O(1)	-C(1)	-C(8a)	-C(8a1)	97.9(2)
C(1)	-C(2)	-C(3)	-C(31)	174.7(2)
C(21)	-C(2)	-C(3)	-C(31)	-4.2(4)
C(21)	-C(2)	-C(3)	-C(4)	177.7(2)
C(2)	-C(3)	-C(4)	-C(41)	-134.3(2)
C(31)	-C(3)	-C(4)	-C(41)	47.5(3)
C(31)	-C(3)	-C(4)	-C(4a)	172.1(2)
C(31)	-C(3)	-C(4)	-O(4)	-67.6(3)
C(3)	-C(4)	-C(4a)	-C(4a1)	163.6(2)
C(41)	-C(4)	-C(4a)	-C(4a1)	-72.9(2)
C(41)	-C(4)	-C(4a)	-C(5)	46.2(2)
C(41)	-C(4)	-C(4a)	-C(8a)	164.4(2)
O(4)	-C(4)	-C(4a)	-C(4a1)	47.7(2)
C(4a1)	-C(4a)	-C(5)	-C(6)	-75.9(2)
C(4)	-C(4a)	-C(8a)	-C(8a1)	59.9(2)
C(4a1)	-C(4a)	-C(8a)	-C(1)	-180.0(2)
C(4a1)	-C(4a)	-C(8a)	-C(8)	59.9(2)
C(4a1)	-C(4a)	-C(8a)	-C(8a1)	-62.7(2)
C(5)	-C(4a)	-C(8a)	-C(8a1)	179.5(2)
C(4a)	-C(5)	-C(6)	-C(61)	166.4(2)
C(5)	-C(6)	-C(7)	-C(71)	178.5(2)
C(61)	-C(6)	-C(7)	-C(71)	-1.8(4)
C(61)	-C(6)	-C(7)	-C(8)	178.1(2)
C(71)	-C(7)	-C(8)	-C(8a)	164.4(2)
C(7)	-C(8)	-C(8a)	-C(8a1)	173.0(2)
C(1)	-C(2)	-C(21)	-H1(21)	-124(3)
C(1)	-C(2)	-C(21)	-H2(21)	130(3)
C(1)	-C(2)	-C(21)	-H3(21)	-9(4)
C(3)	-C(2)	-C(21)	-H1(21)	55(3)
C(3)	-C(2)	-C(21)	-H2(21)	-51(3)
C(3)	-C(2)	-C(21)	-H3(21)	170(4)
C(2)	-C(3)	-C(31)	-H1(31)	-159(2)
C(2)	-C(3)	-C(31)	-H2(31)	91(3)
C(2)	-C(3)	-C(31)	-H3(31)	-38(2)
C(4)	-C(3)	-C(31)	-H1(31)	19(2)
C(4)	-C(3)	-C(31)	-H2(31)	-91(3)
C(4)	-C(3)	-C(31)	-H3(31)	140(2)
C(3)	-C(4)	-C(41)	-H1(41)	175.6(15)
C(3)	-C(4)	-C(41)	-H2(41)	-66(2)
C(3)	-C(4)	-C(41)	-H3(41)	53.0(15)

Table XX (continued)

C(4a)	-C(4)	-C(41)	-H1(41)	50.0(15)
C(4a)	-C(4)	-C(41)	-H2(41)	168(2)
C(4a)	-C(4)	-C(41)	-H3(41)	-72.6(15)
O(4)	-C(4)	-C(41)	-H1(41)	-72.3(15)
O(4)	-C(4)	-C(41)	-H2(41)	46(2)
O(4)	-C(4)	-C(41)	-H3(41)	165.0(15)
C(3)	-C(4)	-O(4)	-H1(O4)	151(2)
C(41)	-C(4)	-O(4)	-H1(O4)	35(2)
C(4a)	-C(4)	-O(4)	-H1(O4)	-87(2)
C(4)	-C(4a)	-C(4a1)	-H1(4a1)	48(2)
C(4)	-C(4a)	-C(4a1)	-H2(4a1)	174(2)
C(4)	-C(4a)	-C(4a1)	-H3(4a1)	-67(2)
C(5)	-C(4a)	-C(4a1)	-H1(4a1)	-72(2)
C(5)	-C(4a)	-C(4a1)	-H2(4a1)	54(2)
C(5)	-C(4a)	-C(4a1)	-H3(4a1)	173(2)
C(8a)	-C(4a)	-C(4a1)	-H1(4a1)	171.2(15)
C(8a)	-C(4a)	-C(4a1)	-H2(4a1)	-62(2)
C(8a)	-C(4a)	-C(4a1)	-H3(4a1)	56(2)
C(4)	-C(4a)	-C(5)	-H1(5)	39.7(12)
C(4)	-C(4a)	-C(5)	-H2(5)	-73.4(14)
C(4a1)	-C(4a)	-C(5)	-H1(5)	159.8(12)
C(4a1)	-C(4a)	-C(5)	-H2(5)	46.7(14)
C(8a)	-C(4a)	-C(5)	-H1(5)	-81.1(12)
C(8a)	-C(4a)	-C(5)	-H2(5)	165.8(14)
H1(5)	-C(5)	-C(6)	-C(61)	-69.1(12)
H1(5)	-C(5)	-C(6)	-C(7)	110.6(12)
H2(5)	-C(5)	-C(6)	-C(61)	43.3(14)
H2(5)	-C(5)	-C(6)	-C(7)	-137.0(14)
C(5)	-C(6)	-C(61)	-H1(61)	41(2)
C(5)	-C(6)	-C(61)	-H2(61)	155(3)
C(5)	-C(6)	-C(61)	-H3(61)	-83(3)
C(7)	-C(6)	-C(61)	-H1(61)	-138(2)
C(7)	-C(6)	-C(61)	-H2(61)	-24(3)
C(7)	-C(6)	-C(61)	-H3(61)	98(3)
C(6)	-C(7)	-C(71)	-H1(71)	122(3)
C(6)	-C(7)	-C(71)	-H2(71)	-139(3)
C(6)	-C(7)	-C(71)	-H3(71)	-6(3)
C(8)	-C(7)	-C(71)	-H1(71)	-58(3)
C(8)	-C(7)	-C(71)	-H2(71)	41(3)
C(8)	-C(7)	-C(71)	-H3(71)	174(3)
C(6)	-C(7)	-C(8)	-H1(8)	-135.1(15)
C(6)	-C(7)	-C(8)	-H2(8)	105.1(14)
C(71)	-C(7)	-C(8)	-H1(8)	44.8(15)
C(71)	-C(7)	-C(8)	-H2(8)	-75.0(14)
H1(8)	-C(8)	-C(8a)	-C(1)	49.4(15)
H1(8)	-C(8)	-C(8a)	-C(4a)	167.8(15)
H1(8)	-C(8)	-C(8a)	-C(8a1)	-65.6(15)
H2(8)	-C(8)	-C(8a)	-C(1)	162.8(14)
H2(8)	-C(8)	-C(8a)	-C(4a)	-78.8(14)
H2(8)	-C(8)	-C(8a)	-C(8a1)	47.8(14)
C(1)	-C(8a)	-C(8a1)	-H1(8a1)	57(2)

Table XX (continued)

C(1)	-C(8a)	-C(8a1)-H2(8a1)	-59(2)
C(1)	-C(8a)	-C(8a1)-H3(8a1)	179.6(15)
C(4a)	-C(8a)	-C(8a1)-H1(8a1)	-62(2)
C(4a)	-C(8a)	-C(8a1)-H2(8a1)	-177(2)
C(4a)	-C(8a)	-C(8a1)-H3(8a1)	61(2)
C(8)	-C(8a)	-C(8a1)-H1(8a1)	175(2)
C(8)	-C(8a)	-C(8a1)-H2(8a1)	59(2)
C(8)	-C(8a)	-C(8a1)-H3(8a1)	-62(2)

CHAPTER IV

6,7-DIMETHYL-4aβ,5,8,8aβ-TETRAHYDRONAPHTHOQUIN-1α,4α-DIOL

Introduction

The crystallographic studies presented thus far were, as previously described, embarked upon with the hope that the structural elucidation would promote an understanding of the photochemical reaction mechanism. While the present compound is similar to the naphthoquinols previously discussed, its crystal structure was studied for a different reason.

Obtaining single crystals for X-ray diffraction work has in many cases been the determining factor in whether or not the solid state structure is solved. This limitation has led to a project of investigating solid state structures by ^{13}C-NMR spectroscopy. McDowell, Naito, Scheffer and Wong (40), have illustrated some advantages of this technique over X-ray structure analysis in their work on conformational analysis of tetrahydronaphthoquinones.

The technique of high resolution solid state ^{13}C-NMR is not discussed here, but some of the results achieved by its use are mentioned. In brief, McDowell et al. have shown that for the tetrahydronaphthoquinones, where chemically equivalent carbons appear as singlets in solution, doublets appear in the solid state. This is attributed to the slight environmental differences experienced by the carbons in the solid state. It was proposed that this discriminating feature of the solid state could be exploited in identifying structurally independent molecules whose ^{13}C-NMR spectra should be readily discernible.

Although the characterization of the two structurally independent molecules of unsubstituted 4aβ,5,8,8aβ-tetrahydro-

1,4-naphthoquinone in the solid state was successful, such was not the case for the present compound. The multitude of peaks in the ^{13}C-NMR spectrum suggested more than one independent molecule in the structure but the evidence did not unambiguously indicate the exact number.

Single crystals of the title compound were obtainable and hence the desire to obtain a complete structural determination by X-ray diffraction techniques seemed compelling. The crystallographic analysis was therefore undertaken in an effort to establish i) the number of structurally independent molecules, ii) their individual conformations and if they differed from each other and iii) to verify the isomer (with respect to the OH positions) present. Of additional interest crystallographically was how the present, fully reduced structure compared with derivatives of 4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol.

Experimental

Colourless acicular crystals of the diol[1] (VIII) , were obtained from a hexanone/n-hexane solution by slow evaporation. Preliminary precession photographs revealed the systematic absences, $0\underline{k}0$, $\underline{k} = 2\underline{n} + 1$; $\underline{h}0\underline{l}$, $\underline{l} = 2\underline{n} + 1$, indicative of the space group $\underline{P}2_1/\underline{c}$.

Crystal data: $C_{12}H_{18}O_2$, MW = 194.28, monoclinic $\underline{a}$ = 13.870(2),

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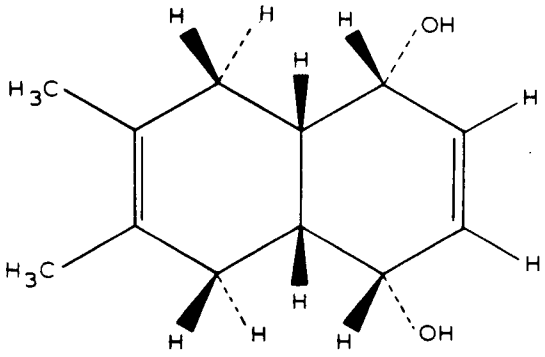
[1] IUPAC name: 1α,4α-dihydroxy-6,7-dimethyl-1,4,4aβ,5,8,8aβ-hexahydronaphthalene.

$\underline{b}$ = 18.025(4), $\underline{c}$ = 9.236(1) Å, β = 108.098(6)°, $\underline{V}$ = 2194.9(6) Å^3, $\underline{Z}$ = 8, $\underline{D}_c$ = 1.176 g cm^{-3}, $\underline{D}_o$ = 1.179 g cm^{-3}, μ(MoKα) = 0.436 cm^{-1}, λ = 0.71073 Å, space group $\underline{P2_1/c}$.



(VIII)

Data were collected with a crystal measuring 0.52 x 0.15 x 0.10 mm^3 between theta limits of 0.0 and 22.5° using an ω-2θ scan and graphite monochromatized MoKα radiation. The omega scan angle, (0.65 + 0.35tanθ)°, was extended by 25% on each side of the peak for background measurement. The vertical aperture remained constant at 4 mm whereas the horizontal aperture was varied according to the expression (2.00 + tanθ) mm. Three reflections were designated as intensity controls and were measured every 3600 seconds of X-ray exposure time. Orientation check reflections were permitted a deviation of up to 0.055° between observed and calculated scattering vectors before reorientation was effected.

Lorentz and polarization corrections were applied to the 2845 reflections collected. Further processing showed 51.4% (1461) of the data were classified as observed having $I \geq 3\sigma(I)$, where $\sigma^2(I) = S + 2B + (0.04(S - B))^2$, S = scan count and B =

the time-averaged background. The decay in the intensities of the three control reflections was negligible over the period of data collection.

Solution and Refinement

The E-statistics, calculated for all the data, closely paralleled the theoretical centric distribution. The N(z) test firmly supported the centric distribution, and so, there existed little doubt concerning the space group assignment of $\underline{P}2_1/\underline{c}$. In the initial stages of MULTAN, 4709 Σ_2-relationships were generated from 312 reflections having $|E| \geq 1.588$. The results of the Σ_1-formula indicated the phases of four reflections, with each indication having a probability greater than the acceptance value of 0.95 and having more than 15 contributors. The phases associated with the three origin defining reflections, chosen in accordance with space group symmetry, the four known phases, from the Σ_1 results and five other phases associated with reflections common to many relationships in the Σ_2-listing made up the starting set. This set of phases was the only one developed and gave excellent figures of merit. Using E's as the coefficients in the three-dimensional Fourier synthesis, an interpretable electron density map was calculated from which the fractional coordinates for all non-hydrogen atoms were obtained. The peaks on the E-map, when joined in a chemically sensible manner, corresponded to two crystallographically independent molecules thereby substantiating the implication from density measurements of there being eight molecules in the unit cell.

In the initial stages of refinement, only non-hydrogens were included and were assigned isotropic thermal parameters. Later, anisotropic temperature factors were incorporated into the refinement of the carbons and oxygens, after which a difference-Fourier synthesis revealed the positions of the 36 hydrogen atoms. Two additional peaks, equivalent in magnitude to the peaks assigned H(O1) and H(O1'), appeared on the electron density map. One peak was positioned approximately 1 Å from O(1) and subtended an angle of roughly 112° with C(1), O(1) being the vertex; the other peak was positioned similarly with respect to O(1'). These positions were given occupancy factors of 0.5 and refined as hydrogens. The initially assigned H(O1) and H(O1') positions also assumed 0.5 occupancies during the refinement. Thermal vibrations of hydrogens were considered to be isotropic and refined accordingly. The final cycle of refinement varied 405 parameters which showed mean and maximum shifts of 0.114 and 1.107σ, respectively. An error of 1.619 was calculated for an observation of unit weight. Final R-values were R = 0.032 and Rw = 0.035 for the 1461 observed data, while R = 0.104 and Rw = 0.035 for the entire data set consisting of 2845 reflections. A difference synthesis following convergence indicated random fluctuations in the electron density with the largest peak corresponding to 0.124 e/Å^3. The absolute weights, $w = 1/\sigma^2(F)$, where $\sigma^2(F)$ is obtained from the previously defined $\sigma^2(I)$, were employed in the refinement. A list of atomic coordinates and temperature factors is presented in Table XXI; anisotropic thermal parameters for non-hydrogen atoms are contained in Table XXII.

Table XXI

Final positional (fractional x 10^4, H x 10^3)

and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)

with estimated standard deviations in parentheses

Atom[2]	x	y	z	Ueq/Uiso
C(1)	2331(3)	1126(2)	3501(3)	49
C(2)	1501(3)	952(2)	2067(4)	55
C(3)	647(3)	1320(2)	1581(4)	49
C(4)	407(2)	1964(2)	2409(3)	41
C(4a)	972(2)	1922(2)	4103(3)	35
C(5)	585(3)	1330(2)	4946(3)	43
C(6)	1287(3)	1165(2)	6529(3)	46
C(61)	789(5)	715(3)	7482(5)	74
C(7)	2242(3)	1393(2)	7001(3)	48
C(71)	2973(4)	1236(3)	8559(5)	78
C(8)	2706(3)	1837(2)	6001(4)	53
C(8a)	2099(2)	1816(2)	4315(3)	41
O(1)	2539(3)	489(1)	4464(3)	70
O(4)	-676(2)	1997(1)	2042(2)	51
C(1')	-4175(2)	801(2)	-2861(3)	42
C(2')	-3370(3)	668(2)	-1378(4)	51
C(3')	-2615(3)	1128(2)	-783(4)	49
C(4')	-2493(2)	1851(2)	-1491(3)	39
C(4a')	-3013(2)	1848(2)	-3194(3)	35
C(5')	-2470(2)	1398(2)	-4087(3)	38
C(6')	-3095(2)	1254(2)	-5716(3)	42
C(61')	-2490(4)	954(3)	-6685(5)	63
C(7')	-4084(3)	1376(2)	-6224(3)	45
C(71')	-4730(4)	1264(3)	-7862(5)	78
C(8')	-4673(3)	1637(2)	-5200(4)	51
C(8a')	-4107(2)	1574(2)	-3508(3)	40
O(1')	-4148(3)	199(1)	-3851(3)	49
O(4')	-1440(2)	2046(1)	-1162(3)	51
H(1)	299(2)	122(1)	326(3)	49(8)
H(2)	160(2)	53(2)	154(4)	67(10)
H(3)	12(2)	121(2)	68(3)	56(9)
H(4)	62(2)	242(1)	209(3)	35(8)
H(4a)	91(2)	239(1)	454(3)	32(7)
H1(5)	-9(2)	145(2)	503(3)	63(10)
H2(5)	44(2)	85(1)	438(3)	36(7)
H1(61)	27(4)	98(3)	770(6)	167(24)

[2] Unprimed atoms correspond to molecule A; primed (') atoms correspond to molecule B.

Table XXI (continued)

H1(61)	27(4)	98(3)	770(6)	167(24)
H2(61)	133(4)	61(2)	834(6)	135(21)
H3(61)	52(4)	26(3)	702(6)	151(23)
H1(71)	337(3)	84(2)	850(4)	95(15)
H2(71)	271(3)	115(2)	937(4)	87(14)
H3(71)	343(3)	169(3)	889(5)	127(19)
H1(8)	278(2)	235(2)	634(3)	72(11)
H2(8)	337(2)	165(2)	611(3)	73(11)
H(8a)	230(2)	220(1)	381(3)	38(8)
H(O1)[3]	306(6)	17(4)	443(6)	70(18)
H(O1)*[4]	247(9)	49(6)	501(13)	163(61)
H(O4)	-85(2)	235(2)	260(4)	76(12)
H(1')	-484(2)	74(1)	-275(3)	38(8)
H(2')	-342(2)	19(2)	-90(3)	69(11)
H(3')	-208(3)	99(2)	12(4)	73(11)
H(4')	-283(2)	226(1)	-110(3)	44(8)
H(4a')	-306(2)	238(1)	-356(3)	32(7)
H1(5')	-189(2)	165(2)	-412(3)	49(9)
H2(5')	-222(2)	90(1)	-360(3)	26(7)
H1(61')	-286(3)	68(2)	-750(4)	96(14)
H2(61')	-200(3)	60(2)	-609(5)	112(18)
H3(61')	-212(3)	130(2)	-695(5)	118(17)
H1(71')	-437(3)	119(2)	-855(5)	117(18)
H2(71')	-514(4)	162(3)	-823(6)	145(27)
H3(71')	-520(4)	85(3)	-794(5)	146(19)
H1(8')	-493(2)	217(2)	-546(3)	59(9)
H2(8')	-532(3)	133(2)	-547(3)	73(10)
H(8a')	-443(2)	193(2)	-292(3)	56(8)
H(O1')	-374(8)	13(6)	-400(12)	50(53)
H(O1')*	-464(8)	7(7)	-464(14)	140(53)
H(O4')	-115(3)	203(2)	-10(5)	107(15)

[3] Hydrogens bonded to O(1) and O(1') are in positions of 50% occupancy.

[4] Asterisks (*) denote additional hydrogen positions arising from the disorder.

Table XXII

Final anisotropic thermal parameters ($\underline{U}ij \times 10^3$ Å^2)

and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
C(1)	46(2)	59(2)	46(2)	16(2)	21(2)	12(2)
C(2)	65(3)	61(2)	44(2)	11(2)	24(2)	-7(2)
C(3)	49(2)	67(2)	30(2)	7(2)	12(2)	-6(2)
C(4)	41(2)	47(2)	34(2)	6(2)	12(1)	4(2)
C(4a)	37(2)	35(2)	31(2)	3(1)	9(1)	0(1)
C(5)	44(2)	52(2)	37(2)	-2(2)	17(2)	-2(2)
C(6)	64(3)	48(2)	29(2)	10(2)	19(2)	1(2)
C(61)	101(4)	83(3)	50(3)	-5(3)	39(3)	15(2)
C(7)	54(2)	51(2)	35(2)	14(2)	6(2)	2(2)
C(71)	91(4)	83(4)	46(3)	33(3)	2(3)	7(2)
C(8)	41(2)	67(3)	42(2)	3(2)	0(2)	-6(2)
C(8a)	40(2)	45(2)	41(2)	0(2)	14(2)	5(2)
O(1)	95(2)	63(2)	57(2)	39(2)	30(2)	15(1)
O(4)	41(1)	74(2)	34(1)	13(1)	5(1)	-6(1)
C(1')	36(2)	46(2)	48(2)	-6(2)	20(2)	-7(2)
C(2')	62(2)	52(2)	38(2)	-10(2)	17(2)	8(2)
C(3')	53(2)	61(2)	31(2)	-6(2)	12(2)	2(2)
C(4')	38(2)	48(2)	30(2)	-7(2)	9(1)	-7(2)
C(4a')	38(2)	32(2)	34(2)	-1(1)	9(1)	-1(1)
C(5')	37(2)	46(2)	32(2)	-6(2)	10(2)	-3(2)
C(6')	53(2)	45(2)	30(2)	-11(2)	15(2)	-2(1)
C(61')	78(3)	80(3)	40(2)	-22(3)	32(2)	-16(2)
C(7')	52(2)	48(2)	29(2)	-14(2)	2(2)	3(1)
C(71')	84(3)	95(4)	38(3)	-32(3)	-5(3)	3(2)
C(8')	39(2)	50(2)	52(2)	1(2)	-2(2)	2(2)
C(8a')	34(2)	45(2)	39(2)	5(2)	8(2)	-5(2)
O(1')	53(2)	44(2)	51(2)	-4(1)	16(2)	-8(1)
O(4')	45(1)	70(2)	31(1)	-14(1)	5(1)	-1(1)

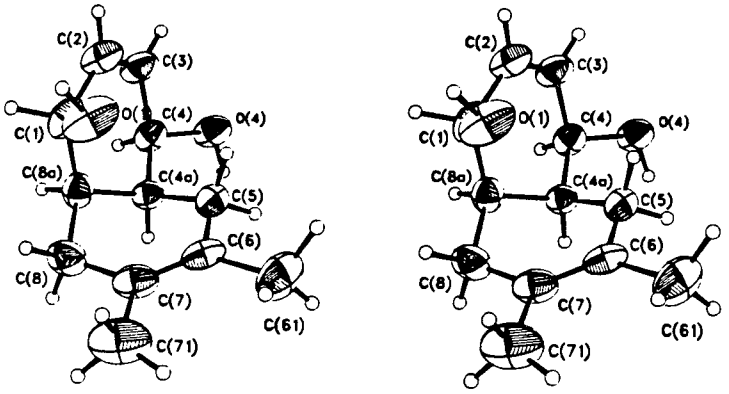


Figure 14

Stereo diagram of a type A molecule of the diol (VIII)

Discussion

The structure consists of two crystallographically independent molecules, A (Fig. 14) and B, per asymmetric unit hydrogen bonded to each other through O(4')-H...O(4) interactions. The molecules are related by a pseudo two-fold rotation axis approximately parallel to b and passing through the mid-point of O(4) and O(4'). Additional hydrogen bonds, linking neighboring asymmetric units, result in a three-dimensional bonding network (Fig. 15) thus increasing the packing energy and rigidity of the structure. Each asymmetric

unit experiences six H-bonds.

The refinement of four hydrogens (around O(1) and O(1')), each with occupancies of 0.5, may be construed as the refinement of the oxygen lone pairs which would explain the short O(1)-H(O1)* and O(1')-H(O1') bonds of 0.54(11) and 0.63(11) Å, respectively (bond lengths and angles are given in Tables XXIII-XXVI). However, it is chemically and structurally reasonable to assume that hydrogen atoms do lie in the vicinity

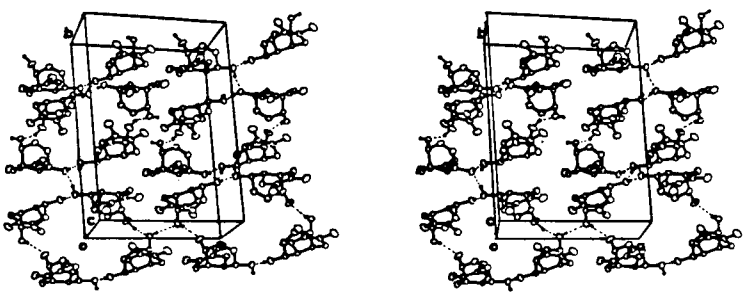


Figure 15

Stereo packing diagram of the diol (VIII)

of the refined centroids of electron density and on the lines through the oxygens and these adjacent centroids. Alternative interpretations of the geometrical arrangements of hydrogens around oxygens O(1) and O(1') invoke what would appear to be physically unrealistic conditions and can result in decreases in the extent of hydrogen bonding. Consider the following situations: i) hydrogens H(O1) and H(O1')* assume full occupancy, ii) hydrogens H(O1) and H(O1') assume full occupancy, iii) hydrogens H(O1)* and H(O1') assume full occupancy and iv) H(O1)* and H(O1')* assume full occupancy. In case (i) the space group symmetry results in a H(O1')*(x,y,z)...H(O1')*(-x-1,-y,-z-1) contact distance of 1.1 Å despite otherwise favorable hydrogen bonding geometry between O(1')(x,y,z) and O(1')(-x-1,-y,-z-1). From the O(1)(x,y,z)-H(O1)...O(1')(-x,-y,-z) angle of 159(12)° and H(O1)...O(1') distance of 1.87(9) Å hydrogen bonding between O(1)(x,y,z) and O(1')(-x,-y,-z) may be inferred; however, if indeed the H(O1') position was occupied by a lone pair of electrons then this bonding may not be inferred, for the O(1)(x,y,z)-H(O1) and O(1')(-x,-y,-z)-(lone pair) vectors are parallel and separated by approximately 1 Å. If instead of H(O1), the H(O1)* position was fully occupied, as in case (iv), the same H(O1')*...H(O1')* contact of 1.1 Å would occur and furthermore, no hydrogen bonding could take place between O(1) and O(1').

Case (ii) invokes similarly drastic conditions with H(O1)(x,y,z) being only 1.1 Å from H(O1')(-x,-y,-z), accompanied by a loss of a hydrogen bond between the symmetry related O(1') atoms at (x,y,z) and (-x-1,-y-1,-z-1). Assigning unit

Table XXIII

Bond lengths (Å) with estimated standard deviations in parentheses

Bond		Length	Bond		Length
C(1)	-C(2)	1.493(4)	C(1')	-C(2')	1.493(4)
C(1)	-C(8a)	1.539(4)	C(1')	-C(8a')	1.529(4)
C(1)	-O(1)	1.426(4)	C(1')	-O(1')	1.428(4)
C(2)	-C(3)	1.309(4)	C(2')	-C(3')	1.316(4)
C(3)	-C(4)	1.485(4)	C(3')	-C(4')	1.491(4)
C(4)	-C(4a)	1.519(4)	C(4')	-C(4a')	1.513(4)
C(4)	-O(4)	1.435(3)	C(4')	-O(4')	1.439(3)
C(4a)	-C(5)	1.514(4)	C(4a')	-C(5')	1.515(4)
C(4a)	-C(8a)	1.525(4)	C(4a')	-C(8a')	1.536(4)
C(5)	-C(6)	1.513(4)	C(5')	-C(6')	1.507(4)
C(6)	-C(61)	1.513(5)	C(6')	-C(61')	1.504(4)
C(6)	-C(7)	1.324(4)	C(6')	-C(7')	1.323(4)
C(7)	-C(71)	1.508(5)	C(7')	-C(71')	1.513(5)
C(7)	-C(8)	1.508(4)	C(7')	-C(8')	1.504(4)
C(8)	-C(8a)	1.523(4)	C(8')	-C(8a')	1.520(4)

Table XXIV

Bond angles (deg) with estimated standard deviations in parentheses

Bonds			Angle	Bonds			Angle
C(2)	-C(1)	-C(8a)	112.4(3)	C(2')	-C(1')	-C(8a)	112.7(3)
C(2)	-C(1)	-O(1)	109.6(3)	C(2')	-C(1')	-O(1')	107.7(3)
C(8a)	-C(1)	-O(1)	112.3(3)	C(8a')	-C(1')	-O(1')	115.1(2)
C(1)	-C(2)	-C(3)	124.3(4)	C(1')	-C(2')	-C(3')	123.6(3)
C(2)	-C(3)	-C(4)	122.9(3)	C(2')	-C(3')	-C(4')	123.5(3)
C(3)	-C(4)	-C(4a)	111.4(3)	C(3')	-C(4')	-C(4a)	111.8(3)
C(3)	-C(4)	-O(4)	107.3(3)	C(3')	-C(4')	-O(4')	111.5(3)
C(4a)	-C(4)	-O(4)	114.4(2)	C(4a')	-C(4')	-O(4')	110.2(2)
C(4)	-C(4a)	-C(5)	114.4(3)	C(4')	-C(4a')	-C(5')	114.2(3)
C(4)	-C(4a)	-C(8a)	108.6(2)	C(4')	-C(4a')	-C(8a)	108.8(2)
C(5)	-C(4a)	-C(8a)	111.0(2)	C(5')	-C(4a')	-C(8a)	110.7(2)
C(4a)	-C(5)	-C(6)	114.2(3)	C(4a')	-C(5')	-C(6')	114.0(3)
C(5)	-C(6)	-C(61)	113.2(4)	C(5')	-C(6')	-C(61')	113.7(3)
C(5)	-C(6)	-C(7)	122.4(3)	C(5')	-C(6')	-C(7')	122.5(3)
C(61)	-C(6)	-C(7)	124.5(4)	C(61')	-C(6')	-C(7')	123.8(3)
C(6)	-C(7)	-C(71)	124.3(4)	C(6')	-C(7')	-C(71')	124.0(4)
C(6)	-C(7)	-C(8)	122.4(3)	C(6')	-C(7')	-C(8')	122.3(3)
C(71)	-C(7)	-C(8)	113.3(4)	C(71')	-C(7')	-C(8')	113.6(4)
C(7)	-C(8)	-C(8a)	114.0(3)	C(7')	-C(8')	-C(8a')	114.5(3)
C(1)	-C(8a)	-C(4a)	113.6(3)	C(1')	-C(8a')	-C(4a')	113.4(2)
C(1)	-C(8a)	-C(8)	112.7(3)	C(1')	-C(8a')	-C(8')	113.3(3)
C(4a)	-C(8a)	-C(8)	110.3(3)	C(4a')	-C(8a')	-C(8')	109.5(3)

Table XXV

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

Bond		Length	Bond		Length
C(1)	-H(1)	1.02(3)	C(1')	-H(1')	0.96(3)
C(2)	-H(2)	0.93(3)	C(2')	-H(2')	0.97(3)
C(3)	-H(3)	0.94(3)	C(3')	-H(3')	0.96(3)
C(4)	-H(4)	0.96(2)	C(4')	-H(4')	1.01(3)
C(4a)	-H(4a)	0.96(2)	C(4a')	-H(4a')	1.00(2)
C(5)	-H1(5)	0.99(3)	C(5')	-H1(5')	0.92(3)
C(5)	-H2(5)	1.00(3)	C(5')	-H2(5')	1.02(2)
C(61)	-H1(61)	0.93(6)	C(61')	-H1(61')	0.91(4)
C(61)	-H2(61)	0.92(5)	C(61')	-H2(61')	0.96(4)
C(61)	-H3(61)	0.95(5)	C(61')	-H3(61')	0.90(4)
C(71)	-H1(71)	0.91(4)	C(71')	-H1(71')	0.93(4)
C(71)	-H2(71)	0.94(4)	C(71')	-H2(71')	0.85(5)
C(71)	-H3(71)	1.02(4)	C(71')	-H3(71')	0.98(5)
C(8)	-H1(8)	0.97(3)	C(8')	-H1(8')	1.03(3)
C(8)	-H2(8)	0.96(3)	C(8')	-H2(8')	1.02(3)
C(8a)	-H(8a)	0.93(3)	C(8a')	-H(8a')	1.03(3)
O(1)	-H(O1)	0.93(9)	O(1')	-H(O1')	0.63(11)
O(1)	-H(O1)*	0.54(11)	O(1')	-H(O1')*	0.86(10)
O(4)	-H(O4)	0.90(3)	O(4')	-H(O4')	0.94(4)

Table XXVI

Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses

Bonds			Angle	Bonds			Angle
C(2)	-C(1)	-H(1)	109.6(14)	C(2')	-C(1')	-H(1')	110.3(15)
C(8a)	-C(1)	-H(1)	107.9(14)	C(8a')	-C(1')	-H(1')	109.3(14)
O(1)	-C(1)	-H(1)	104.7(14)	O(1')	-C(1')	-H(1')	101.2(15)
C(1)	-C(2)	-H(2)	116(2)	C(1')	-C(2')	-H(2')	115(2)
C(3)	-C(2)	-H(2)	120(2)	C(3')	-C(2')	-H(2')	122(2)
C(2)	-C(3)	-H(3)	124(2)	C(2')	-C(3')	-H(3')	120(2)
C(4)	-C(3)	-H(3)	113(2)	C(4')	-C(3')	-H(3')	116(2)
C(3)	-C(4)	-H(4)	112.5(14)	C(3')	-C(4')	-H(4')	110.9(14)
C(4a)	-C(4)	-H(4)	104.5(15)	C(4a')	-C(4')	-H(4')	104.6(14)
O(4)	-C(4)	-H(4)	106.8(14)	O(4')	-C(4')	-H(4')	107.6(14)
C(4)	-C(4a)	-H(4a)	107.6(14)	C(4')	-C(4a')	-H(4a')	107.9(13)
C(5)	-C(4a)	-H(4a)	108.3(14)	C(5')	-C(4a')	-H(4a')	108.6(13)
C(8a)	-C(4a)	-H(4a)	106.6(14)	C(8a')	-C(4a')	-H(4a')	106.3(13)
C(4a)	-C(5)	-H1(5)	112(2)	C(4a')	-C(5')	-H1(5')	110(2)
C(4a)	-C(5)	-H2(5)	112.6(14)	C(4a')	-C(5')	-H2(5')	112.8(12)
C(6)	-C(5)	-H1(5)	108(2)	C(6')	-C(5')	-H1(5')	107(2)
C(6)	-C(5)	-H2(5)	107.3(15)	C(6')	-C(5')	-H2(5')	107.6(13)
H1(5)	-C(5)	-H2(5)	102(2)	H1(5')	-C(5')	-H2(5')	106(2)
C(6)	-C(61)	-H1(6)	112(3)	C(6')	-C(61')	-H1(6')	114(2)
C(6)	-C(61)	-H2(6)	102(3)	C(6')	-C(61')	-H2(6')	109(2)
C(6)	-C(61)	-H3(6)	113(3)	C(6')	-C(61')	-H3(6')	113(3)
H1(61)	-C(61)	-H2(6)	113(4)	H1(61')	-C(61')	-H2(6')	103(3)
H1(61)	-C(61)	-H3(6)	108(4)	H1(61')	-C(61')	-H3(6')	112(3)
H2(61)	-C(61)	-H3(6)	108(4)	H2(61')	-C(61')	-H3(6')	105(4)
C(7)	-C(71)	-H1(7)	109(2)	C(7')	-C(71')	-H1(7')	115(3)
C(7)	-C(71)	-H2(7)	119(2)	C(7')	-C(71')	-H2(7')	114(4)
C(7)	-C(71)	-H3(7)	108(2)	C(7')	-C(71')	-H3(7')	110(3)
H1(71)	-C(71)	-H2(7)	108(3)	H1(71')	-C(71')	-H2(7')	106(4)
H1(71)	-C(71)	-H3(7)	109(4)	H1(71')	-C(71')	-H3(7')	108(4)
H2(71)	-C(71)	-H3(7)	105(3)	H2(71')	-C(71')	-H3(7')	101(4)
C(7)	-C(8)	-H1(8)	109(2)	C(7')	-C(8')	-H1(8')	111.6(15)
C(7)	-C(8)	-H2(8)	110(2)	C(7')	-C(8')	-H2(8')	107(2)
C(8a)	-C(8)	-H1(8)	109(2)	C(8a')	-C(8')	-H1(8')	109.9(15)
C(8a)	-C(8)	-H2(8)	108(2)	C(8a')	-C(8')	-H2(8')	110(2)
H1(8)	-C(8)	-H2(8)	107(3)	H1(8')	-C(8')	-H2(8')	103(2)
C(1)	-C(8a)	-H(8a)	102.6(15)	C(1')	-C(8a')	-H(8a')	105.9(15)
C(4a)	-C(8a)	-H(8a)	107.3(15)	C(4a')	-C(8a')	-H(8a')	105.1(15)
C(8)	-C(8a)	-H(8a)	109.8(15)	C(8')	-C(8a')	-H(8a')	109(2)
C(1)	-O(1)	-H(O1)	119(3)	C(1')	-O(1')	-H(O1')	119(3)
C(1)	-O(1)	-H(O1)	*120(12)	C(1')	-O(1')	-H(O1')	*126(9)
H(O1)	-O(1)	-H(O1)	*113(13)	H(O1')	-O(1')	-H(O1')	*107(11)
C(4)	-O(4)	-H(O4)	110(2)	C(4')	-O(4')	-H(O4')	106(2)

occupancies to H(O1) and H(O1') is to construe H(O1')* as a refined lone pair and this implication leads to a close O1'(lone pair)(x,y,z)...O1'(lone pair)(-x-1,-y,-z-1) contact of 1.1 Å – an unstable configuration.

The third case does not entail close atomic contacts, however, the number of hydrogen bonds is reduced as in (ii).

The most favorable interpretation, alluded to earlier, takes into consideration a disordered arrangement of the hydrogens on O(1) and O(1'), namely fractional occupancy for each of the four hydrogens, effecting linkage of the asymmetric units via bonding between O(1) and O(1') by O(1)(x,y,z)-H(O1)...O(1')(-x,-y,-z)-H(O1')*...O(1')(1+x,y,1+z)-H(O1')...O(1)(1-x,-y,1-z)-H(O1)*. Three important aspects concerning this arrangement are firstly, that the occupancy of each hydroxyl hydrogen is restricted to exactly 50% – the reader may convince himself that any other degree of occupancy would result in physically unrealistic H...H contacts (vide supra) – secondly, that such an arrangement provides a link between asymmetric units along the a-direction[5] and lastly, that the chain length involving this sequence of bonds (i.e. O(1)...O(1') type) is four molecules beginning with and then terminating at an O(1) atom. However, the chains formed by a combination of O(1)...O(1') and O(4)...O(4') links are infinite in length (Fig. 15 and Table XXVII).

The conformation adopted by each molecule consists of a

[5] This linkage is also accomplished in case (i) at the expense of close H...H contacts; cases (ii) and (iii) do not afford any link along a.

half-chair cyclohexene ring cis-fused to a half-chair cyclohexen-diol moiety. Although the gross molecular conformations are the same for both molecules in the asymmetric unit, detailed differences are noticeable. Deviations of up to 4.2° are observed in corresponding (heavy atom) angles involving

Table XXVII

Hydrogen bonding geometries

Distances are in Angstroms and angles in degrees.

	O-H	H...O	O-H...O
O(4')(x,y,z)-H...O(4)(x,y,z)	0.94(4)	1.88(4)	176(3)
O(4)(x,y,z)-H...O(4')(x,1/2-y,1/2+z)	0.90(3)	1.93(3)	169(3)
O(1)(x,y,z)-H...O(1')(-x,-y,-z)	0.93(9)	1.87(9)	158(5)
O(1')(x,y,z)-H...O(1)(-x,-y,-z)	0.63(11)	2.16(12)	159(12)
O(1')(x,y,z)-H*...O(1')(-x-1,-y,-z-1)	0.86(10)	1.89(10)	170(12)

oxygens in A and B, and may be attributed to the effects of hydrogen bonding. Bond lengths and other bond angles do not differ significantly between molecules. Examination of the torsion angles (Table XXVIII) indicates further minor conformational differences.

The OH configurations in each molecule are both anti with respect to the bridgehead hydrogens. This confirms the expected major isomer formed by the reduction of the 1,4-dione by $NaBH_4$, the method by which the present compound was prepared.

Despite the favorable geometry for a hydrogen abstraction reaction involving the upper hydrogen on C(5) (Fig. 14), and the C(3) atom, such a reaction does not proceed photochemically (at ≥350 nm) due to the lack of a suitable chromophore. Bonds joining atoms C(1), C(2), C(3), C(4), C(4a) and C(5), and similarly C(1'), C(2'), C(3'), C(4'), C(4a') and C(5') are all shorter than accepted values. This may be due to slight hybridization deviations from the formal sp^3 and sp^2 states. The larger than normal endocyclic bond angles at these centers are consistent with this rationale.

Comparison with Tetrahydronaphthoquin-4α-ols

The present molecular conformations are similar to the least energy conformations predicted by Bucourt and Hainaut (38) and found in previously studied naphthoquinols (Chapters I-III and reference 32). Many of the structural trends noted in these past studies are also observed in the current diol compound. Not unlike the other naphthoquinols, the cis-fused rings in the diol molecules, so joined, form three approximate planes – two planes defined by each of the double bonds (C(1), C(2), C(3), C(4) and C(5), C(6), C(7), C(8)) are almost perpendicular to each other (with a dihedral angle of 96°) and each of these planes subtends an angle of approximately 141° with respect to the third plane containing atoms C(4)-C(4a)-C(8a)-C(8) (and similarly C(4')-C(4a')-C(8a')-C(8') in the other molecule).

Since the molecules in the asymmetric unit are very similar, structural features and values for B molecules will be

Table XXVIII

Torsion angles (deg) with estimated standard deviations in parentheses

Atoms				Value
C(8a)	-C(1)	-C(2)	-C(3)	-3.1(4)
O(1)	-C(1)	-C(2)	-C(3)	122.5(4)
C(2)	-C(1)	-C(8a)	-C(4a)	32.1(4)
C(2)	-C(1)	-C(8a)	-C(8)	158.5(3)
O(1)	-C(1)	-C(8a)	-C(4a)	-92.0(3)
O(1)	-C(1)	-C(8a)	-C(8)	34.4(4)
C(1)	-C(2)	-C(3)	-C(4)	0.4(5)
C(2)	-C(3)	-C(4)	-C(4a)	-26.5(4)
C(2)	-C(3)	-C(4)	-O(4)	-152.4(3)
C(3)	-C(4)	-C(4a)	-C(5)	-71.8(4)
C(3)	-C(4)	-C(4a)	-C(8a)	52.8(4)
O(4)	-C(4)	-C(4a)	-C(5)	50.0(4)
O(4)	-C(4)	-C(4a)	-C(8a)	174.7(3)
C(4)	-C(4a)	-C(5)	-C(6)	166.4(3)
C(8a)	-C(4a)	-C(5)	-C(6)	43.0(4)
C(4)	-C(4a)	-C(8a)	-C(1)	-57.2(3)
C(4)	-C(4a)	-C(8a)	-C(8)	175.1(3)
C(5)	-C(4a)	-C(8a)	-C(1)	69.4(3)
C(5)	-C(4a)	-C(8a)	-C(8)	-58.2(4)
C(4a)	-C(5)	-C(6)	-C(61)	166.4(3)
C(4a)	-C(5)	-C(6)	-C(7)	-14.2(4)
C(5)	-C(6)	-C(7)	-C(71)	-179.3(3)
C(5)	-C(6)	-C(7)	-C(8)	0.2(5)
C(61)	-C(6)	-C(7)	-C(71)	0.0(5)
C(61)	-C(6)	-C(7)	-C(8)	179.5(4)
C(6)	-C(7)	-C(8)	-C(8a)	-16.0(5)
C(71)	-C(7)	-C(8)	-C(8a)	163.5(3)
C(7)	-C(8)	-C(8a)	-C(1)	-83.7(4)
C(7)	-C(8)	-C(8a)	-C(4a)	44.5(4)
C(8a')	-C(1')	-C(2')	-C(3')	-7.6(4)
O(1')	-C(1')	-C(2')	-C(3')	120.5(4)
C(2')	-C(1')	-C(8a')	-C(4a')	35.7(3)
C(2')	-C(1')	-C(8a')	-C(8')	161.3(3)
O(1')	-C(1')	-C(8a')	-C(4a')	-88.3(4)
O(1')	-C(1')	-C(8a')	-C(8')	37.3(4)
C(1')	-C(2')	-C(3')	-C(4')	2.3(5)
C(2')	-C(3')	-C(4')	-C(4a')	-25.0(4)
C(2')	-C(3')	-C(4')	-O(4')	-148.8(3)
C(3')	-C(4')	-C(4a')	-C(5')	-73.7(3)
C(3')	-C(4')	-C(4a')	-C(8a')	50.6(3)
O(4')	-C(4')	-C(4a')	-C(5')	50.9(3)
O(4')	-C(4')	-C(4a')	-C(8a')	175.1(2)
C(4')	-C(4a')	-C(5')	-C(6')	167.1(3)
C(8a')	-C(4a')	-C(5')	-C(6')	43.9(3)
C(4')	-C(4a')	-C(8a')	-C(1')	-57.8(3)
C(4')	-C(4a')	-C(8a')	-C(8')	174.6(3)

Table XXVIII (continued)

C(5')	-C(4a')	-C(8a')	-C(1')	68.5(3)
C(5')	-C(4a')	-C(8a')	-C(8')	-59.1(3)
C(4a')	-C(5')	-C(6')	-C(61')	167.6(3)
C(4a')	-C(5')	-C(6')	-C(7')	-13.2(4)
C(5')	-C(6')	-C(7')	-C(71')	177.7(4)
C(5')	-C(6')	-C(7')	-C(8')	-2.6(5)
C(61')	-C(6')	-C(7')	-C(71')	-3.1(5)
C(61')	-C(6')	-C(7')	-C(8')	176.5(3)
C(6')	-C(7')	-C(8')	-C(8a')	-13.9(5)
C(71')	-C(7')	-C(8')	-C(8a')	165.8(3)
C(7')	-C(8')	-C(8a')	-C(1')	-83.7(4)
C(7')	-C(8')	-C(8a')	-C(4a')	44.0(4)
C(8a)	-C(1)	-C(2)	-H(2)	-179(2)
O(1)	-C(1)	-C(2)	-H(2)	-53(2)
H(1)	-C(1)	-C(2)	-C(3)	-123.0(15)
H(1)	-C(1)	-C(2)	-H(2)	61(3)
C(2)	-C(1)	-C(8a)	-H(8a)	-83(2)
O(1)	-C(1)	-C(8a)	-H(8a)	152.5(15)
H(1)	-C(1)	-C(8a)	-C(4a)	153.2(15)
H(1)	-C(1)	-C(8a)	-C(8)	-80(2)
H(1)	-C(1)	-C(8a)	-H(8a)	38(2)
C(2)	-C(1)	-O(1)	-H(O1)	94(4)
C(2)	-C(1)	-O(1)	-H(O1)*	-115(15)
C(8a)	-C(1)	-O(1)	-H(O1)	-140(4)
C(8a)	-C(1)	-O(1)	-H(O1)*	10(15)
H(1)	-C(1)	-O(1)	-H(O1)	-23(4)
H(1)	-C(1)	-O(1)	-H(O1)*	127(15)
C(1)	-C(2)	-C(3)	-H(3)	-179(2)
H(2)	-C(2)	-C(3)	-C(4)	176(2)
H(2)	-C(2)	-C(3)	-H(3)	-3(3)
C(2)	-C(3)	-C(4)	-H(4)	91(2)
H(3)	-C(3)	-C(4)	-C(4a)	153(2)
H(3)	-C(3)	-C(4)	-O(4)	27(2)
H(3)	-C(3)	-C(4)	-H(4)	-90(2)
C(3)	-C(4)	-C(4a)	-H(4a)	167.9(15)
O(4)	-C(4)	-C(4a)	-H(4a)	-70.3(15)
H(4)	-C(4)	-C(4a)	-C(5)	166.4(14)
H(4)	-C(4)	-C(4a)	-C(8a)	-68.9(15)
H(4)	-C(4)	-C(4a)	-H(4a)	46(2)
C(3)	-C(4)	-O(4)	-H(O4)	173(2)
C(4a)	-C(4)	-O(4)	-H(O4)	49(2)
H(4)	-C(4)	-O(4)	-H(O4)	-66(3)
C(4)	-C(4a)	-C(5)	-H1(5)	-70(2)
C(4)	-C(4a)	-C(5)	-H2(5)	44(2)
C(8a)	-C(4a)	-C(5)	-H1(5)	166(2)
C(8a)	-C(4a)	-C(5)	-H2(5)	-80(2)
H(4a)	-C(4a)	-C(5)	-C(6)	-73.7(15)
H(4a)	-C(4a)	-C(5)	-H1(5)	50(2)
H(4a)	-C(4a)	-C(5)	-H2(5)	164(2)
C(4)	-C(4a)	-C(8a)	-H(8a)	56(2)
C(5)	-C(4a)	-C(8a)	-H(8a)	-178(2)

Table XXVIII (continued)

H(4a)	-C(4a)	-C(8a)	-C(1)	-172.9(15)
H(4a)	-C(4a)	-C(8a)	-C(8)	59.5(15)
H(4a)	-C(4a)	-C(8a)	-H(8a)	-60(2)
H1(5)	-C(5)	-C(6)	-C(61)	41(2)
H1(5)	-C(5)	-C(6)	-C(7)	-140(2)
H2(5)	-C(5)	-C(6)	-C(61)	-68.1(14)
H2(5)	-C(5)	-C(6)	-C(7)	111.4(14)
C(5)	-C(6)	-C(61)	-H1(61)	-66(4)
C(5)	-C(6)	-C(61)	-H2(61)	173(3)
C(5)	-C(6)	-C(61)	-H3(61)	57(3)
C(7)	-C(6)	-C(61)	-H1(61)	114(4)
C(7)	-C(6)	-C(61)	-H2(61)	-7(3)
C(7)	-C(6)	-C(61)	-H3(61)	-123(3)
C(6)	-C(7)	-C(71)	-H1(71)	98(3)
C(6)	-C(7)	-C(71)	-H2(71)	-25(3)
C(6)	-C(7)	-C(71)	-H3(71)	-144(3)
C(8)	-C(7)	-C(71)	-H1(71)	-81(3)
C(8)	-C(7)	-C(71)	-H2(71)	155(3)
C(8)	-C(7)	-C(71)	-H3(71)	36(3)
C(6)	-C(7)	-C(8)	-H1(8)	106(2)
C(6)	-C(7)	-C(8)	-H2(8)	-137(2)
C(71)	-C(7)	-C(8)	-H1(8)	-74(2)
C(71)	-C(7)	-C(8)	-H2(8)	42(2)
C(7)	-C(8)	-C(8a)	-H(8a)	163(2)
H1(8)	-C(8)	-C(8a)	-C(1)	154(2)
H1(8)	-C(8)	-C(8a)	-C(4a)	-78(2)
H1(8)	-C(8)	-C(8a)	-H(8a)	40(3)
H2(8)	-C(8)	-C(8a)	-C(1)	38(2)
H2(8)	-C(8)	-C(8a)	-C(4a)	167(2)
H2(8)	-C(8)	-C(8a)	-H(8a)	-75(2)
C(8a')	-C(1')	-C(2')	-H(2')	176(2)
O(1')	-C(1')	-C(2')	-H(2')	-56(2)
H(1')	-C(1')	-C(2')	-C(3')	-130.0(15)
H(1')	-C(1')	-C(2')	-H(2')	54(2)
C(2')	-C(1')	-C(8a')	-H(8a')	-79(2)
O(1')	-C(1')	-C(8a')	-H(8a')	157(2)
H(1')	-C(1')	-C(8a')	-C(4a')	159(2)
H(1')	-C(1')	-C(8a')	-C(8')	-76(2)
H(1')	-C(1')	-C(8a')	-H(8a')	44(2)
C(2')	-C(1')	-O(1')	-H(O1')	-57(11)
C(2')	-C(1')	-O(1')	-H(O1')*	158(11)
C(8a')	-C(1')	-O(1')	-H(O1')	68(11)
C(8a')	-C(1')	-O(1')	-H(O1')*	-74(11)
H(1')	-C(1')	-O(1')	-H(O1')	-173(11)
H(1')	-C(1')	-O(1')	-H(O1')*	43(11)
C(1')	-C(2')	-C(3')	-H(3')	-173(2)
H(2')	-C(2')	-C(3')	-C(4')	178(2)
H(2')	-C(2')	-C(3')	-H(3')	3(3)
C(2')	-C(3')	-C(4')	-H(4')	91.3(15)
H(3')	-C(3')	-C(4')	-C(4a')	150(2)
H(3')	-C(3')	-C(4')	-O(4')	26(2)
H(3')	-C(3')	-C(4')	-H(4')	-93(3)

Table XXVIII (continued)

C(3')	-C(4')	-C(4a')	-H(4a')	165.4(13)
O(4')	-C(4')	-C(4a')	-H(4a')	-70.0(13)
H(4')	-C(4')	-C(4a')	-C(5')	166.3(14)
H(4')	-C(4')	-C(4a')	-C(8a')	-69.5(14)
H(4')	-C(4')	-C(4a')	-H(4a')	45(2)
C(3')	-C(4')	-O(4')	-H(O4')	-54(2)
C(4a')	-C(4')	-O(4')	-H(O4')	-179(2)
H(4')	-C(4')	-O(4')	-H(O4')	68(3)
C(4')	-C(4a')	-C(5')	-H1(5')	-73(2)
C(4')	-C(4a')	-C(5')	-H2(5')	44.0(14)
C(8a')	-C(4a')	-C(5')	-H1(5')	164(2)
C(8a')	-C(4a')	-C(5')	-H2(5')	-79.1(14)
H(4a')	-C(4a')	-C(5')	-C(6')	-72.4(14)
H(4a')	-C(4a')	-C(5')	-H1(5')	47(2)
H(4a')	-C(4a')	-C(5')	-H2(5')	165(2)
C(4')	-C(4a')	-C(8a')	-H(8a')	57(2)
C(5')	-C(4a')	-C(8a')	-H(8a')	-176(2)
H(4a')	-C(4a')	-C(8a')	-C(1')	-173.7(13)
H(4a')	-C(4a')	-C(8a')	-C(8')	58.7(14)
H(4a')	-C(4a')	-C(8a')	-H(8a')	-58(2)
H1(5')	-C(5')	-C(6')	-C(61')	46(2)
H1(5')	-C(5')	-C(6')	-C(7')	-134(2)
H2(5')	-C(5')	-C(6')	-C(61')	-66.5(13)
H2(5')	-C(5')	-C(6')	-C(7')	112.7(13)
C(5')	-C(6')	-C(61')	-H1(61')	154(2)
C(5')	-C(6')	-C(61')	-H2(61')	40(3)
C(5')	-C(6')	-C(61')	-H3(61')	-76(3)
C(7')	-C(6')	-C(61')	-H1(61')	-25(3)
C(7')	-C(6')	-C(61')	-H2(61')	-140(3)
C(7')	-C(6')	-C(61')	-H3(61')	105(3)
C(6')	-C(7')	-C(71')	-H1(71')	-11(3)
C(6')	-C(7')	-C(71')	-H2(71')	-134(4)
C(6')	-C(7')	-C(71')	-H3(71')	112(3)
C(8')	-C(7')	-C(71')	-H1(71')	170(3)
C(8')	-C(7')	-C(71')	-H2(71')	46(4)
C(8')	-C(7')	-C(71')	-H3(71')	-68(3)
C(6')	-C(7')	-C(8')	-H1(8')	112(2)
C(6')	-C(7')	-C(8')	-H2(8')	-136(2)
C(71')	-C(7')	-C(8')	-H1(8')	-68(2)
C(71')	-C(7')	-C(8')	-H2(8')	43(2)
C(7')	-C(8')	-C(8a')	-H(8a')	158.5(15)
H1(8')	-C(8')	-C(8a')	-C(1')	150(2)
H1(8')	-C(8')	-C(8a')	-C(4a')	-83(2)
H1(8')	-C(8')	-C(8a')	-H(8a')	32(2)
H2(8')	-C(8')	-C(8a')	-C(1')	37(2)
H2(8')	-C(8')	-C(8a')	-C(4a')	164(2)
H2(8')	-C(8')	-C(8a')	-H(8a')	-81(2)

recorded in brackets following the corresponding quantities for the A molecules.

Ring twist, which is strictly defined as the H(4a)-C(4a)-C(8a)-H(8a) torsion angle (-60(3)°) [-58(2)°] is also described to a good approximation by the more accurately determined C(1)-C(8a)-C(4a)-C(5) torsion angle of 69.4(3)° [68.5(3)°]. The latter torsion angles are slightly larger in the present structures than in any other 4a-naphthoquinol studied in the series and appear to be due to steric interactions between O(1) and carbons C(2), C(8), C(8a) and C(7). Short contacts (less than the van der Waals radii sum for O and C of 3.22 Å) between these atoms result in these four carbons tending to force the exocyclic oxygen into a more sterically favored position, i.e. one which minimizes crowding. The pressure exerted by C(8a), C(8) and C(7) is greater than, and opposed by, that exerted by C(2) resulting in a slight increase in the twist angle C(1)-C(8a)-C(4a)-C(5).

The C(6)=C(7) bond length of 1.324(4) Å [1.323(4) Å] is not significantly longer than that in similarly substituted tetrahydro-1-naphthoquin-4a-ol derivatives (Chapter III and reference 32). The increased endocyclic angles around C(6) and C(7) in the present structure follow the previously noted trend of internal angle enlargement accompanying increased substitution at these centers. The C(5)-C(6) and C(7)-C(8) bonds are longer in the diol than in the unsubstituted tetrahydronaphthoquinol, as expected on the basis of previous trends observed in the naphthoquinols with methyl substituents at C(6) and C(7).

Asymmetric Unit Size - Structure Comparison

The obvious difference between the diol (VIII) and other tetrahydronaphthoquin-4α-ols studied is the presence of a hydroxyl group in place of a carbonyl oxygen bonded to C(1). The additional mode for hydrogen bonding is probably a factor in determining the size of the asymmetric unit by permitting molecules to associate in pairs while allowing H-bonding to adjacent units via the other hydroxyl group, thus enabling efficient packing in the crystal – the packing coefficient is about 0.67 for this structure. Similar situations are found, for example, in hydroxyimino(N,N'-dimethyl)malonamide (41) and (±)-cis-5,6-dihydro-5,6-dihydroxy-7,12-dimethylbenz(a)anthracene (42) where molecular association through hydrogen bonding seems to account for the presence of two molecules in the asymmetric unit. Conversely, the literature shows many examples where multiple modes of hydrogen bonding exist but only one molecule is accomodated in the asymmetric unit. The many interrelated factors (such as the geometric shape of the molecule, the type of atoms involved, electronic and steric effects, etc.) involved in the growth of the crystal make it difficult to predict the size of the asymmetric unit.

Although hydrogen bonding undoubtedly contributes to the associative interaction in the present case, it is not necessarily the only reason for the increased number of molecules in the asymmetric unit. As an illustration of this point, it is interesting to compare two compounds whose parent ring structures and conformations are essentially the same as

the diol, namely cis-4a,5,8,8a-tetrahydro-1,4-naphthoquinone (43) and 5α,8α-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol (44). Both structures crystallize in monoclinic space groups – the former in $\underline{P}2_1/\underline{c}$ with $\underline{Z}$ = 8 and the latter in $\underline{P}2_1/\underline{n}$ with $\underline{Z}$ = 8. In sharp contrast with the present structure, the naphthoquinone molecule lacks any facility for hydrogen bonding and therefore an alternative explanation for the greater than expected number of molecules in the asymmetric unit must be sought, but is beyond the scope of this discussion. The 5α,8α-dimethylnaphthoquinol, on the other hand, despite its ability to hydrogen bond, does so only between symmetry related molecules and not between A and B molecules in the asymmetric unit.

PART II

CHAPTER V

A TWISTANE DERIVATIVE

(TWISTENONE)

Introduction

The solution photochemistry of (I) (Figure 16) has been recently reinvestigated by Scheffer and Walsh (35). It was found that a slight modification in the method of photolysis had a marked effect on the ratios of the photoproducts formed. The modification, which involved irradiating internally rather than externally[1] as previously done (25) gave rise to (II) and (III) and an additional photoproduct at the expense of (II). In the original investigation, Scheffer et al. (24,25) had not observed this additional product, though it may have been present in trace amounts.

A crystallographic study was carried out on this unknown photoproduct in an attempt to elucidate its molecular structure. It was hoped that the structural solution would aid in the derivation of a mechanism for the reaction. Although infrared and NMR techniques were available, neither afforded a readily interpretable spectrum and for this reason the methods of X-ray crystal structure analysis were exploited. The structure is now shown to be (IV)[2].

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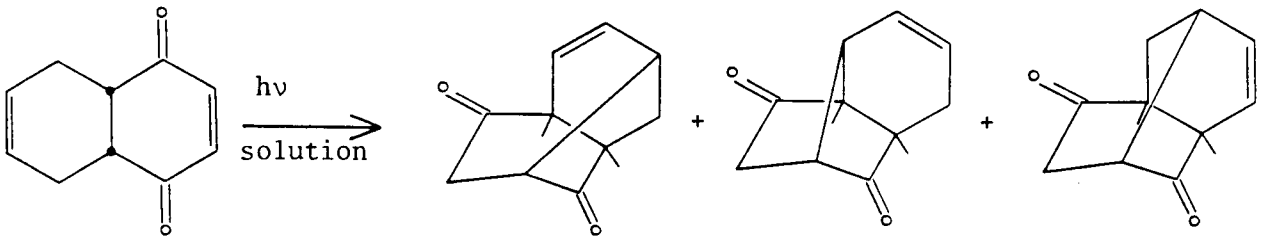
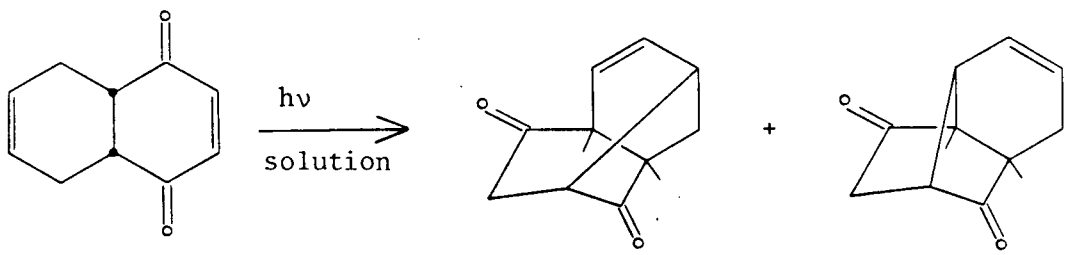
[1] Internal irradiation is performed by inserting the lamp into the hollow of the immersion well reactor vessel; external irradiation is carried out by placing the lamp by the exterior wall of the reactor vessel.

[2] IUPAC name: tricyclo[4.4.0.$0^{3,8}$]dec-9-ene-2,5-dione.



(I) (II) (III) (IV)

Scheffer and Walsh (1981) (35).



(I) (II) (III)

Scheffer, Bhandari, Gayler and Wostradowski (1974) (24).

Figure 16

Reaction schemes illustrating the different results from internal (top) and external (bottom) irradiation.

Experimental

Thin crystals were obtained by slow evaporation of a hexane/acetone solution. X-ray data were measured with a crystal of dimensions 0.2 x 0.3 x 0.3 mm^3 under the following conditions: graphite monochromatized MoKα radiation; a theta range from 0.0 to 27.5 degrees; an omega scan angle given by (0.80 + 0.35tanθ) degrees; a variable horizontal aperture width (variation according to the expression (2.00 + tanθ) mm); an ω-2(4/6)θ scan type; and scan speeds in the the range 1.34-10.06 deg min^{-1}. Intensity and orientation controls were monitored regularly throughout data collection. Accurate cell parameters were obtained by least squares fit to the observed sinθ values for 21 centered reflections.

Crystal data: $C_{10}H_{10}O_2$, MW = 162.19, monoclinic $\underline{a}$ = 6.381(2), $\underline{b}$ = 19.454(2), $\underline{c}$ = 6.708(2) Å, β = 106.24(1)°, $\underline{V}$ = 799.5(3) $Å^3$, $\underline{Z}$ = 4, $\underline{D}_c$ = 1.347 g cm^{-3}, μ(MoKα) = 0.870 cm^{-1}, λ = 0.71073 Å, space group $\underline{P2_1/n}$, from absences and structure analysis.

Intensities were corrected for Lorentz and polarization effects but not for absorption. The decay of the three standards' intensities — $(2\bar{5}\bar{3})$ 1.93%; $(\bar{1}3\bar{1})$, 5.85%; $(\bar{1}6\bar{2})$, 4.15% — necessitated the application of a decay correction. Of the 1828 unique reflections, 930 (50.8%) had $I \geq 3\sigma(I)$ where $\sigma^2(I) = S + 2B + (0.04(S - B))^2$, S being the scan count and B the time-averaged background.

Solution and Refinement

A cursory analysis of the data showed reflections of the types $\underline{h}0\underline{l}$, $\underline{h} + \underline{l}$ = odd and $0\underline{k}0$, $\underline{k}$ = odd were the only reflections classified as unobserved systematically; this suggested $\underline{P}2_1/\underline{n}$ symmetry. The intensity statistics tended more toward a centric distribution than an acentric one – consistent with the suggested space group. The structure was solved by MULTAN employing 3296 Σ_2-relationships which involved 248 normalized structure factors. The starting set of phases was made up of eight reflections: three origin defining reflections, chosen in accordance with space group restrictions and given phases of 0; one reflection whose phase was determined by the Σ_1-formula; and four other general reflections, prominent in the Σ_2-listing and initially assigned phases of 0. Fourteen permutations of the two phases, 0 and π, among the four general reflections resulted in one outstanding phase set. A Fourier synthesis, calculated with this set of phases, produced a map on which the top twelve peaks corresponded to the non-hydrogen atom positions.

Refinement was initiated in the space group $\underline{P}2_1/\underline{n}$ (which was confirmed by subsequent refinement as the correct space group). In the early stages of refinement carbon and oxygen atoms were assigned isotropic temperature factors but later were converted to anisotropic for further cycling. Hydrogen atoms were easily identified on a difference-Fourier map and were subsequently included in the full matrix least squares refinement. Those reflections for which $I < 3\sigma(I)$ were excluded

from the refinement. Convergence was reached at R = 0.037, Rw = 0.043 for 149 variables and 930 reflections. Mean and maximum parameter shifts were 0.019 and 0.170σ, respectively. The standard deviation in an observation of unit weight was 1.844. A weighting analysis confirmed the suitability of the chosen weights, $w = 1/\sigma^2(F)$, where $\sigma^2(F)$ is derived from the previously defined $\sigma^2(I)$. Fluctuations of ± 0.17 e/Å^3 on the final difference map appeared to be random. Atomic coordinates and temperature factors are given in Table XXIX. Anisotropic thermal parameters for non-hydrogen atoms are listed in Table XXX.

Discussion

The structure was found to be a twistane (31) derivative, unsaturated at C(9) and C(10), and having carbonyl substituents at positions 2 and 5. This appears to be the first example of an X-ray crystal structure determination of an unsaturated twistane derivative and therefore, structural comparisons are limited to the relatively few twistanes whose crystal structures are known.

Generally, bond lengths are comparable to accepted values (33) with the exception of C(9)=C(10) (1.310(4) Å) and the bridging bonds, C(3)-C(8) (1.559(3) Å) and C(1)-C(6) (1.574(3) Å) (Table XXXI). However, the lengthening of the latter two bonds is not unusual for this type of system; similar lengthening of C(sp^3)-C(sp^3) bonds has been reported for bridged ring hydrocarbons (see for example, references 45 and 46).

Atom C(2) deviates by 0.0083(19) Å from the mean plane through C(1), C(2), C(3) and O(2) (Table XXXII); the other

Table XXIX

Final positional (fractional x 10^5, H x 10^4)

and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)

with estimated standard deviations in parentheses

Atom	x	y	z	Ueq/Uiso
C(1)	43183(30)	9198(11)	73230(32)	42
C(2)	46946(32)	16445(10)	81296(30)	43
C(3)	68270(35)	18800(11)	78540(33)	50
C(4)	84231(40)	15878(13)	98328(40)	55
C(5)	79127(29)	8327(11)	99726(31)	43
C(6)	66087(30)	5539(10)	79168(29)	40
C(7)	78841(39)	7886(12)	64120(37)	51
C(8)	71086(37)	15293(13)	58557(36)	55
C(9)	49048(43)	14393(14)	43397(36)	62
C(10)	35198(41)	10864(12)	50506(36)	56
O(2)	34914(28)	19664(9)	89031(27)	70
O(5)	85239(26)	5020(9)	115598(24)	67
H(1)	3304(37)	696(11)	7830(32)	53(6)
H(3)	6943(38)	2367(14)	7803(36)	68(7)
H1(4)	8257(47)	1812(14)	11038(47)	84(9)
H2(4)	9855(43)	1611(11)	9740(34)	59(6)
H(6)	6439(32)	82(13)	7943(31)	52(6)
H1(7)	7583(39)	488(13)	5098(41)	75(7)
H2(7)	9442(38)	766(10)	7115(34)	58(6)
H(8)	8141(38)	1794(13)	5341(35)	67(7)
H(9)	4646(47)	1596(15)	3003(48)	91(9)
H(10)	2038(40)	995(12)	4290(37)	68(7)

Table XXX

Final anisotropic thermal parameters ($\underline{U}ij \times 10^4$ Å^2)

and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
C(1)	324(10)	437(12)	483(12)	-57(9)	104(9)	-24(10)
C(2)	434(11)	437(12)	405(11)	77(9)	105(8)	-6(9)
C(3)	552(13)	298(12)	628(15)	-70(10)	138(11)	18(10)
C(4)	437(13)	567(15)	589(14)	-118(10)	66(10)	-79(12)
C(5)	364(10)	496(13)	429(12)	39(9)	114(8)	48(10)
C(6)	433(11)	296(11)	449(11)	15(8)	98(9)	27(9)
C(7)	481(13)	637(15)	456(12)	168(11)	187(10)	65(12)
C(8)	568(14)	553(14)	599(14)	35(11)	292(11)	197(12)
C(9)	758(16)	684(16)	385(12)	301(13)	114(12)	119(12)
C(10)	483(13)	604(15)	489(13)	138(11)	-17(11)	-102(11)
O(2)	691(10)	717(12)	766(11)	205(9)	306(9)	-146(9)
O(5)	715(11)	786(11)	456(9)	81(8)	67(8)	179(9)

Table XXXI

Bond lengths (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1) -C(2)	1.505(3)	C(5) -C(6)	1.499(3)
C(1) -C(10)	1.501(3)	C(5) -O(5)	1.211(2)
C(2) -C(3)	1.495(3)	C(6) -C(7)	1.533(3)
C(2) -O(2)	1.214(2)	C(6) -C(1)	1.573(3)
C(3) -C(4)	1.538(3)	C(7) -C(8)	1.535(3)
C(3) -C(8)	1.559(3)	C(8) -C(9)	1.497(4)
C(4) -C(5)	1.513(3)	C(9) -C(10)	1.310(4)

Bond lengths (Å) involving hydrogen atoms with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1) -H(1)	0.92(2)	C(7) -H1(7)	1.03(3)
C(3) -H(3)	0.95(3)	C(7) -H2(7)	0.98(2)
C(4) -H1(4)	0.95(3)	C(8) -H(8)	0.97(2)
C(4) -H2(4)	0.93(3)	C(9) -H(9)	0.92(3)
C(6) -H(6)	0.92(2)	C(10) -H(10)	0.96(2)

carbonyl group is essentially planar with an average deviation from the least squares plane of 0.0027 Å. The alkene moiety is distorted noticeably from an unstrained planar configuration showing a C(8)-C(9)-C(10)-C(1) torsion angle of 7.4°. Other torsion angles in the five unique six-membered rings of the twistenone (IV) are recorded in Figure 17. As to be expected,

Table XXXII

Least squares planes

(x, y, z are fractional coordinates referred to the monoclinic cell)

Plane 1 defined by atoms C(1), C(2), C(3) and O(2)

Equation: 1.5130x - 6.9114y + 5.3785z - 3.9547 = 0

Deviations from the plane:

atom	deviation (Å)
C(1)	0.0018(20)
C(2)	-0.0083(19)
C(3)	0.0035(22)
O(2)	0.0030(18)

Plane 2 defined by atoms C(4), C(5), C(6) and O(5)

Equation: 6.0315x - 4.5660y - 3.2341z - 1.1718 = 0

Deviations from the plane:

atom	deviation (Å)
C(4)	0.0036(28)
C(5)	-0.0047(18)
C(6)	0.0010(19)
O(5)	0.0017(16)

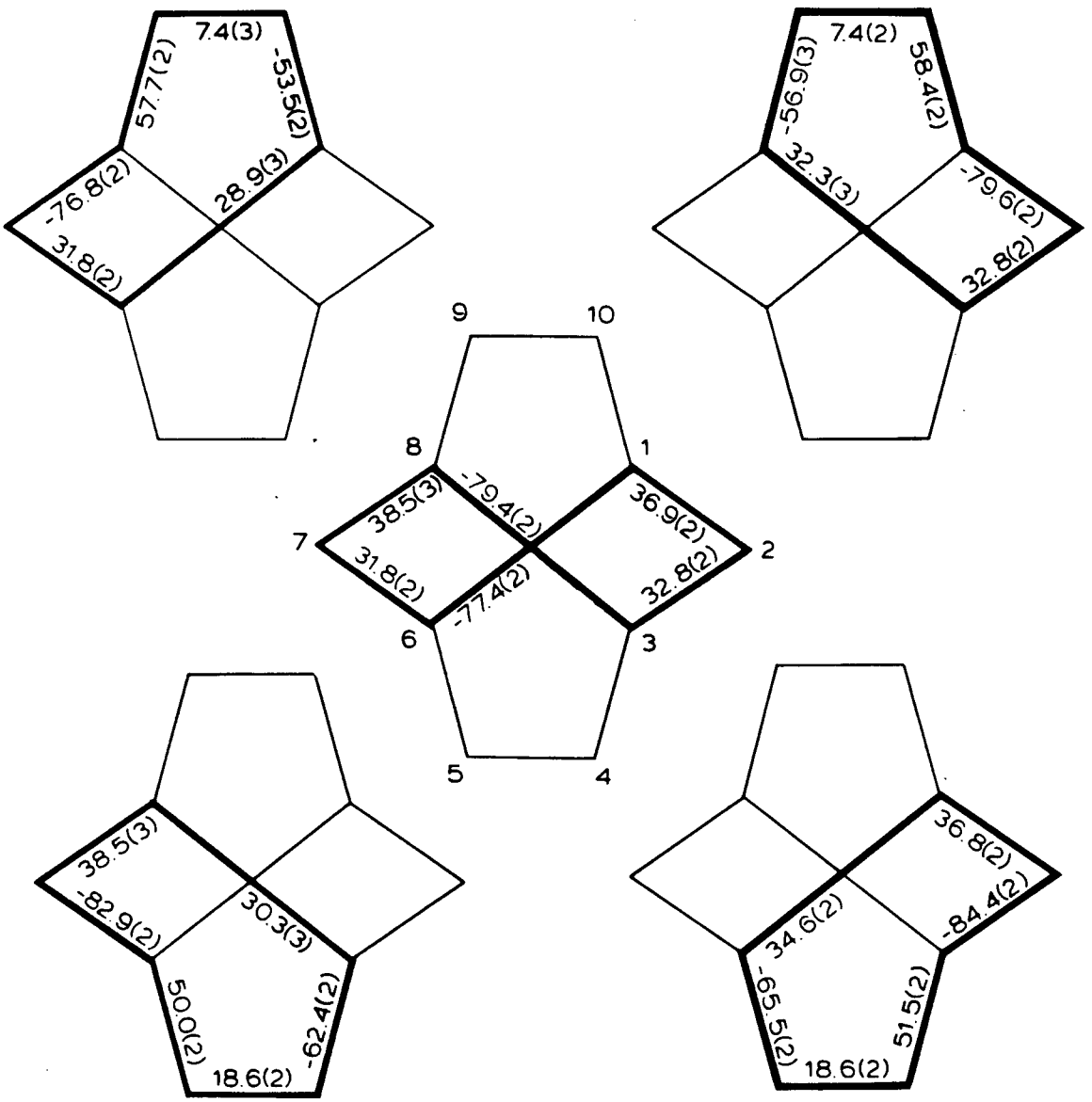


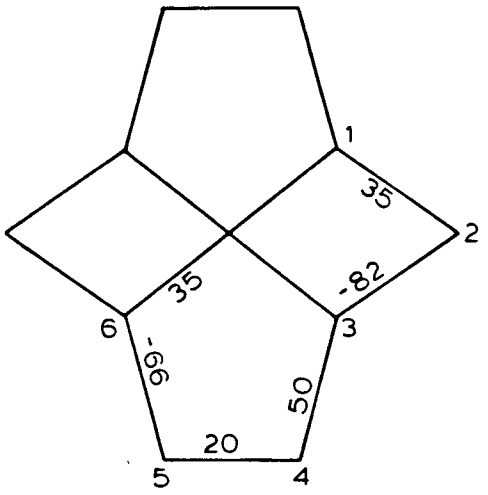
Figure 17

Torsion angles for twistenone (IV)

the presence of the double bond within the tricyclic skeleton introduces marked deviations from the twistane geometry where the five rings approach twist-boat conformations. Ideal torsion angles for twist-boat conformers (38) are presented in Figure 18 along with torsion angles for twistane obtained by empirical force-field calculations (47). Despite significant differences between twistane torsion angles (and similarly those of the present molecule) and the idealized twist-boat torsion angles, these angles seem more consistent with this conformation than with any other.

The D_2-symmetry of the twistane is drastically reduced to C_1 with the addition of O(2) and O(5). Notwithstanding the change in hybridization at carbons 2 and 5, exclusion of the oxygens leaves the tricyclic skeleton with symmetry closely approximating C_2 (see Fig. 19). The rotation axis passes through the center of, and is perpendicular to bonds C(9)=C(10) and C(4)-C(5), similar to the pseudo C_2-axis in aza-twistanone (48).

In addition to torsional strain, twistenone (IV) suffers from considerable angular strain. Compared with normal values, endocyclic angles are observed to deviate up to 12.4° with the most noticeable divergence from accepted values occurring for angles involving the oxygen bearing carbon atoms as vertices; C(1)-C(2)-C(3), 107.6(2)° and C(4)-C(5)-C(6), 111.6(2)° (Table XXXIII). Of similar magnitude is the difference between the C(2)-C(1)-C(10) angle of 97.9(2)° and the normal tetrahedral value of 109.5° suggesting marked deviation from sp^3 hybridization at C(1). Other angles which include one bridging carbon, flanked on either side by carbons not involved in a



(a)

C(1)	C(2)	C(3)	C(4)	-70.6
C(2)	C(3)	C(4)	C(5)	33.1
C(3)	C(4)	C(5)	C(6)	33.1
C(4)	C(5)	C(6)	C(1)	-70.6
C(5)	C(6)	C(1)	C(2)	33.1
C(6)	C(1)	C(2)	C(3)	33.1

(b)

Figure 18

Torsion angles in twistane (a) and in the idealized twist-boat conformation (b). Values in (a) are from empirical force-field calculations (47); those in (b) are from reference 38.

bridge (e.g. C(2)-C(3)-C(4)), show a mean compression of 6.8° from the ideal tetrahedral value.

Despite the accuracy with which the bond lengths were obtained, it is still insufficient to allow one to quantify detailed hybridization differences strictly on the basis of small changes (<0.01 Å) in various bond distances. However, from the overall bonding geometry the fraction of s-character in the hybrid orbitals associated with each atom may be calculated approximately, thereby giving a clearer indication as to the hybridization within particular bonds. For example, the

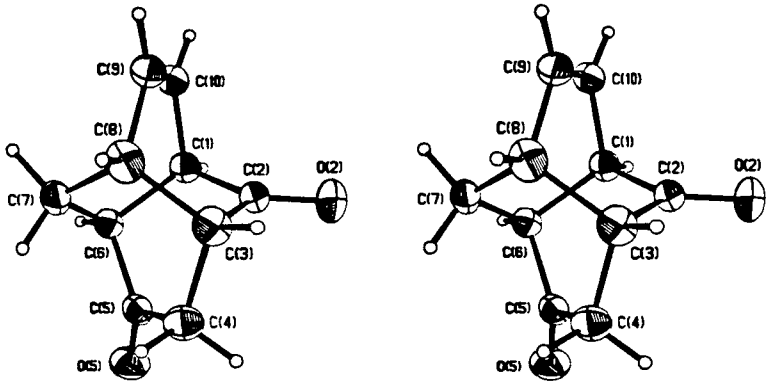


Figure 19

Stereo diagram of the twistenone (IV)

fractional s-character at the carbon atom C(1), in the bond C(1)-C(2), is about 0.145, suggesting the involvement of a hybrid orbital quite different from sp^3. An almost equal value of 0.186 for the fractional s-character at C(3), in the C(2)-C(3) bond, implies similar hybridization. These values, not uncommon in strained systems, reflect the distribution of the electrons accomodating that part of the structure. As mentioned above, the C(9)-C(10) bond, 1.310(4) Å, is significantly different from the accepted $C(sp^2)$-$C(sp^2)$ length of 1.335(5) Å, but this does not appear to be accompanied by hybridization differences. The amount of s-character was calculated to be 32% at both C(9) and C(10), as expected for sp^2 hybrids; however, the twist of 7.4(3)° about the C(9)-C(10) bond, expected to result in a decrease in the p-orbital overlap between these

Table XXXIII

Bond angles (deg) with estimated standard deviations in parentheses

Bonds			Angle	Bonds			Angle
C(1)	-C(1)	-C(6)	106.8(2)	C(4)	-C(5)	-O(5)	123.2(2)
C(1)	-C(1)	-C(10)	97.9(2)	C(6)	-C(5)	-O(5)	125.2(2)
C(6)	-C(1)	-C(10)	112.5(2)	C(5)	-C(6)	-C(7)	103.8(2)
C(3)	-C(1)	-C(1)	107.6(2)	C(5)	-C(6)	-C(1)	107.8(2)
C(3)	-C(1)	-O(1)	126.9(2)	C(7)	-C(6)	-C(1)	109.0(2)
C(1)	-C(1)	-O(1)	125.5(2)	C(6)	-C(7)	-C(8)	104.2(2)
C(1)	-C(3)	-C(4)	100.7(2)	C(3)	-C(8)	-C(7)	108.0(2)
C(1)	-C(3)	-C(8)	107.5(2)	C(3)	-C(8)	-C(9)	108.8(2)
C(4)	-C(3)	-C(8)	111.9(2)	C(7)	-C(8)	-C(9)	103.5(2)
C(3)	-C(4)	-C(5)	108.1(2)	C(8)	-C(9)	-C(10)	114.5(2)
C(4)	-C(5)	-C(6)	111.6(2)	C(9)	-C(10)	-C(1)	114.3(2)

Bond angles (deg) involving hydrogen atoms with estimated standard deviations in parentheses

Bonds			Angle	Bonds			Angle
C(1)	-C(1)	-H(1)	111.6(13)	C(1)	-C(6)	-H(6)	110.4(12)
C(6)	-C(1)	-H(1)	113.0(14)	C(6)	-C(7)	-H1(7)	112.8(13)
C(10)	-C(1)	-H(1)	113.8(13)	C(6)	-C(7)	-H2(7)	109.0(13)
C(1)	-C(3)	-H(2)	113.1(14)	C(8)	-C(7)	-H1(7)	110.8(14)
C(4)	-C(3)	-H(2)	111.1(15)	C(8)	-C(7)	-H2(7)	112.1(12)
C(8)	-C(3)	-H(2)	112.1(14)	H1(7)	-C(7)	-H2(7)	108.0(18)
C(3)	-C(4)	-H1(4)	111.1(18)	C(3)	-C(8)	-H(8)	109.0(13)
C(3)	-C(4)	-H2(4)	110.4(14)	C(7)	-C(8)	-H(8)	112.3(14)
C(5)	-C(4)	-H1(4)	108.4(16)	C(9)	-C(8)	-H(8)	115.0(14)
C(5)	-C(4)	-H2(4)	106.4(13)	C(8)	-C(9)	-H(9)	120.2(18)
H1(4)	-C(4)	-H2(4)	112.2(22)	C(10)	-C(9)	-H(9)	125.1(18)
C(5)	-C(6)	-H(6)	112.3(13)	C(9)	-C(10)	-H(10)	124.7(14)
C(7)	-C(6)	-H(6)	113.3(12)	C(1)	-C(10)	-H(10)	120.3(14)

atoms, should lengthen the bond. Crystal packing is unlikely to cause the decrease in the bond length; all intermolecular contacts correspond to normal van der Waals distances. A packing diagram is presented in Figure 20.

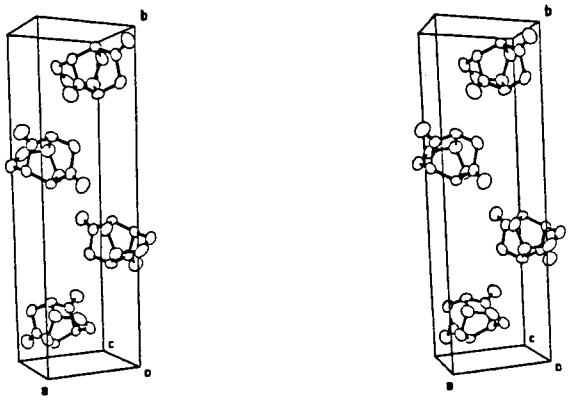


Figure 20

Stereo packing diagram of twistenone (IV)

CHAPTER VI

5-(2,3-DIMETHYLPHENYL)-γ-BUTYROLACTONE

Introduction

Photochemical studies combined with crystal structure analyses on substituted 4aβ,5,8,8aβ-tetrahydro-1,4-naphthoquinones and 4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4-ols have provided valuable insights into such photochemical reactions as H-abstractions (Part I and references 26,30,32,34), dimerizations (34) and [2+2] intramolecular cycloadditions (26,49). However, some reactions, though designed to clarify or confirm a particular aspect of a previously interpreted mechanism, have led to interesting results which strayed slightly from the original theme of the study. It has been observed, for example, that minor modifications in technique along the photochemical experimentation route, as in the case of the photolysis of the unsubstituted tetrahydronaphthoquinone (see Chapter V), has an interesting and significant effect on the resulting product ratios. The present compound, shown by X-ray analysis to be a 2,3-dimethylphenyl substituted γ-butyrolactone[1], and its formation sequence are regarded with equal interest. Its immediate precursor, resulting from the photolysis of 6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1,4-naphthoquinone has not yet been characterized. It was hoped that the structural elucidation of the present compound would aid in the determination of the intermediate compound in the reaction scheme.

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[1] Alternative IUPAC name: 5-(2,3-dimethylphenyl)-tetrahydro-2-furanone.

Experimental

Photolysis of 6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1,4-naphthoquinone (V) (Fig. 21) gave the previously observed γ-hydrogen abstraction product (VI) and a new product X.

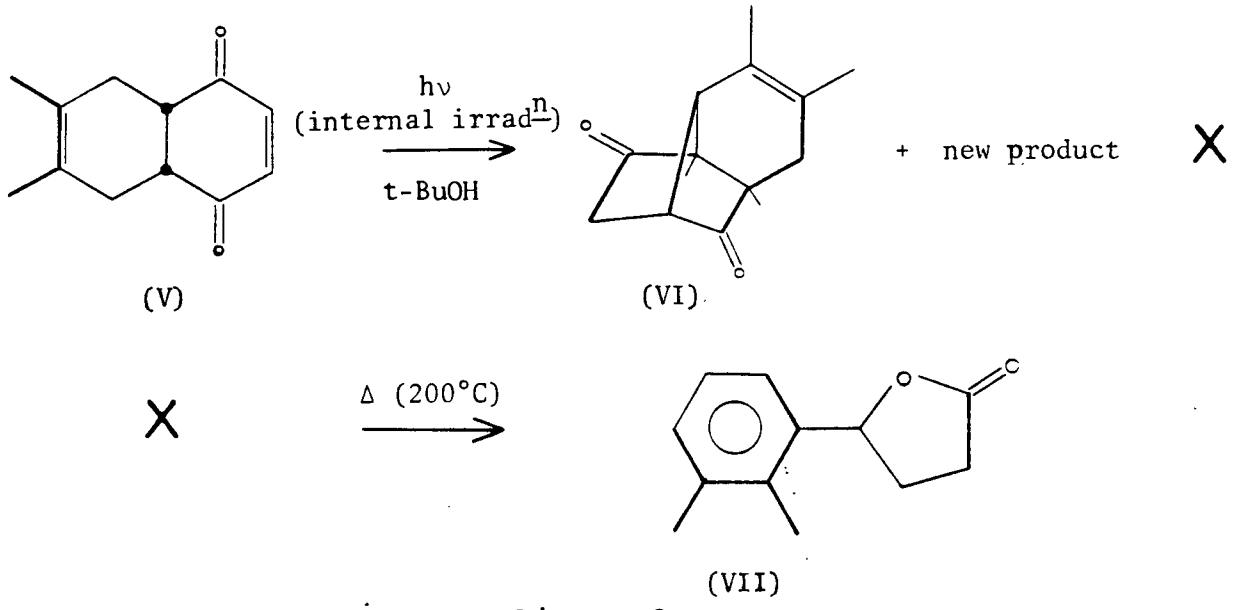


Figure 21

Reaction scheme leading to the lactone (VII).

Thermolysis of the minor product X yielded the title compound (VII) which was recrystallized from a petroleum ether/ethanol solution. The crystal chosen for structure analysis was bounded by six well-defined faces ±(102), ±(10$\bar{1}$) and ±(01$\bar{1}$), and measured 0.14 x 0.04 x 0.06 mm^3.

Crystal data: $C_{12}H_{14}O_2$, MW = 190.24, monoclinic $\underline{a}$ = 10.847(3), $\underline{b}$ = 6.924(1), $\underline{c}$ = 13.654(4) Å, β = 95.22(1)°, $\underline{V}$ = 1021.3(5) Å^3, $\underline{Z}$ = 4, $\underline{D}_c$ = 1.237 g cm^{-3}, $\underline{D}_o$ = 1.244 g cm^{-3}, μ(MoKα) = 0.468 cm^{-1}, λ = 0.71073 Å, space group $\underline{P2_1/n}$, from structure analysis.

Data were collected between 0.0 and 22.5° (graphite monochromatized MoKα radiation) with ω-2θ scans and speeds ranging from 1.44 to 10.06 deg min^{-1}. The omega scan angle was given by $(0.90 + 0.35\tan\theta)^{\circ}$. The horizontal aperture width was calculated from the expression $(2.00 + \tan\theta)$ mm and the vertical aperture remained constant at 4 mm. Intensity control reflections were monitored every 3600 seconds of X-ray exposure time and crystal orientation was checked after every 100 reflections collected. Final cell parameters were obtained by least squares fit of the parameters to the $\sin\theta$ values for 18 centered reflections.

Data processing included corrections for Lorentz and polarization effects but not for absorption. The maximum decay in the intensity controls was 2.98% over the entire data collection. 569 of the 1341 reflections collected had $I \geq 3\sigma(I)$, where $\sigma^2(I) = S + 2B + (0.04(S - B))^2$, S = scan count, B = time-averaged background.

Solution and Refinement

The crystal density of 1.24 g cm^{-3} suggested 14 non-hydrogen atoms per asymmetric unit and the E-statistics indicated a centric distribution of these atoms throughout the cell. From the 256 largest E's, 5301 Σ_2-relationships were generated for use in the phase determining process. No phases were determined by the Σ_1-formula and so MULTAN was permitted to choose additional starting reflections with relatively large E values and which occurred frequently in the Σ_2-listing. The

phases of the general reflections were to be permuted, thereby generating different phase sets during the phase determination. Three origin defining reflections were chosen according to the centrosymmetric monoclinic space group criteria. The set of phases accepted as the true solution had the best figures of merit. A subsequent Fourier synthesis using the normalized structures factors (with their newly found phases) as coefficients revealed the positions of all non-hydrogen atoms.

Full matrix least squares refinement was initiated in the space group $\underline{P}2_1/\underline{n}$, with the inclusion of non-hydrogen atoms with isotropic temperature factors. Unit weights were employed in the initial stages of the refinement. Conversion to anisotropic temperature factors was followed by further cycling and a difference synthesis which revealed coordinates for all hydrogen atoms. The hydrogens assumed isotropic thermal parameters during subsequent refinement. The weighting scheme was changed to $w = 1/\sigma^2(F)$ (where $\sigma^2(F)$ is obtained from the $\sigma^2(I)$ defined above) in order to reflect the accuracy of the data.

As the refinement proceeded it was noted that what initially appeared as reasonable bonding geometries for hydrogens on C(8) and C(9) had become chemically unreasonable, for each pair of hydrogens at these carbons had coalesced into single peaks. At this point, bond lengths and angles were calculated in an effort to determine the bond order between C(8) and C(9). All bore reasonable semblance to accepted values (33) with the exception of those including C(8) and C(9). For example, the C(8)-C(9) bond length of 1.42 Å seemed very short for a single bond in that environment, and yet, was extremely

long for a double bond. Excluding the affected hydrogens, the remainder of the molecule accounted for 186 mass units (m.u.) which was 4 m.u. less than the parent ion peak observed in the mass spectrum. This left little doubt as to the number of missing hydrogens, and so it was concluded that C(8) and C(9) were methylene carbons. Inspection of the thermal parameters for these 2 carbons revealed anomalously large r.m.s. vibrations, up to 0.5 Å for C(8), roughly perpendicular to the mean plane of the five-membered ring. This situation of apparent high thermal motion out of the plane, combined with unusual bonding geometry around C(8) and C(9) closely parallels that found in the five-membered ring metal complexes, $Me_2XCR^1R^2.CF_2XMe_2.M(CO)_4$ (50) where the presence of disorder accounted for the seemingly unreasonable geometry. Similar disorder was thought to occur in the present structure. The limited number of data restricted the handling of the disorder to C(8) and its corresponding hydrogens.

Two carbon atoms with isotropic temperature factors replaced the original C(8) in the refinement and were initially given equal occupancies 1 Å apart on the vector normal to the mean plane of the furanose ring and passing through the original C(8) coordinates. From the magnitude of the temperature factors after several cycles of refinement, it was concluded that the positions of C(8)' and C(8)" were occupied in the ratio of 60:40. Four hydrogen atoms were found via a difference map and refined along with their isotropic thermal parameters.

The standard deviation in an observation of unit weight was 3.3 when $w = 1/\sigma^2(F)$ (which was probably due to the incomplete

handling of the disorder). In the final cycle the polynomial weighting scheme $w = (A + BFo + CFo^2 + DFo^3)^{-1}$, where A = 0.3957, B = 0.00000, C = -0.004568 and D = 0.000384, was employed. This gave constant averages of $w\Delta^2$ over ranges of Fo. Mean and maximum parameter shifts on the last cycle of refinement were 0.233 and 1.201σ, respectively; the maximum shift occurred in the temperature factor of C(8)". The final R-value for 569 reflections with $I \geq 3\sigma(I)$ was 0.057 while that for Rw was 0.065. For the entire data set (1341 reflections) R = 0.141 and Rw = 0.066. A difference-Fourier synthesis following refinement showed random fluctuations between 0.156 and -0.220 e/Å^3. A list of coordinates and temperature factors is given in Table XXXIV. Anisotropic thermal parameters are presented in Table XXXV.

Discussion

The structure consists of a 2,3-dimethylphenyl substituent bonded to the γ-carbon of a butyrolactone moiety. Considering only the gross conformation, the molecule may be described as two ring-containing moieties (Fig. 22) whose mean planes through the rings subtend a dihedral angle of 70°. The molecules pack with the lactone rings back-to-back and lie almost parallel to the $(30\bar{1})$ plane. This is consistent with the relatively large E-magnitude of 3.23 found for the $30\bar{1}$ reflection. Similarly, the proximity of the phenyl ring atoms to the (113) plane seems to account for its E-magnitude of 4.66, the largest in the data set.

Table XXXIV

Final positional (fractional x 10^4,H x 10^3)

and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)

with estimated standard deviations in parentheses

Atom[2]	x	y	z	Ueq/Uiso
C(1)	5386(6)	-879(7)	1867(4)	71
C(2)	5493(6)	813(7)	1313(4)	66
C(21)	4454(11)	2262(11)	1216(8)	90
C(3)	6569(7)	1174(9)	854(4)	74
C(31)	6724(13)	2952(12)	256(7)	110
C(4)	7510(8)	-167(12)	944(6)	89
C(5)	7437(9)	-1804(11)	1500(6)	92
C(6)	6373(9)	-2176(10)	1939(5)	87
C(7)	4233(11)	-1263(9)	2366(7)	100
C(8)'	3958(17)	-326(17)	3301(11)	76(4)
C(8)"	4691(20)	-464(22)	3555(12)	62(4)
C(9)	4208(7)	-1940(10)	4050(5)	102
C(10)	4101(6)	-3764(9)	3463(6)	82
O(1)	3999(5)	-5396(7)	3737(4)	121
O(2)	4078(5)	-3332(5)	2526(4)	105
H1(21)	372(7)	214(10)	158(5)	121(31)
H2(21)	478(7)	330(12)	147(6)	114(31)
H3(21)	395(11)	221(14)	60(9)	188(49)
H1(31)	604(7)	313(11)	-26(6)	120(31)
H2(31)	742(8)	327(13)	-5(7)	129(38)
H3(31)	687(7)	421(12)	72(6)	147(27)
H(4)	820(5)	3(7)	68(4)	61(20)
H(5)	807(7)	-280(11)	157(5)	106(24)
H(6)	623(6)	-317(11)	236(5)	104(23)
H(7)	361(6)	-86(10)	189(6)	98(28)
H1(8)'	306(9)	-32(12)	348(6)	77(28)
H2(8)'	459(7)	107(12)	340(5)	50(22)
H1(8)"	547(11)	-86(15)	383(7)	39(30)
H2(8)"	424(10)	-13(16)	302(10)	20(32)
H1(9)*	496	-194	447	136
H2(9)*	353	-181	443	136

[2] Primed (') atoms are at 60% occupancy; double primed (") atoms are at 40% occupancy; asterisks (*) denote atoms in calculated positions.

Table XXXV

Final anisotropic thermal parameters ($\underline{U}ij \times 10^3$ Å^2)

and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
C(1)	107(5)	48(4)	58(4)	17(4)	1(4)	-5(3)
C(2)	87(5)	47(3)	61(4)	10(3)	-13(3)	-11(3)
C(21)	106(7)	55(4)	106(6)	23(5)	-8(6)	-6(4)
C(3)	96(5)	58(4)	63(4)	4(4)	-11(4)	-19(3)
C(31)	167(10)	73(5)	90(6)	-25(6)	14(8)	3(4)
C(4)	91(6)	83(5)	93(5)	-6(5)	17(5)	-32(4)
C(5)	105(7)	78(5)	89(5)	32(5)	-12(5)	-19(4)
C(6)	124(7)	60(4)	75(4)	28(5)	5(5)	6(3)
C(7)	171(9)	48(4)	85(5)	10(5)	34(6)	2(4)
C(9)	136(7)	67(4)	103(5)	-9(5)	12(5)	-17(4)
C(10)	87(5)	53(4)	110(5)	-11(4)	42(4)	-11(4)
O(1)	165(5)	56(3)	153(5)	-18(3)	73(4)	0(3)
O(2)	175(5)	49(3)	95(3)	-6(3)	29(3)	-13(3)

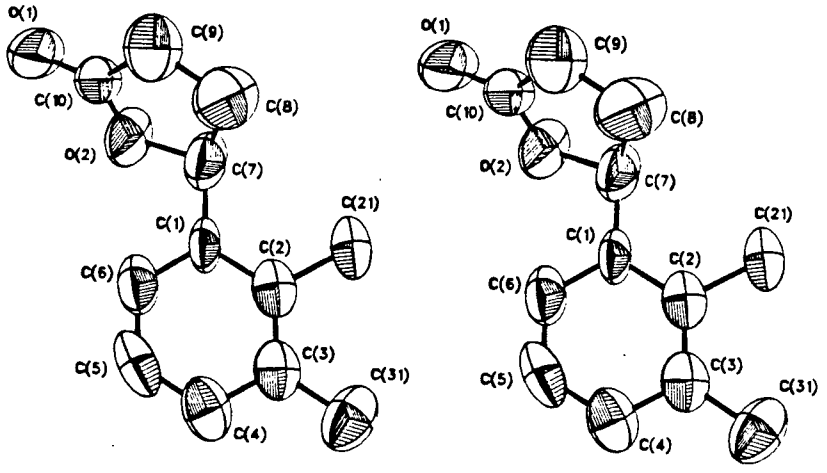


Figure 22

Stereo view of the lactone (VII).

A detailed description of the structure is limited by the accuracy of the derived quantities, which in turn is adversely affected by the disorder in the structure. Some general aspects, however, are noteworthy and are described below.

Butyrolactone rings usually assume an envelope conformation (51,52) where the only atom deviating significantly from the plane of the remaining four is the β-carbon. The planarity of the remaining atoms in the ring stems from the carbonyl group and the partial sp^2-character of the hetero-oxygen atom. Incomplete handling of the disorder prevented observation of

this conformation in the present structure, however, the conformation may be inferred from the nature of the disorder. Generally, the bond lengths and angles (Tables XXXVI and XXXVII) agree with those given by Harlow and Simonsen (52), for a similar γ-lactone. Deviations in these derived quantities involving C(8)' and C(8)" indicate that the disorder is not confined to only one atom in the ring. Examination of the r.m.s. thermal displacements of each of the lactone atoms reveals the extent of the disorder. The stereo diagrams included in Figures 22 and 23 show the relative sizes of the thermal ellipsoids before the disorder at C(8) was refined.

The phenyl ring is significantly non-planar as indicated by the chi-squared value of 8.9 for 3 degrees of freedom. C(4) and

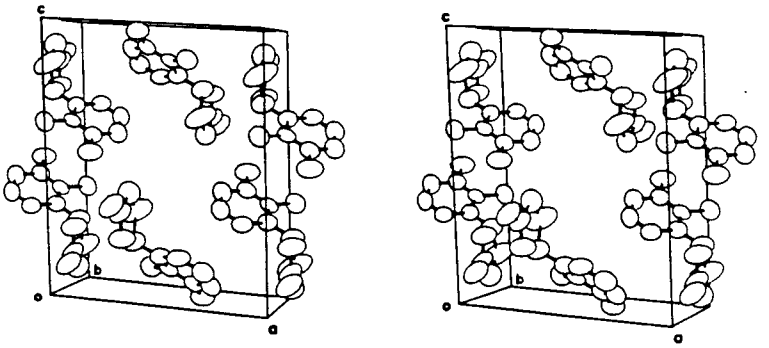


Figure 23

Stereo view of the contents of the unit cell.

Table XXXVI

Bond lengths (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(1) -C(2)	1.405(7)	C(7) -C(8)'	1.49(2)
C(1) -C(6)	1.394(9)	C(7) -C(8)"	1.74(2)
C(1) -C(7)	1.502(10)	C(7) -O(2)	1.461(8)
C(2) -C(21)	1.505(10)	C(8) -C(9)	1.523(15)
C(2) -C(3)	1.397(8)	C(8)" -C(9)	1.357(15)
C(3) -C(31)	1.496(10)	C(9) -C(10)	1.495(8)
C(3) -C(4)	1.377(9)	C(10) -O(1)	1.199(7)
C(4) -C(5)	1.371(11)	C(10) -O(2)	1.312(8)
C(5) -C(6)	1.372(10)		

Bond angles (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(1) -C(6)	118.3(7)	C(1) -C(7) -O(2)	110.7(6)
C(2) -C(1) -C(7)	120.3(6)	C(8)'-C(7) -C(8)"	28.9(7)
C(6) -C(1) -C(7)	121.3(6)	C(8)'-C(7) -O(2)	105.4(7)
C(1) -C(2) -C(21)	120.3(7)	C(8)"-C(7) -O(2)	101.5(8)
C(1) -C(2) -C(3)	120.2(5)	C(7) -C(8)'-C(9)	102.7(8)
C(21)-C(2) -C(3)	119.4(7)	C(7) -C(8)"-C(9)	97.7(10)
C(2) -C(3) -C(31)	122.2(7)	C(8)'-C(9) -C(8)"	33.5(9)
C(2) -C(3) -C(4)	118.9(6)	C(8)'-C(9) -C(10)	105.0(7)
C(31)-C(3) -C(4)	119.0(8)	C(8)"-C(9) -C(10)	112.6(8)
C(3) -C(4) -C(5)	121.8(8)	C(9) -C(10)-O(1)	129.3(7)
C(4) -C(5) -C(6)	119.3(8)	C(9) -C(10)-O(2)	108.9(5)
C(1) -C(6) -C(5)	121.3(7)	O(1) -C(10)-O(2)	121.7(6)
C(1) -C(7) -C(8)'	123.6(11)	C(7) -O(2) -C(10)	112.1(6)
C(1) -C(7) -C(8)"	100.8(9)		

Table XXXVII

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

Bond	Length	Bond	Length
C(21) -H1(21)	0.99(7)	C(6) -H(6)	0.92(7)
C(21) -H2(21)	0.86(8)	C(7) -H(7)	0.94(7)
C(21) -H3(21)	0.96(12)	C(8) -H1(8)'	1.02(8)
C(31) -H1(31)	0.99(8)	C(8)' -H2(8)'	1.19(8)
C(31) -H2(31)	0.92(8)	C(8)" -H1(8)"	0.94(11)
C(31) -H3(31)	1.08(8)	C(8)" -H2(8)"	0.87(11)
C(4) -H(4)	0.87(5)	C(9) -H1(9)	0.95(8)
C(5) -H(5)	0.97(8)	C(9) -H2(9)	0.95(8)

Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(2) -C(21)-H1(21)	122(4)	C(8)" -C(7) -H(7)	133(4)
C(2) -C(21)-H2(21)	104(5)	O(2) -C(7) -H(7)	108(4)
C(2) -C(21)-H3(21)	114(6)	C(7) -C(8)'-H1(8)'	118(5)
H1(21)-C(21)-H2(21)	101(7)	C(7) -C(8)'-H2(8)'	107(4)
H1(21)-C(21)-H3(21)	91(7)	C(9) -C(8)'-H1(8)'	88(5)
H2(21)-C(21)-H3(21)	124(8)	C(9) -C(8)'-H2(8)'	117(4)
C(3) -C(31)-H1(31)	112(4)	H1(8)'-C(8)'-H2(8)'	122(6)
C(3) -C(31)-H2(31)	126(6)	C(7) -C(8)"-H1(8)"	117(6)
C(3) -C(31)-H3(31)	111(4)	C(7) -C(8)"-H2(8)"	38(8)
H1(31)-C(31)-H2(31)	104(7)	C(9) -C(8)"-H1(8)"	88(6)
H1(31)-C(31)-H3(31)	112(7)	C(9) -C(8)"-H2(8)"	114(7)
H2(31)-C(31)-H3(31)	89(7)	H1(8)"-C(8)"-H2(8)"	146.7(1)
C(3) -C(4) -H(4)	121(4)	C(8)' -C(9) -H1(9)	119.6(9)
C(5) -C(4) -H(4)	117(4)	C(8)' -C(9) -H2(9)	101.2(9)
C(4) -C(5) -H(5)	124(4)	C(8)" -C(9) -H1(9)	87.2(1)
C(6) -C(5) -H(5)	116(4)	C(8)" -C(9) -H2(9)	123.7(1)
C(1) -C(6) -H(6)	111(4)	C(10) -C(9) -H1(9)	110.0(6)
C(5) -C(6) -H(6)	128(4)	C(10) -C(9) -H2(9)	110.4(6)
C(1) -C(7) -H(7)	102(4)	H1(9) -C(9) -H2(9)	110.1(7)
C(8)' -C(7) -H(7)	106(5)		

Table XXXVIII

Torsion angles (deg) with estimated standard deviations in parentheses

Atoms				Value
C(6)	-C(1)	-C(2)	-C(21)	-179.8(7)
C(6)	-C(1)	-C(2)	-C(3)	0.4(8)
C(7)	-C(1)	-C(2)	-C(21)	0.2(9)
C(7)	-C(1)	-C(2)	-C(3)	179.6(7)
C(2)	-C(1)	-C(6)	-C(5)	1.4(8)
C(7)	-C(1)	-C(6)	-C(5)	-178.5(7)
C(2)	-C(1)	-C(7)	-C(8)'	-78.1(12)
C(2)	-C(1)	-C(7)	-C(8)"	-97.6(9)
C(2)	-C(1)	-C(7)	-O(2)	155.7(6)
C(6)	-C(1)	-C(7)	-C(8)'	101.8(10)
C(6)	-C(1)	-C(7)	-C(8)"	82.4(8)
C(6)	-C(1)	-C(7)	-O(2)	-24.4(11)
C(1)	-C(2)	-C(3)	-C(31)	179.9(6)
C(1)	-C(2)	-C(3)	-C(4)	0.9(7)
C(21)	-C(2)	-C(3)	-C(31)	0.7(9)
C(21)	-C(2)	-C(3)	-C(4)	-179.7(7)
C(2)	-C(3)	-C(4)	-C(5)	-2.6(9)
C(31)	-C(3)	-C(4)	-C(5)	178.4(7)
C(3)	-C(4)	-C(5)	-C(6)	3.6(10)
C(4)	-C(5)	-C(6)	-C(1)	-3.0(9)
C(1)	-C(7)	-C(8)'	-C(9)	-104.9(10)
C(8)"	-C(7)	-C(8)'	-C(9)	-62.3(14)
O(2)	-C(7)	-C(8)'	-C(9)	23.6(15)
C(1)	-C(7)	-C(8)"	-C(9)	-136.8(10)
C(8)'	-C(7)	-C(8)"	-C(9)	78(2)
O(2)	-C(7)	-C(8)"	-C(9)	-22.9(13)
C(1)	-C(7)	-O(2)	-C(10)	118.0(7)
C(8)'	-C(7)	-O(2)	-C(10)	-17.8(13)
C(8)"	-C(7)	-O(2)	-C(10)	11.7(11)
C(7)	-C(8)'	-C(9)	-C(8)"	86(2)
C(7)	-C(8)'	-C(9)	-C(10)	-21.8(13)
C(7)	-C(8)"	-C(9)	-C(8)'	-56.9(15)
C(7)	-C(8)"	-C(9)	-C(10)	26.3(14)
C(8)'	-C(9)	-C(10)	-O(1)	-165.0(10)
C(8)'	-C(9)	-C(10)	-O(2)	12.2(10)
C(8)"	-C(9)	-C(10)	-O(1)	160.5(12)
C(8)"	-C(9)	-C(10)	-O(2)	-22.3(13)
C(9)	-C(10)	-O(2)	-C(7)	3.2(9)
O(1)	-C(10)	-O(2)	-C(7)	-179.3(7)
C(2)	-C(1)	-C(6)	-H(6)	175(5)
C(7)	-C(1)	-C(6)	-H(6)	-5(5)
C(2)	-C(1)	-C(7)	-H(7)	41(4)
C(6)	-C(1)	-C(7)	-H(7)	-139(4)
C(1)	-C(2)	-C(21)	-H1(21)	6(5)

Table XXXVIII (continued)

C(1)	-C(2)	-C(21)	-H2(21)	119(5)
C(1)	-C(2)	-C(21)	-H3(21)	-102(7)
C(3)	-C(2)	-C(21)	-H1(21)	-173(5)
C(3)	-C(2)	-C(21)	-H2(21)	-60(5)
C(3)	-C(2)	-C(21)	-H3(21)	78(7)
C(2)	-C(3)	-C(31)	-H1(31)	-53(5)
C(2)	-C(3)	-C(31)	-H2(31)	179(7)
C(2)	-C(3)	-C(31)	-H3(31)	74(4)
C(4)	-C(3)	-C(31)	-H1(31)	125(5)
C(4)	-C(3)	-C(31)	-H2(31)	-2(7)
C(4)	-C(3)	-C(31)	-H3(31)	-107(4)
C(2)	-C(3)	-C(4)	-H(4)	-179(4)
C(31)	-C(3)	-C(4)	-H(4)	2(4)
C(3)	-C(4)	-C(5)	-H(5)	178(5)
H(4)	-C(4)	-C(5)	-C(6)	180(4)
H(4)	-C(4)	-C(5)	-H(5)	-5(6)
C(4)	-C(5)	-C(6)	-H(6)	-176(5)
H(5)	-C(5)	-C(6)	-C(1)	-178(5)
H(5)	-C(5)	-C(6)	-H(6)	9(7)
C(1)	-C(7)	-C(8)'	-H1(8)'	161(6)
C(1)	-C(7)	-C(8)'	-H2(8)'	19(4)
C(8)"	-C(7)	-C(8)'	-H1(8)'	-156(6)
C(8)"	-C(7)	-C(8)'	-H2(8)'	61(4)
O(2)	-C(7)	-C(8)'	-H1(8)'	-71(6)
O(2)	-C(7)	-C(8)'	-H2(8)'	147(4)
H(7)	-C(7)	-C(8)'	-C(9)	138(4)
H(7)	-C(7)	-C(8)'	-H1(8)'	44(7)
H(7)	-C(7)	-C(8)'	-H2(8)'	-98(6)
C(1)	-C(7)	-C(8)"	-H1(8)"	-46(7)
C(1)	-C(7)	-C(8)"	-H2(8)"	104(12)
C(8)'	-C(7)	-C(8)"	-H1(8)"	169(8)
C(8)'	-C(7)	-C(8)"	-H2(8)"	-41(12)
O(2)	-C(7)	-C(8)"	-H1(8)"	68(7)
O(2)	-C(7)	-C(8)"	-H2(8)"	-142(12)
H(7)	-C(7)	-C(8)"	-C(9)	105(6)
H(7)	-C(7)	-C(8)"	-H1(8)"	-164(9)
H(7)	-C(7)	-C(8)"	-H2(8)"	-13(13)
H(7)	-C(7)	-O(2)	-C(10)	-131(5)
C(7)	-C(8)'	-C(9)	-H1(9)	102.2(11)
C(7)	-C(8)'	-C(9)	-H2(9)	-136.8(11)
H1(8)'	-C(8)'	-C(9)	-C(8)"	-155(5)
H1(8)'	-C(8)'	-C(9)	-C(10)	96(5)
H1(8)'	-C(8)'	-C(9)	-H1(9)	-140(5)
H1(8)'	-C(8)'	-C(9)	-H2(9)	-19(5)
H2(8)'	-C(8)'	-C(9)	-C(8)"	-31(4)
H2(8)'	-C(8)'	-C(9)	-C(10)	-139(4)
H2(8)'	-C(8)'	-C(9)	-H1(9)	-15(5)
H2(8)'	-C(8)'	-C(9)	-H2(9)	106(4)
C(7)	-C(8)"	-C(9)	-H1(9)	136.7(10)
C(7)	-C(8)"	-C(9)	-H2(9)	-110.8(10)
H1(8)"	-C(8)"	-C(9)	-C(8)'	-174(7)

Table XXXVIII (continued)

H1(8)"-C(8)"	-C(9)	-C(10)		-91(6)
H1(8)"-C(8)"	-C(9)	-H1(9)		20(6)
H1(8)"-C(8)"	-C(9)	-H2(9)		132(6)
H2(8)"-C(8)"	-C(9)	-C(8)'		-20(9)
H2(8)"-C(8)"	-C(9)	-C(10)		63(10)
H2(8)"-C(8)"	-C(9)	-H1(9)		173(10)
H2(8)"-C(8)"	-C(9)	-H2(9)		-74(10)
H1(9) -C(9)	-C(10)	-O(1)		65.1(10)
H1(9) -C(9)	-C(10)	-O(2)		-117.7(7)
H2(9) -C(9)	-C(10)	-O(1)		-56.7(11)
H2(9) -C(9)	-C(10)	-O(2)		120.5(7)

C(5) deviate from the mean plane calculated through all six ring carbons by 0.015 and -0.017 Å, respectively. Intra-annular torsion angles range from -3.0(9) to 3.6(10), Table XXXVIII. Slight differences in bond lengths and angles compared to benzene (53) reflect the electronic distribution within the ring.

CHAPTER VII

1,3,4,5,6,9-HEXAMETHYL-8-EXO-METHYLENETRICYCLO[4.4.0.$0^{3,9}$]DEC-4-ENE-2-ONE

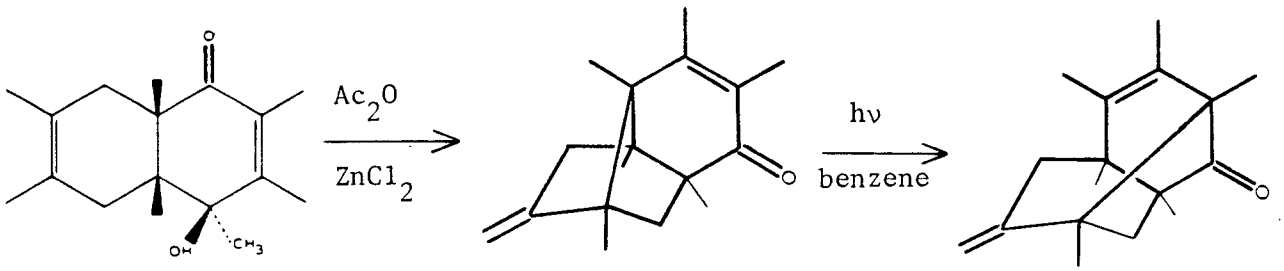
Introduction

Attempts to acetylate the heptamethyl-4β-ol (VIII) led to the formation of the exo-methylene ketone (IX) rather than the acetate. Replacing OH with OAc would have removed the facility for hydrogen bonding via the hydroxyl group hence, the reactivity in the absence of H-bonding could have been studied. However, with the production of the methylene ketone, interest was diverted to its photochemistry. The following crystal structure analysis showed that a 1,3-shift resulted from the photolysis of (IX) in solution leading to the isomeric exo-methylene ketone (X).

Experimental

Figure 24 shows the reaction scheme for the generation of the title compound from 2,3,4α,4aβ,6,7,8aβ-heptamethyl-4aβ,5,8,8aβ-tetrahydronaphthoquin-4β-ol (VIII) via the intermediate 1,3,6,7,8,9-hexamethyl-4-exo-methylenetricyclo [4.4.0.$0^{3,7}$]dec-7-ene-10-one, (IX). Recrystallization of methylene ketone (X) from a hexane/acetone solution yielded translucent crystals whose faces appeared related by a two-fold rotation axis parallel to the long axis of the crystals.

Crystal data: $C_{17}H_{24}O$, MW = 244.36, monoclinic $\underline{a}$ = 12.374(2), $\underline{b}$ = 8.771(1), $\underline{c}$ = 13.743(2) Å, β = 104.027(6)°, $\underline{V}$ = 1446.9(3) Å^3, $\underline{Z}$ = 4, $\underline{D}_{\underline{c}}$ = 1.122 g cm^{-3}, μ(MoKα) = 0.626 cm^{-1}, λ = 0.71073 Å, space group $\underline{P}2_1/\underline{a}$, from systematic absences and structure analysis.



(VIII) (IX) (X)

Figure 24

Reaction scheme showing the production of the methylene ketone (X).

Data were collected with a crystal measuring 0.3 x 0.2 x 0.3 mm^3 using graphite monochromatized MoKα radiation. An ω-2(5/6)θ scan was employed in collecting 3297 unique reflections between 0.0 and 27.5°. Omega scan widths varied according to the expression $(0.65 + 0.35\tan\theta)^{\circ}$ and were extended 25% on each side for background measurement. Horizontal aperture settings were varied with theta, the width being given by $(2.00 + \tan\theta)$ mm; and the vertical aperture remained constant at 4 mm. Scan speeds ranged from 0.91 to 10.06 deg min^{-1}, the former limit corresponding to 75 s scans.

Data processing, which included application of Lorentz and polarization corrections, indicated that 41.5% (1369 reflections) of the total reflections measured (3297) were classified as observed having $I \geq 3\sigma(I)$, where $\sigma^2(I) = (S + 2B + (0.06(S - B))^2$, S = scan count, B = time-averaged background.

Solution and Refinement

The processed data revealed that reflections of the types $\underline{h}0\underline{l}$, $\underline{h} = 2\underline{n} + 1$ and $0\underline{k}0$, $\underline{k} = 2\underline{n} + 1$ were classified as unobserved thereby suggesting the space group $\underline{P}2_1/\underline{a}$. The intensity statistics compared favorably with the theoretical centric distribution – consistent with the centrosymmetric space group suggested. The structure was solved by direct methods employed in MULTAN using 272 of the largest E-values to generate 2448 phase relationships. No phases indicated by the Σ_1-relationships had a probability of greater than 0.90, which was less than the minimum value of 0.95 for acceptance. The three origin fixing reflections, chosen to fit the criteria for origin specification, were assigned initial phases of 0. Four other reflections which were involved in many Σ_2-relationships were given starting values of 0, but were permuted with 0 and π to yield 16 sets of phases (total phase sets = n^p, where n = number of starting phases and p = number of possible starting values for these phases). The set of phases with the highest degree of internal consistency (calculated as a figure of merit) was the correct set which, when used in conjunction with the E's in calculating a Fourier synthesis, resulted in an electron density map on which the positions of the 18 non-hydrogen atoms were located.

Refinement was initiated in the space group $\underline{P}2_1/\underline{a}$ (later confirmed to be the correct space group assignment) with 16 carbon atoms and 2 oxygen atoms assuming isotropic temperature factors. Subsequent cycles with these atoms and anisotropic

thermal parameters were followed by difference syntheses which revealed the positions of the 24 hydrogens. Convergence was reached after several cycles of refinement which included all atoms and resulted in an R-value of 0.040, Rw = 0.040. A list of planes, where $||Fo| - k|Fc||$ divided by the error in an observation of unit weight was greater than 3.0, showed several reflections which appeared to suffer from extinction effects. An isotropic Type I (domain misorientation) extinction correction was applied assuming the mosaic spread distribution to be Gaussian. Three further refinement cycles produced the final g-value, 5.44×10^{4}, where g is the secondary extinction coefficient in the expression $|Fo|^2 = |Fc|^2 \exp(-g\gamma/2|Fc|^2)$*. The refinement, with extinction corrections, converged at R = 0.037, Rw = 0.039 with mean and maximum parameter shifts of 0.079 and 0.465σ, respectively on the final cycle which had 260 variables fitted to the 1369 data having $I \geq 3\sigma(I)$. For all data R = 0.132 and Rw = 0.075. Reflections were assigned weights, $w = 1/\sigma^2(F)$ where $\sigma^2(F)$ is derived from the $\sigma^2(I)$ defined above. The standard error in an observation of unit weight was 0.7371. Following convergence a difference-synthesis showed random fluctuations up to $0.15 e/Å^3$. A list of atomic coordinates and temperature factors is presented in Table XXXIX and anisotropic thermal parameters for non-hydrogen atoms are given in Table XL.

$$^{*}\gamma = \left(\frac{1+\cos^4 2\theta}{1+\cos^2 2\theta}\right)\left(\frac{\overline{T}}{\sin 2\theta}\right)\left(\frac{\lambda^3}{V^2}\right) \times \frac{-2}{12.593}$$

where V is the volume and $\overline{T}$ is the mean transmission path length

Table XXXIX

Final positional (fractional x 10^5, H x 10^3)

and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)

with estimated standard deviations in parentheses

Atom	x	y	z	Ueq/Uiso
C(1)	55042(23)	13913(33)	65380(19)	45
C(2)	60655(21)	-160(32)	70552(19)	42
C(21)	53993(39)	-14597(49)	66836(35)	71
C(3)	60690(21)	4181(33)	81383(19)	45
C(31)	56373(40)	-7121(57)	87757(31)	76
C(4)	64132(22)	18184(35)	84397(20)	46
C(41)	64072(42)	24161(63)	94693(28)	78
C(4a)	69955(23)	27705(32)	77830(20)	51
C(4a1)	70615(53)	44767(46)	80587(38)	88
C(5)	81862(25)	21046(40)	80195(26)	59
C(6)	81535(21)	4419(36)	77570(20)	49
C(61)	88274(32)	-5574(61)	83079(31)	79
C(7)	72670(21)	625(32)	68131(19)	44
C(71)	75583(38)	-13489(49)	62815(31)	73
C(8)	71454(27)	14881(37)	61453(23)	51
C(8a)	64186(24)	25406(33)	66145(20)	48
C(8a1)	60276(53)	39753(49)	60040(36)	85
O	45341(16)	15105(25)	60954(15)	70
H1(21)	534(3)	-157(3)	598(3)	84(12)
H2(21)	576(3)	-241(5)	706(3)	101(14)
H3(21)	465(3)	-131(4)	675(3)	97(14)
H1(31)	584(3)	-40(5)	948(3)	118(14)
H2(31)	485(4)	-83(4)	856(3)	115(15)
H3(31)	599(4)	-176(6)	873(4)	162(22)
H1(41)	598(4)	181(5)	983(3)	143(20)
H2(41)	711(3)	250(4)	984(3)	96(14)
H3(41)	614(4)	352(6)	939(4)	161(22)
H1(4a1)	750(3)	496(5)	765(3)	118(17)
H2(4a1)	625(4)	503(5)	800(3)	124(16)
H3(4a1)	747(3)	461(4)	875(3)	88(11)
H1(5)	853(2)	229(3)	876(2)	58(8)
H2(5)	863(2)	267(3)	762(2)	71(9)
H1(61)	936(3)	-24(3)	893(2)	79(10)
H2(61)	876(3)	-160(4)	812(2)	77(12)
H1(71)	828(3)	-112(4)	615(3)	108(15)
H2(71)	700(3)	-151(3)	560(3)	84(11)
H3(71)	759(3)	-235(4)	669(3)	100(13)
H1(8)	673(2)	122(3)	542(2)	57(8)
H2(8)	786(3)	193(3)	610(2)	76(10)
H1(8a1)	562(3)	368(4)	533(3)	98(13)
H2(8a1)	668(3)	462(5)	598(3)	114(17)
H3(8a1)	550(3)	452(4)	633(3)	92(14)

Table XL

Final anisotropic thermal parameters ($\underline{U}ij \times 10^4$ Å^2) and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
C(1)	389(16)	604(20)	354(15)	73(16)	103(13)	-36(14)
C(2)	385(14)	440(16)	430(15)	-40(14)	104(11)	-15(14)
C(21)	781(29)	643(27)	709(28)	-228(23)	166(22)	-119(22)
C(3)	359(15)	569(21)	428(16)	-11(14)	129(12)	43(15)
C(31)	743(28)	982(34)	593(25)	-219(26)	254(21)	127(23)
C(4)	436(16)	577(20)	370(15)	43(15)	83(12)	-16(14)
C(41)	859(30)	989(36)	468(20)	-15(28)	142(21)	-157(23)
C(4a)	570(19)	418(18)	513(17)	-46(15)	62(14)	-27(15)
C(4a1)	1287(43)	519(25)	755(30)	-130(27)	81(30)	-123(21)
C(5)	462(19)	768(27)	511(20)	-172(18)	57(15)	47(19)
C(6)	323(15)	692(23)	487(17)	57(15)	141(13)	106(16)
C(61)	631(24)	1009(37)	676(25)	210(25)	58(19)	112(26)
C(7)	414(15)	490(18)	424(15)	72(14)	139(12)	24(15)
C(71)	771(28)	755(29)	690(26)	265(24)	235(22)	-51(23)
C(8)	452(17)	657(22)	440(18)	-27(17)	150(14)	67(16)
C(8a)	573(18)	428(17)	435(16)	52(15)	85(14)	92(14)
C(8a1)	1186(40)	590(26)	681(27)	147(29)	60(28)	156(22)
O	399(13)	1040(19)	605(14)	167(12)	9(10)	-71(12)

Discussion

The structure consists of molecules composed of a twisted half-chair cyclohexenone ring cis-fused to a twisted boat cyclohexane moiety. In addition to the bridging bond C(4a)-C(8a)[1], the two six-membered rings are joined via atoms C(2) and C(7) forming a five-membered ring with atoms C(1), C(8a) and C(8) (see Figure 25, page 171). The molecule is highly strained, as evidenced by marked deviations from the expected values of angles associated with atoms of given hybridizations (Tables XLI and XLII). The endocyclic angles of the five-membered ring which includes a formally sp^2-hybridized carbon atom, range from 94° to 105°; the experimental value for the angles of unsubstituted cyclopentane is 111.7° (54) and for planar aromatic cyclopentadienyl is 108°. Further angular strain is noticeable in those angles containing methyl groups. Each methyl substituent is eclipsed with at least one other methyl group on an adjacent carbon. Except for C(31)-C(3)-C(2)-C(21) (11.5(3)°) and C(41)-C(4)-C(4a)-C(4a1) (-24.4(4)°), H_3C-C-C-CH_3 torsion angles range from -1.2(3) to -2.9(4) (Table XLIII). The steric repulsion of the eclipsed substituents results in widening the H_3C-C-C angles by as much as 7.4° in the case of C(8a1)-C(8a)-C(4a); the combined effect at the bridgeheads is a net increase of 8.5°.

The overall stress in the molecule is alleviated somewhat by the lengthening of the bridging bonds C(4a)-C(8a) and C(2)-

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[1] Note, atom labels refer to the same system used in naming the naphthoquinol progenitor (VIII).

Table XLI

Bond angles (°) with estimated standard deviations in parentheses; expected values are enclosed in brackets

$C(sp^3)-C(sp^3)-C(sp^3)$	[109.5]
C(21) -C(2) -C(7)	114.7(3)
C(4a1)-C(4a) -C(5)	108.9(3)
C(4a1)-C(4a) -C(8a)	110.6(3)
C(5) -C(4a) -C(8a)	109.5(2)
C(2) -C(7) -C(71)	113.8(3)
C(2) -C(7) -C(8)	101.4(2)
C(71) -C(7) -C(8)	112.0(3)
C(7) -C(8) -C(8a)	102.8(2)
C(4a) -C(8a) -C(8)	109.4(2)
C(4a) -C(8a) -C(8a1)	116.9(3)
C(8) -C(8a) -C(8a1)	113.9(3)
$C(sp^3)-C(sp^3)-C(sp^2)$	[109.5]
C(21) -C(2) -C(1)	111.8(3)
C(21) -C(2) -C(3)	113.8(3)
C(7) -C(2) -C(1)	102.2(2)
C(7) -C(2) -C(3)	114.0(2)
C(4a1)-C(4a) -C(4)	112.9(3)
C(5) -C(4a) -C(4)	103.3(2)
C(8a) -C(4a) -C(4)	111.3(2)
C(4a) -C(5) -C(6)	110.4(2)
C(2) -C(7) -C(6)	110.3(2)
C(71) -C(7) -C(6)	112.4(3)
C(8) -C(7) -C(6)	106.1(2)
C(4a) -C(8a) -C(1)	107.4(2)
C(8) -C(8a) -C(1)	94.3(2)
C(8a1)-C(8a) -C(1)	112.5(3)
$C(sp^2)-C(sp^3)-C(sp^2)$	[109.5]
C(1) -C(2) -C(3)	98.4(2)

Table XLI (continued)

$X(sp^2)$-$C(sp^2)$-$C(sp^3)$			[120.0]
O	-C(1)	-C(2)	126.5(3)
O	-C(1)	-C(8a)	128.0(3)
C(2)	-C(1)	-C(8a)	105.3(2)
C(4)	-C(3)	-C(2)	117.1(2)
C(4)	-C(3)	-C(31)	123.9(3)
C(3)	-C(4)	-C(41)	122.5(3)
C(3)	-C(4)	-C(4a)	118.7(2)

$C(sp^3)$-$C(sp^2)$-$C(sp^3)$			[120.0]
C(2)	-C(1)	-C(8a)	105.3(2)
C(2)	-C(3)	-C(31)	118.9(3)
C(41)	-C(4)	-C(4a)	118.2(3)
C(5)	-C(6)	-C(61)	122.2(3)
C(5)	-C(6)	-C(7)	113.0(2)
C(61)	-C(6)	-C(7)	124.8(3)

Table XLII

Bond angles (deg) involving hydrogen atoms with estimated standard deviations in parentheses

Bonds	Angle
C(2) -C(21) -H1(21)	109(2)
C(2) -C(21) -H2(21)	112(2)
C(2) -C(21) -H3(21)	108(2)
H1(21)-C(21) -H2(21)	110(3)
H1(21)-C(21) -H3(21)	105(3)
H2(21)-C(21) -H3(21)	112(3)
C(3) -C(31) -H1(31)	110(2)
C(3) -C(31) -H2(31)	111(2)
C(3) -C(31) -H3(31)	110(3)
H1(31)-C(31) -H2(31)	110(3)
H1(31)-C(31) -H3(31)	108(4)
H2(31)-C(31) -H3(31)	108(4)
C(4) -C(41) -H1(41)	115(3)
C(4) -C(41) -H2(41)	110(2)
C(4) -C(41) -H3(41)	108(3)
H1(41)-C(41) -H2(41)	109(3)
H1(41)-C(41) -H3(41)	112(4)
H2(41)-C(41) -H3(41)	103(3)
C(4a) -C(4a1)-H1(4a1)	106(2)
C(4a) -C(4a1)-H2(4a1)	115(2)
C(4a) -C(4a1)-H3(4a1)	110(2)
H1(4a1)-C(4a1)-H2(4a1)	113(3)
H1(4a1)-C(4a1)-H3(4a1)	107(3)
H2(4a1)-C(4a1)-H3(4a1)	106(3)

Bonds	Angle
C(4a) -C(5) -H1(5)	107(2)
C(4a) -C(5) -H2(5)	109(2)
C(6) -C(5) -H1(5)	112(2)
C(6) -C(5) -H2(5)	109(2)
H1(5) -C(5) -H2(5)	109(2)
C(6) -C(61) -H1(61)	121(2)
C(6) -C(61) -H2(61)	119(2)
H1(61)-C(61) -H2(61)	120(3)
C(7) -C(71) -H1(71)	105(2)
C(7) -C(71) -H2(71)	111(2)
C(7) -C(71) -H3(71)	115(2)
H1(71)-C(71) -H2(71)	108(3)
H1(71)-C(71) -H3(71)	110(3)
H2(71)-C(71) -H3(71)	108(3)
C(7) -C(8) -H1(8)	110(2)
C(7) -C(8) -H2(8)	113(2)
H1(8) -C(8) -H2(8)	106(2)
C(8a) -C(8a1)-H1(8a1)	109(2)
C(8a) -C(8a1)-H2(8a1)	110(2)
C(8a) -C(8a1)-H3(8a1)	107(2)
H1(8a1)-C(8a1)-H2(8a1)	111(3)
H1(8a1)-C(8a1)-H3(8a1)	108(3)
H2(8a1)-C(8a1)-H3(8a1)	112(3)

Table XLIII

Torsion angles (deg) with estimated standard deviations in parentheses

Atoms				Value
C(8a)	-C(1)	-C(2)	-C(21)	-156.0(3)
C(8a)	-C(1)	-C(2)	-C(3)	84.1(2)
O	-C(1)	-C(2)	-C(21)	19.2(4)
O	-C(1)	-C(2)	-C(3)	-100.7(3)
C(2)	-C(1)	-C(8a)	-C(4a)	-57.8(3)
C(2)	-C(1)	-C(8a)	-C(8a1)	172.2(3)
O	-C(1)	-C(8a)	-C(4a)	127.1(3)
O	-C(1)	-C(8a)	-C(8a1)	-2.9(4)
C(1)	-C(2)	-C(3)	-C(31)	129.9(3)
C(1)	-C(2)	-C(3)	-C(4)	-47.1(3)
C(21)	-C(2)	-C(3)	-C(31)	11.5(4)
C(21)	-C(2)	-C(3)	-C(4)	-165.5(3)
C(2)	-C(3)	-C(4)	-C(41)	177.1(3)
C(2)	-C(3)	-C(4)	-C(4a)	-12.2(3)
C(31)	-C(3)	-C(4)	-C(41)	0.2(5)
C(31)	-C(3)	-C(4)	-C(4a)	170.9(3)
C(3)	-C(4)	-C(4a)	-C(4a1)	164.5(3)
C(3)	-C(4)	-C(4a)	-C(5)	-78.0(3)
C(3)	-C(4)	-C(4a)	-C(8a)	39.4(3)
C(41)	-C(4)	-C(4a)	-C(4a1)	-24.4(4)
C(41)	-C(4)	-C(4a)	-C(5)	93.1(3)
C(41)	-C(4)	-C(4a)	-C(8a)	-149.5(3)
C(4)	-C(4a)	-C(5)	-C(6)	59.9(3)
C(4a1)	-C(4a)	-C(5)	-C(6)	-179.8(3)
C(8a)	-C(4a)	-C(5)	-C(6)	-58.7(3)
C(4)	-C(4a)	-C(8a)	-C(1)	-2.4(3)
C(4)	-C(4a)	-C(8a)	-C(8a1)	125.1(4)
C(4a1)	-C(4a)	-C(8a)	-C(1)	-128.7(3)
C(4a1)	-C(4a)	-C(8a)	-C(8a1)	-1.2(5)
C(5)	-C(4a)	-C(8a)	-C(1)	111.2(3)
C(5)	-C(4a)	-C(8a)	-C(8a1)	-121.3(4)
C(4a)	-C(5)	-C(6)	-C(61)	-142.2(3)
C(4a)	-C(5)	-C(6)	-C(7)	37.2(3)
C(5)	-C(6)	-C(7)	-C(71)	153.2(3)
C(5)	-C(6)	-C(7)	-C(8)	30.5(3)
C(61)	-C(6)	-C(7)	-C(71)	-27.4(4)
C(61)	-C(6)	-C(7)	-C(8)	-150.1(3)
C(1)	-C(2)	-C(21)	-H1(21)	61(2)
C(1)	-C(2)	-C(21)	-H2(21)	-177(2)
C(1)	-C(2)	-C(21)	-H3(21)	-53(2)
C(3)	-C(2)	-C(21)	-H1(21)	171(2)
C(3)	-C(2)	-C(21)	-H2(21)	-67(2)
C(3)	-C(2)	-C(21)	-H3(21)	57(2)
C(2)	-C(3)	-C(31)	-H1(31)	167(2)

Table XLIII (continued)

C(2)	-C(3)	-C(31)	-H2(31)	-71(3)
C(2)	-C(3)	-C(31)	-H3(31)	49(3)
C(4)	-C(3)	-C(31)	-H1(31)	-16(3)
C(4)	-C(3)	-C(31)	-H2(31)	106(3)
C(4)	-C(3)	-C(31)	-H3(31)	-135(3)
C(3)	-C(4)	-C(41)	-H1(41)	-14(3)
C(3)	-C(4)	-C(41)	-H2(41)	109(3)
C(3)	-C(4)	-C(41)	-H3(41)	-139(3)
C(4a)	-C(4)	-C(41)	-H1(41)	176(3)
C(4a)	-C(4)	-C(41)	-H2(41)	-62(3)
C(4a)	-C(4)	-C(41)	-H3(41)	50(3)
C(4)	-C(4a)	-C(4a1)	-H1(4a1)	175(3)
C(4)	-C(4a)	-C(4a1)	-H2(4a1)	-60(2)
C(4)	-C(4a)	-C(4a1)	-H3(4a1)	60(2)
C(5)	-C(4a)	-C(4a1)	-H1(4a1)	61(3)
C(5)	-C(4a)	-C(4a1)	-H2(4a1)	-174(2)
C(5)	-C(4a)	-C(4a1)	-H3(4a1)	-54(2)
C(8a)	-C(4a)	-C(4a1)	-H1(4a1)	-60(3)
C(8a)	-C(4a)	-C(4a1)	-H2(4a1)	66(2)
C(8a)	-C(4a)	-C(4a1)	-H3(4a1)	-175(2)
C(4)	-C(4a)	-C(5)	-H1(5)	-63(2)
C(4)	-C(4a)	-C(5)	-H2(5)	-180(2)
C(4a1)	-C(4a)	-C(5)	-H1(5)	58(2)
C(4a1)	-C(4a)	-C(5)	-H2(5)	-60(2)
C(8a)	-C(4a)	-C(5)	-H1(5)	179(2)
C(8a)	-C(4a)	-C(5)	-H2(5)	61(2)
H1(5)	-C(5)	-C(6)	-C(61)	-23(2)
H1(5)	-C(5)	-C(6)	-C(7)	157(2)
H2(5)	-C(5)	-C(6)	-C(61)	98(2)
H2(5)	-C(5)	-C(6)	-C(7)	-83(2)
C(5)	-C(6)	-C(61)	-H1(61)	3(2)
C(5)	-C(6)	-C(61)	-H2(61)	178(2)
C(7)	-C(6)	-C(61)	-H1(61)	-177(2)
C(7)	-C(6)	-C(61)	-H2(61)	-1(2)
C(6)	-C(7)	-C(71)	-H1(71)	-57(2)
C(6)	-C(7)	-C(71)	-H2(71)	-173(2)
C(6)	-C(7)	-C(71)	-H3(71)	65(2)
C(8)	-C(7)	-C(71)	-H1(71)	63(2)
C(8)	-C(7)	-C(71)	-H2(71)	-53(2)
C(8)	-C(7)	-C(71)	-H3(71)	-176(2)
C(6)	-C(7)	-C(8)	-H1(8)	164.3(15)
C(6)	-C(7)	-C(8)	-H2(8)	45(2)
C(71)	-C(7)	-C(8)	-H1(8)	41(2)
C(71)	-C(7)	-C(8)	-H2(8)	-78(2)
C(1)	-C(8a)	-C(8a1)	-H1(8a1)	-48(2)
C(1)	-C(8a)	-C(8a1)	-H2(8a1)	-170(2)
C(1)	-C(8a)	-C(8a1)	-H3(8a1)	68(2)
C(4a)	-C(8a)	-C(8a1)	-H1(8a1)	-173(2)
C(4a)	-C(8a)	-C(8a1)	-H2(8a1)	65(3)
C(4a)	-C(8a)	-C(8a1)	-H3(8a1)	-57(2)

C(7) to distances of 1.604(4) and 1.602(4) Å, respectively (Table XLIV). This increase in length of approximately 0.07 Å over accepted values (33) for $C(sp^3)$-$C(sp^3)$ bonds is not enough to eliminate the repulsive effect of the eclipsed methyls (vide supra).

The strain induced in the cyclohexenone ring on bonding C(2) to C(7) is compensated somewhat by the stretching of the bridge C(4a)-C(8a); in addition, bonds C(2)-C(3) and C(4a)-C(4) show increases as well, averaging 0.024 Å greater than the accepted value of 1.510 Å for $C(sp^3)$-$C(sp^2)$. Other bonds within the structure (Table XLV) do not deviate significantly from accepted values. Intermolecular contacts generally correspond to van der Waals distances.

The photochemical reaction, illustrated in Figure 24, involves a shift in the secondary bridge from C(4)-C(7) to C(2)-C(7). The reactant energy, relative to the product, is not easily deduced from this study, but Dreiding models of both molecules suggest that (IX) is the higher energy isomer manifesting two very strained five-membered rings as opposed to only one of these rings in (X). It is interesting to note that molecular mechanics calculations (47) on the unsaturated, unsubstituted tricyclo analogs of (IX) and (X) indicate strains of 23.59 and 30.90 kcal/mole, respectively. The effect of adding substituents and sp^2-hybridized ring members is likely to increase the energy of both molecules but even the relative magnitudes of the increases would be difficult to predict. However, a less than rigorous comparison of conformations tends to confirm the molecular mechanics indication of (X) as the

Table XLIV

Bond lengths (Å) with standard deviations in parentheses; accepted values[2] are enclosed in brackets

Bond	Length
$C(sp^3)-C(sp^3)$	[1.537(5)]
C(2) -C(21)	1.530(4)
C(2) -C(7)	1.602(4)
C(4a) -C(4a1)	1.541(5)
C(4a) -C(5)	1.544(4)
C(4a) -C(8a)	1.604(4)
C(7) -C(71)	1.524(5)
C(7) -C(8)	1.537(4)
C(8) -C(8a)	1.536(6)
C(8a) -C(8a1)	1.525(5)
$C(sp^3)-C(sp^2)$	[1.510(5)]
C(2) -C(1)	1.507(4)
C(8a) -C(1)	1.500(4)
C(2) -C(3)	1.535(4)
C(31) -C(3)	1.504(4)
C(41) -C(4)	1.511(4)
C(4a) -C(4)	1.532(4)
C(5) -C(6)	1.500(5)
C(7) -C(6)	1.519(4)
$C(sp^2)-C(sp^2)$	[1.335(5)]
C(3) -C(4)	1.333(4)
C(6) -C(61)	1.316(6)
$C(sp^2)-O$	[1.215(5)]
C(1) -O	1.212(3)

[2] From reference 33.

Table XLV

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

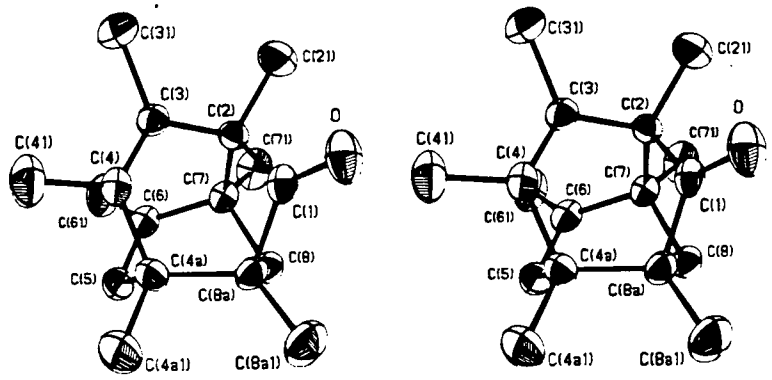
Bond	Length	Bond	Length
C(21) -H1(21)	0.95(4)	C(5) -H1(5)	1.01(3)
C(21) -H2(21)	1.03(4)	C(5) -H2(5)	1.00(3)
C(21) -H3(21)	0.97(4)	C(61) -H1(61)	0.99(3)
C(31) -H1(31)	0.97(4)	C(61) -H2(61)	0.95(3)
C(31) -H2(31)	0.95(4)	C(71) -H1(71)	0.98(4)
C(31) -H3(31)	1.02(5)	C(71) -H2(71)	1.04(4)
C(41) -H1(41)	0.97(5)	C(71) -H3(71)	1.04(4)
C(41) -H2(41)	0.90(3)	C(8) -H1(8)	1.03(3)
C(41) -H3(41)	1.02(5)	C(8) -H2(8)	0.98(3)
C(4a1)-H1(4a1)	0.97(4)	C(8a1)-H1(8a1)	0.97(4)
C(4a1)-H2(4a1)	1.10(4)	C(8a1)-H2(8a1)	0.99(4)
C(4a1)-H3(4a1)	0.98(3)	C(8a1)-H3(8a1)	1.00(4)

higher energy isomer:

	(IX)	kcal	(X)
1) conformation of the six-membered rings	i) boat	2 >	twisted boat
	ii) half-chair	3 >	twisted half-chair
2) stereochemistry of substituents	all are at relatively least energy positions	< 10	two pairs of methyls are eclipsed; axial hydrogens on C(5) and C(8) are in close proximity

The indication is that from molecular strain and steric arguments alone, (X) is approximately 5 kcal higher in energy than its precursor (IX). This is in contrast to the Dreiding model suggestion. Although such models nicely illustrate torsional and angular strain, they are less effective in showing steric effects.

Stereo diagrams of the molecule and the unit cell contents are displayed in Figure 25.



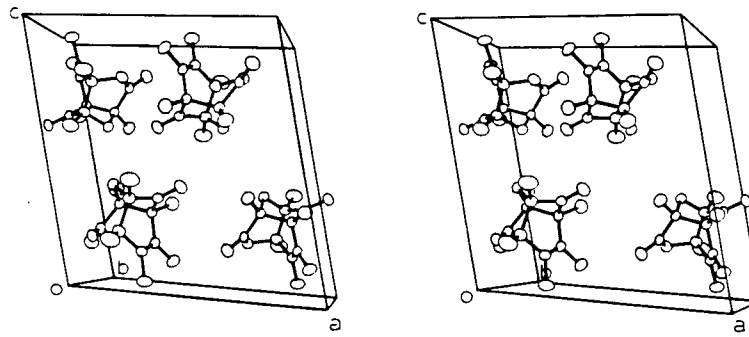


Figure 25

Stereo view of the methylene-ketone molecule, (X) (top) and the contents of the unit cell (bottom).

CHAPTER VIII

1,2,3,5,6,8-HEXAMETHYL-4-MESYL-7-HYDROXY-TETRACYCLO[4.2.1.1^{2,5}.0^{3,7}]DECANE

Introduction

Not unlike the other structures presented in this part of the thesis, the present compound was produced as an unexpected result (55). An intramolecular pinacolization of a symmetrical diketone cage compound was attempted, but instead of forming the symmetric pinacol, the reaction produced a ketol. Efforts to obtain crystals of the ketol met with little success. However, a hydroxy mesylate derivative afforded crystals of sufficiently good quality to be employed in a crystal structure analysis. The analysis was carried out in an effort to confirm the structure of the ketol, and on the basis of its structure a mechanism for its formation from the diketone was suggested (55).

Experimental

Photolysis of the hexamethyl-4α-ol (XI) (Fig. 26) in solution yielded the cage compound (XII), which upon oxidation by pyridinium chlorochromate led to the diketone (XIII). Subsequent treatment of (XIII) with zinc amalgam and HCl at reflux resulted in the formation of the hydroxy ketone (XIV). Reduction of (XIV) with sodium borohydride gave the two intermediate diols, (XV) and (XVI), of which the minor product (XV) was reacted with methane sulfonyl chloride to yield the hydroxy mesylate (XVII). After several attempts at recrystallization of (XVII), a crystal of fair quality was obtained from a hexane/acetone solution. This crystal measured 0.45 x 0.43 x 1.03 mm^3 and was not cut to a smaller size for fear of shattering it. Preliminary Weissenberg and precession

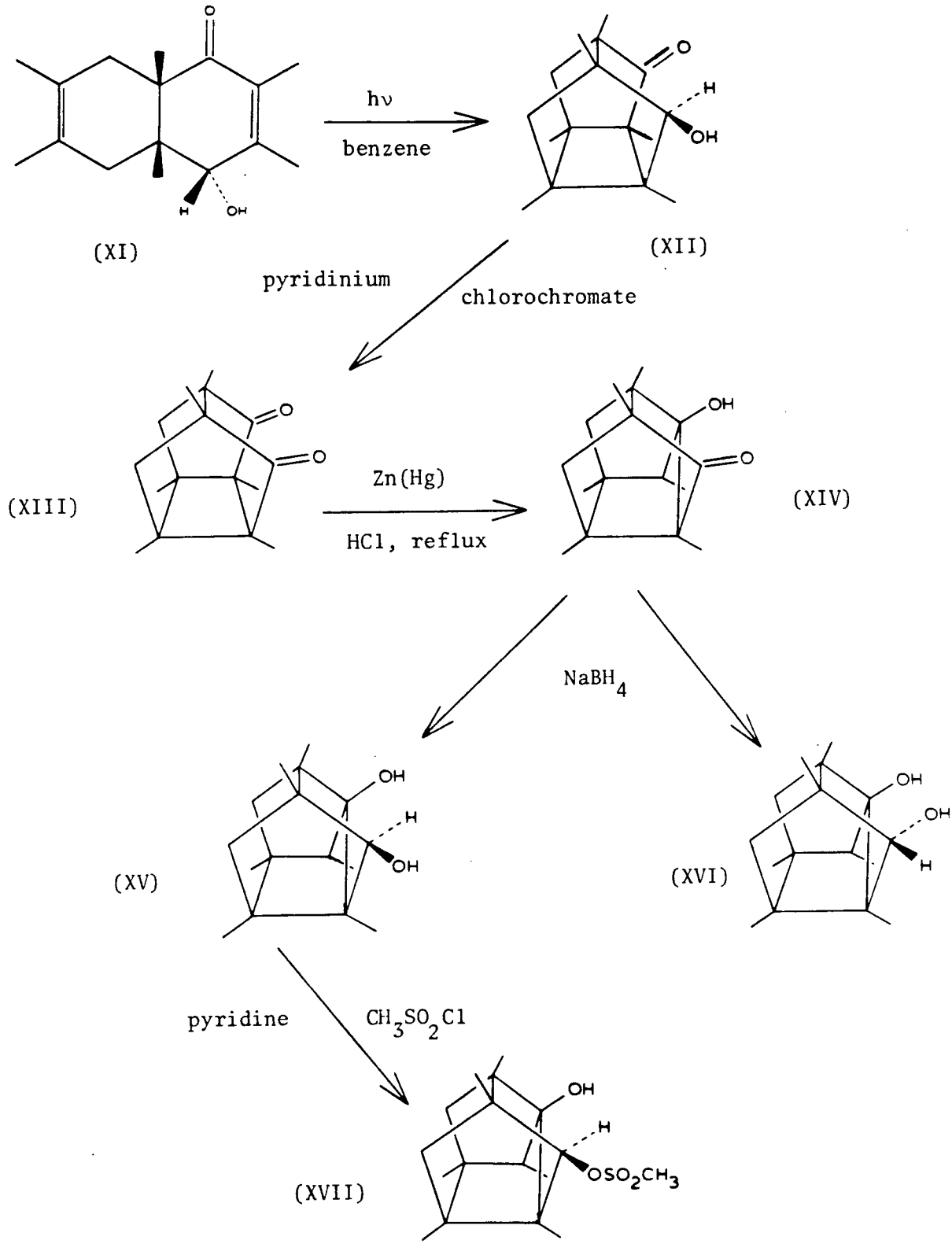


Figure 26

Reaction scheme showing the development of the title compound (XVII).

photographs indicated monoclinic symmetry 2/m and absence conditions 0$\underline{k}$0, $\underline{k}$ = 2$\underline{n}$ + 1, h0$\underline{l}$, $\underline{l}$ = 2$\underline{n}$ + 1, uniquely defining the space group $\underline{P}2_1/\underline{c}$.

Crystal data: $C_{17}H_{28}O_4S$, MW = 328.48, monoclinic $\underline{a}$ = 9.246(2), $\underline{b}$ = 10.938(1), $\underline{c}$ = 17.335(4) Å, β = 102.11(1)°, $\underline{V}$ = 1714.1(6) Å^3, $\underline{Z}$ = 4, $\underline{D}_c$ = 1.273 g cm^{-3}, μ(MoKα) = 1.944 cm^{-1}, λ = 0.71073 Å, space group $\underline{P}2_1/\underline{c}$.

Data were measured between theta limits of 0.0 and 27.5° with graphite monochromatized MoKα radiation and scan speeds ranging from 1.44 to 10.06 deg min^{-1}. ω-2(5/6)θ scans were employed with the omega scan angle calculated from (0.90 + 0.35 tanθ)°. The large mosaic spread in the crystal (inferred from the relatively large peak widths of several reflections analyzed) and the size of the crystal necessitated the use of horizontal aperture widths between 3.00 and 3.52 mm which were derived from the theta-dependent expression (3.00 + tanθ) mm. The vertical aperture was fixed at 4 mm. The setting angles of three reflections were checked after every 100 reflections collected to ensure proper crystal orientation. Three additional reflections served as intensity controls and were monitored periodically throughout data collection.

Lorentz and polarization corrections, along with an isotropic decay correction were applied during data reduction. Of the 3911 unique data measured, 2997 or 76.6% had I $\geq$ 3σ(I), where σ^2(I) is defined as S + 2B + (0.040(S - B))^2; S is the scan count and B, the time-averaged background.

Solution and Refinement

The E-statistics closely paralleled the theoretical centric distribution. The largest 188 E's ranging from 1.98 to 3.82 were used in generating 1169 Σ_2-relationships. Five phases were accepted from the Σ_1 calculations which required only that the probability of the suggested phase be greater than 0.95. In addition to the five reflections associated with these phases, three origin defining reflections and two general reflections with permutable phases made up the starting set. Of the four solutions generated by MULTAN, the outstanding solution was shown to be the correct one. A Fourier synthesis produced a readily interpretable E-map from which the coordinates of all non-hydrogen atoms were obtained.

Full matrix least squares refinement of the non-hydrogen atom coordinates and isotropic temperature factors converged rapidly. After two subsequent cycles, with anisotropic thermal parameters, a difference-Fourier synthesis indicated most of the hydrogen positions. Further refinement and difference syntheses revealed the remaining hydrogens. All hydrogen atoms were refined with isotropic temperature factors. Anomalous scattering factors were included for the sulfur atom. The $\bar{1}02$ reflection was removed from the data set in the latter stages of refinement due to the discrepancy between its observed and calculated structure factors, Fc = 259.5 and Fo = 87.5. On examination of the processed data, a warning was found beside this reflection which cautioned that the detection system experienced difficulty in measuring the intensity of the peak even with the attenuator

in place. In view of the unreliability in the measurement of intensities of this magnitude, it was considered justified to eliminate this reflection from the data set. A structure factor calculation prior to further refinement led to an R of 0.046 and Rw of 0.070 compared to R = 0.050 and Rw = 0.083 calculated before deletion of the $\bar{1}02$ reflection. Towards the end of refinement the weighting scheme was changed from $w = 1/\sigma^2(F)$ (where $\sigma^2(F)$ is derived from the $\sigma^2(I)$ defined previously) to the polynomial scheme $w = (A + BFo + CFo^2 + DFo^3)^{-1}$. This gave uniform averages of $w\Delta^2$ ($\Delta = |Fo| - k|Fc|$) over ranges of Fo. The weakest reflection in the data set, the 229 reflection (Fo = 1.5, Fc = 2.0), appeared anomalous in the weighting analysis of reflections in ranges of Fo. Rw for the 229 was 0.351 and the error associated with this plane was 1.81, the largest in the data set. Due to the apparent abnormality of this reflection, it too was removed from the data set. Upon removal, Rw was reduced significantly from 0.066 to 0.061 while R remained unchanged at 0.043. The refinement converged at R = 0.042 and Rw = 0.058. 311 parameters were varied on the final cycle in which the mean and maximum shifts were 0.218 and 0.981σ, respectively. Final values for the polynomial weighing scheme parameters were A = 0.1986, B = 0.01147, C = -0.000743 and D = 0.000075. A difference-Fourier map, calculated following convergence, indicated a peak of 0.484 $e/Å^3$, midway between S and C(1S); other peaks ranging from -0.34 to 0.36 $e/Å^3$ appeared at random positions. Atomic coordinates and anisotropic thermal parameters are listed in Tables XLVI and XLVII, respectively.

Table XLVI

Final positional (fractional x 10^5, H x 10^3)
and isotropic thermal parameters ($\underline{U}$ x 10^3 Å^2)
with estimated standard deviations in parentheses

Atom	x	y	z	Ueq/Uiso
S	83184(5)	52807(4)	89249(3)	43
O(1)	84901(14)	38764(10)	90544(8)	41
O(2)	72994(19)	55187(13)	82021(10)	64
O(3)	97730(16)	57429(14)	90274(10)	59
O(4)	50043(17)	21623(13)	74732(9)	53
C(1S)	75588(39)	57845(30)	97079(21)	73
C(1)	76462(19)	-1049(16)	83729(11)	39
C(11)	84945(30)	-12879(20)	83556(21)	65
C(2)	86229(18)	11101(15)	85669(11)	38
C(21)	101656(25)	10284(25)	83793(22)	66
C(3)	76017(18)	21744(14)	81113(9)	32
C(31)	80665(31)	28463(22)	74364(13)	55
C(4)	72686(18)	30234(15)	87511(10)	33
C(5)	71416(21)	20454(16)	93569(10)	39
C(51)	68076(40)	24510(29)	101354(15)	69
C(6)	59675(19)	11802(16)	88225(11)	37
C(61)	43891(27)	13283(26)	89295(19)	62
C(7)	61455(18)	14684(14)	79342(10)	33
C(8)	65000(21)	2214(16)	76188(11)	39
C(81)	69640(40)	1689(26)	68292(15)	65
C(9)	65705(23)	-1238(17)	89386(12)	42
C(10)	86609(22)	14523(17)	94287(11)	44
H(O4)	435(3)	173(3)	730(2)	78(9)
H1(1S)	738(4)	660(4)	962(2)	114(13)
H2(1S)	816(4)	554(3)	1022(2)	93(10)
H3(1S)	664(4)	542(3)	968(2)	87(10)
H1(11)	908(4)	-120(3)	789(2)	97(11)
H2(11)	781(3)	-195(3)	825(2)	72(8)
H3(11)	920(4)	-144(3)	887(2)	101(11)
H1(21)	1064(3)	190(3)	846(2)	83(9)
H2(21)	1005(4)	74(3)	777(2)	97(11)
H3(21)	1076(3)	46(3)	869(2)	83(10)
H1(31)	841(3)	232(3)	705(2)	94(9)
H2(31)	881(3)	341(3)	765(2)	67(7)
H3(31)	724(3)	337(3)	716(2)	81(9)
H(4)	643(2)	343(2)	856(1)	46(6)

Table XLVI (continued)

H1(51)	592(4)	296(3)	1006(2)	101(11)
H2(51)	654(3)	177(3)	1045(2)	97(10)
H3(51)	763(4)	301(4)	1043(2)	109(12)
H1(61)	411(3)	219(3)	889(2)	69(8)
H2(61)	370(3)	80(3)	855(2)	83(9)
H3(61)	427(3)	107(3)	948(2)	87(9)
H(8)	569(2)	-32(2)	758(1)	42(6)
H1(81)	788(3)	42(3)	684(2)	64(8)
H2(81)	693(3)	-69(3)	665(2)	85(9)
H3(81)	630(4)	67(4)	644(2)	111(12)
H1(9)	705(3)	-33(2)	947(2)	60(7)
H2(9)	579(3)	-71(2)	878(1)	59(6)
H1(10)	945(2)	202(2)	960(1)	48(6)
H2(10)	889(3)	69(3)	981(2)	72(8)

Table XLVII

Final anisotropic thermal parameters ($\underline{U}ij \times 10^4$ Å^2)

and their estimated standard deviations

Atom	$\underline{U}_{11}$	$\underline{U}_{22}$	$\underline{U}_{33}$	$\underline{U}_{12}$	$\underline{U}_{13}$	$\underline{U}_{23}$
S	420(3)	262(2)	533(3)	-10(2)	-66(2)	5(2)
O(1)	401(6)	251(6)	505(7)	-26(5)	-97(5)	12(5)
O(2)	675(10)	362(7)	722(11)	28(7)	-240(8)	92(7)
O(3)	509(8)	404(7)	805(11)	-129(6)	-3(7)	31(7)
O(4)	468(8)	349(7)	632(9)	-27(6)	-199(7)	68(6)
C(1S)	790(19)	558(15)	866(21)	167(14)	201(16)	-100(14)
C(1)	391(9)	266(8)	495(10)	-4(6)	81(7)	15(7)
C(11)	565(13)	329(10)	1005(21)	80(9)	62(14)	-58(11)
C(2)	313(8)	298(8)	511(10)	-1(6)	54(7)	24(7)
C(21)	356(10)	531(13)	1108(22)	-5(9)	211(12)	-65(14)
C(3)	358(8)	282(7)	323(8)	-55(6)	53(6)	34(6)
C(31)	759(15)	468(11)	457(11)	-192(11)	214(11)	59(9)
C(4)	312(8)	270(7)	389(8)	-19(6)	-3(6)	6(6)
C(5)	485(10)	356(8)	337(8)	-51(7)	85(7)	2(7)
C(51)	995(21)	682(16)	461(12)	-160(16)	296(13)	-118(12)
C(6)	367(8)	339(8)	429(9)	-47(7)	123(7)	17(7)
C(61)	479(12)	616(14)	869(18)	-89(11)	346(12)	-78(13)
C(7)	329(8)	279(7)	359(8)	-23(6)	-7(6)	36(6)
C(8)	440(9)	301(8)	405(9)	-63(7)	61(7)	-33(7)
C(81)	941(21)	569(14)	494(13)	-174(14)	241(13)	-161(11)
C(9)	493(10)	323(8)	445(10)	-71(7)	87(8)	91(7)
C(10)	473(10)	337(8)	426(10)	-32(8)	-82(8)	88(7)

Discussion

The structure consists of molecules well-separated along the c-axis (Fig. 27). Chains of molecules running along the b-direction are linked by O(2)...H-O(4)(1-x,1/2+y,1+1/2-z) hydrogen bonds in which the O...H distance and O...H-O angle are 2.07(3) Å and 177(3)°, respectively; the O...O distance is

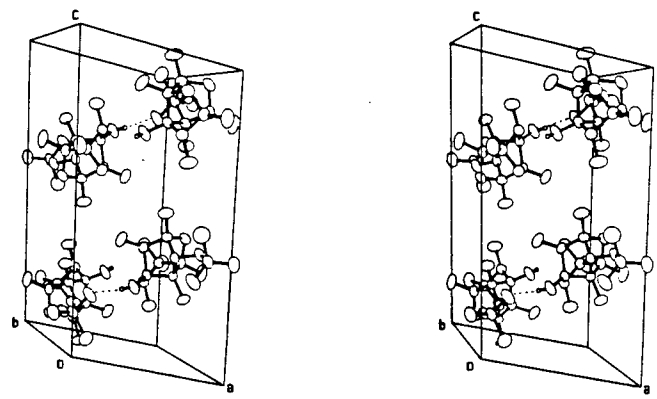


Figure 27

Stereo packing diagram of the mesyl derivative (XVII).

2.845(2) Å.

The tetracyclo[4.2.1.$1^{2,5}$.$0^{3,7}$]decane ring system (Fig. 28) symmetry is altered slightly by the effect of substituents on the ring conformations; however, the symmetry of the ring system can still be best described as C_2, with the rotation axis passing through the center of the six-membered ring and the mid-point of the C(3)-C(7) bond. The five-membered rings assume approximate envelope conformations (in which one atom deviates markedly from the mean plane through the remaining four) while the lone six-membered ring adopts a twist-boat conformation with the amount of twist shown by the torsion angles C(11)-C(1)-C(2)-C(21) and C(51)-C(5)-C(6)-C(61) of 23.9(3)° and 27.9(3)°, respectively (Table XLVIII).

Although most agree with accepted values, some bond lengths and angles within the rings (Tables XLIX and L) are indicative of a highly strained system; deviations of up to 0.077 Å larger than accepted C(sp^3)-C(sp^3) bond lengths of 1.537 Å (33) are observed in the cage structure. Many bond angles differ significantly from tetrahedral values, which is not surprising for a cage structure including four five-membered rings. The geometry of the methyl sulfonyl group compares favorably with that in other structures (cf. 56,57). Methyl to carbon bond lengths, with the exception of C(21)-C(2), are significantly shorter than accepted values which suggests slight differences from sp^3 hybridization at the attached ring carbons. The short C(7)-O(4) bond (1.405(2) Å) is consistent with an increase in s-character in the C(7) orbital directed along that bond. The

Table XLVIII

Torsion angles (deg) with estimated standard deviations in parentheses

Atoms				Value
O(2)	-S	-O(1)	-C(4)	-30.5(2)
O(3)	-S	-O(1)	-C(4)	-159.57(14)
C(1S)	-S	-O(1)	-C(4)	86.2(2)
S	-O(1)	-C(4)	-C(3)	114.24(14)
S	-O(1)	-C(4)	-C(5)	-137.36(13)
C(11)	-C(1)	-C(2)	-C(21)	23.9(3)
C(11)	-C(1)	-C(2)	-C(3)	150.3(2)
C(11)	-C(1)	-C(2)	-C(10)	-102.7(2)
C(8)	-C(1)	-C(2)	-C(21)	-105.6(2)
C(8)	-C(1)	-C(2)	-C(3)	20.8(2)
C(8)	-C(1)	-C(2)	-C(10)	127.83(15)
C(9)	-C(1)	-C(2)	-C(21)	152.4(2)
C(9)	-C(1)	-C(2)	-C(3)	-81.2(2)
C(9)	-C(1)	-C(2)	-C(10)	25.9(2)
C(11)	-C(1)	-C(8)	-C(7)	-175.0(2)
C(11)	-C(1)	-C(8)	-C(81)	-49.4(3)
C(2)	-C(1)	-C(8)	-C(7)	-45.69(15)
C(2)	-C(1)	-C(8)	-C(81)	79.9(2)
C(9)	-C(1)	-C(8)	-C(7)	63.64(14)
C(9)	-C(1)	-C(8)	-C(81)	-170.8(2)
C(11)	-C(1)	-C(9)	-C(6)	178.5(2)
C(2)	-C(1)	-C(9)	-C(6)	48.8(2)
C(8)	-C(1)	-C(9)	-C(6)	-58.2(2)
C(1)	-C(2)	-C(3)	-C(31)	-114.8(2)
C(1)	-C(2)	-C(3)	-C(4)	115.28(15)
C(1)	-C(2)	-C(3)	-C(7)	14.0(2)
C(21)	-C(2)	-C(3)	-C(31)	11.5(3)
C(21)	-C(2)	-C(3)	-C(4)	-118.4(2)
C(21)	-C(2)	-C(3)	-C(7)	140.3(2)
C(10)	-C(2)	-C(3)	-C(31)	133.4(2)
C(10)	-C(2)	-C(3)	-C(4)	3.5(2)
C(10)	-C(2)	-C(3)	-C(7)	-97.81(14)
C(1)	-C(2)	-C(10)	-C(5)	-78.2(2)
C(21)	-C(2)	-C(10)	-C(5)	154.3(2)
C(3)	-C(2)	-C(10)	-C(5)	31.2(2)
C(2)	-C(3)	-C(4)	-O(1)	80.28(15)
C(2)	-C(3)	-C(4)	-C(5)	-36.65(15)
C(31)	-C(3)	-C(4)	-O(1)	-53.3(2)
C(31)	-C(3)	-C(4)	-C(5)	-170.2(2)
C(7)	-C(3)	-C(4)	-O(1)	-179.04(12)
C(7)	-C(3)	-C(4)	-C(5)	64.03(14)
C(2)	-C(3)	-C(7)	-O(4)	-175.96(14)
C(2)	-C(3)	-C(7)	-C(6)	61.33(14)
C(2)	-C(3)	-C(7)	-C(8)	-46.25(15)
C(31)	-C(3)	-C(7)	-O(4)	-45.8(2)

Table XLVIII (continued)

C(31)	-C(3)	-C(7)	-C(6)	-168.5(2)
C(31)	-C(3)	-C(7)	-C(8)	83.9(2)
C(4)	-C(3)	-C(7)	-O(4)	76.7(2)
C(4)	-C(3)	-C(7)	-C(6)	-46.05(14)
C(4)	-C(3)	-C(7)	-C(8)	-153.63(13)
O(1)	-C(4)	-C(5)	-C(51)	61.7(2)
O(1)	-C(4)	-C(5)	-C(6)	-170.97(13)
O(1)	-C(4)	-C(5)	-C(10)	-61.6(2)
C(3)	-C(4)	-C(5)	-C(51)	179.8(2)
C(3)	-C(4)	-C(5)	-C(6)	-52.87(15)
C(3)	-C(4)	-C(5)	-C(10)	56.50(15)
C(4)	-C(5)	-C(6)	-C(61)	-100.1(2)
C(4)	-C(5)	-C(6)	-C(7)	24.0(2)
C(4)	-C(5)	-C(6)	-C(9)	131.18(15)
C(51)	-C(5)	-C(6)	-C(61)	27.9(3)
C(51)	-C(5)	-C(6)	-C(7)	152.1(2)
C(51)	-C(5)	-C(6)	-C(9)	-100.8(2)
C(10)	-C(5)	-C(6)	-C(61)	157.6(2)
C(10)	-C(5)	-C(6)	-C(7)	-78.2(2)
C(10)	-C(5)	-C(6)	-C(9)	28.9(2)
C(4)	-C(5)	-C(10)	-C(2)	-56.1(2)
C(51)	-C(5)	-C(10)	-C(2)	177.8(2)
C(6)	-C(5)	-C(10)	-C(2)	46.4(2)
C(5)	-C(6)	-C(7)	-O(4)	-106.2(2)
C(5)	-C(6)	-C(7)	-C(3)	13.5(2)
C(5)	-C(6)	-C(7)	-C(8)	122.85(14)
C(61)	-C(6)	-C(7)	-O(4)	19.4(2)
C(61)	-C(6)	-C(7)	-C(3)	139.0(2)
C(61)	-C(6)	-C(7)	-C(8)	-111.6(2)
C(9)	-C(6)	-C(7)	-O(4)	142.60(14)
C(9)	-C(6)	-C(7)	-C(3)	-97.72(14)
C(9)	-C(6)	-C(7)	-C(8)	11.6(2)
C(5)	-C(6)	-C(9)	-C(1)	-81.4(2)
C(61)	-C(6)	-C(9)	-C(1)	149.7(2)
C(7)	-C(6)	-C(9)	-C(1)	27.6(2)
O(4)	-C(7)	-C(8)	-C(1)	-175.00(15)
O(4)	-C(7)	-C(8)	-C(81)	59.3(3)
C(3)	-C(7)	-C(8)	-C(1)	59.17(15)
C(3)	-C(7)	-C(8)	-C(81)	-66.6(2)
C(6)	-C(7)	-C(8)	-C(1)	-45.44(15)
C(6)	-C(7)	-C(8)	-C(81)	-171.2(2)

Table XLIX

Bond lengths (Å) with estimated standard deviations in parentheses

Bond		Length	Bond		Length
S	-O(1)	1.5556(12)	C(3)	-C(31)	1.518(2)
S	-O(2)	1.4248(15)	C(3)	-C(4)	1.527(2)
S	-O(3)	1.4128(15)	C(3)	-C(7)	1.526(2)
S	-C(1S)	1.743(3)	C(4)	-C(5)	1.521(2)
O(1)	-C(4)	1.474(2)	C(5)	-C(51)	1.513(3)
O(4)	-C(7)	1.405(2)	C(5)	-C(6)	1.584(2)
C(1)	-C(11)	1.517(3)	C(5)	-C(10)	1.529(3)
C(1)	-C(2)	1.602(2)	C(6)	-C(61)	1.518(3)
C(1)	-C(8)	1.542(2)	C(6)	-C(7)	1.614(2)
C(1)	-C(9)	1.536(3)	C(6)	-C(9)	1.529(2)
C(2)	-C(21)	1.531(3)	C(7)	-C(8)	1.530(2)
C(2)	-C(3)	1.599(2)	C(8)	-C(81)	1.519(3)
C(2)	-C(10)	1.533(3)			

Bond lengths involving hydrogen atoms (Å) with estimated standard deviations in parentheses

Bond		Length	Bond		Length
O(4)	-H(O4)	0.78(3)	C(51)	-H1(51)	0.98(4)
C(1S)	-H1(1S)	0.91(4)	C(51)	-H2(51)	0.99(4)
C(1S)	-H2(1S)	0.97(4)	C(51)	-H3(51)	1.03(4)
C(1S)	-H3(1S)	0.93(3)	C(61)	-H1(61)	0.97(3)
C(11)	-H1(11)	1.06(4)	C(61)	-H2(61)	0.99(3)
C(11)	-H2(11)	0.95(3)	C(61)	-H3(61)	1.02(3)
C(11)	-H3(11)	1.00(4)	C(8)	-H(8)	0.95(2)
C(21)	-H1(21)	1.05(3)	C(81)	-H1(81)	0.89(3)
C(21)	-H2(21)	1.09(4)	C(81)	-H2(81)	0.99(3)
C(21)	-H3(21)	0.92(3)	C(81)	-H3(81)	0.98(4)
C(31)	-H1(31)	0.99(3)	C(9)	-H1(9)	0.97(3)
C(31)	-H2(31)	0.94(3)	C(9)	-H2(9)	0.96(3)
C(31)	-H3(31)	0.99(3)	C(10)	-H1(10)	0.96(2)
C(4)	-H(4)	0.90(2)	C(10)	-H2(10)	1.05(3)

Table L

Bond angles (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
O(1) -S -O(2)	109.64(8)	O(1) -C(4) -C(5)	111.30(13)
O(1) -S -O(3)	105.64(8)	C(3) -C(4) -C(5)	97.49(13)
O(1) -S -C(1S)	104.20(13)	C(4) -C(5) -C(51)	118.0(2)
O(2) -S -O(3)	118.79(11)	C(4) -C(5) -C(6)	99.16(13)
O(2) -S -C(1S)	109.08(15)	C(4) -C(5) -C(10)	98.75(14)
O(3) -S -C(1S)	108.50(15)	C(51)-C(5) -C(6)	117.0(2)
S -O(1) -C(4)	121.74(10)	C(51)-C(5) -C(10)	114.1(2)
C(11)-C(1) -C(2)	116.1(2)	C(6) -C(5) -C(10)	107.42(14)
C(11)-C(1) -C(8)	116.6(2)	C(5) -C(6) -C(61)	115.0(2)
C(11)-C(1) -C(9)	114.1(2)	C(5) -C(6) -C(7)	104.28(12)
C(2) -C(1) -C(8)	104.05(13)	C(5) -C(6) -C(9)	107.10(15)
C(2) -C(1) -C(9)	106.80(15)	C(61)-C(6) -C(7)	112.9(2)
C(8) -C(1) -C(9)	97.03(14)	C(61)-C(6) -C(9)	114.6(2)
C(1) -C(2) -C(21)	114.6(2)	C(7) -C(6) -C(9)	101.56(14)
C(1) -C(2) -C(3)	104.58(13)	O(4) -C(7) -C(3)	111.50(13)
C(1) -C(2) -C(10)	107.68(15)	O(4) -C(7) -C(6)	115.69(14)
C(21)-C(2) -C(3)	114.7(2)	O(4) -C(7) -C(8)	118.02(14)
C(21)-C(2) -C(10)	112.9(2)	C(3) -C(7) -C(6)	99.74(12)
C(3) -C(2) -C(10)	101.18(13)	C(3) -C(7) -C(8)	106.07(14)
C(2) -C(3) -C(31)	120.0(2)	C(6) -C(7) -C(8)	103.84(13)
C(2) -C(3) -C(4)	105.80(13)	C(1) -C(8) -C(7)	93.67(13)
C(2) -C(3) -C(7)	97.79(12)	C(1) -C(8) -C(81)	118.8(2)
C(31)-C(3) -C(4)	113.47(15)	C(7) -C(8) -C(81)	118.5(2)
C(31)-C(3) -C(7)	118.05(15)	C(1) -C(9) -C(6)	99.82(13)
C(4) -C(3) -C(7)	98.63(13)	C(2) -C(10)-C(5)	101.03(13)
O(1) -C(4) -C(3)	112.82(14)		

Table L (continued)

Bond angles involving hydrogen atoms (deg) with estimated standard deviations in parentheses

Bonds	Angle	Bonds	Angle
C(7) -O(4) -H(O4)	109(2)	C(5) -C(51)-H3(51)	111(2)
S -C(1S)-H1(1S)	105(2)	H1(51)-C(51)-H2(51)	102(3)
S -C(1S)-H2(1S)	112(2)	H1(51)-C(51)-H3(51)	104(3)
S -C(1S)-H3(1S)	110(2)	H2(51)-C(51)-H3(51)	114(3)
H1(1S)-C(1S)-H2(1S)	118(3)	C(6) -C(61)-H1(61)	110(2)
H1(1S)-C(1S)-H3(1S)	106(3)	C(6) -C(61)-H2(61)	111(2)
H2(1S)-C(1S)-H3(1S)	106(3)	C(6) -C(61)-H3(61)	112(2)
C(1) -C(11)-H1(11)	106(2)	H1(61)-C(61)-H2(61)	113(2)
C(1) -C(11)-H2(11)	109(2)	H1(61)-C(61)-H3(61)	105(2)
C(1) -C(11)-H3(11)	112(2)	H2(61)-C(61)-H3(61)	106(2)
H1(11)-C(11)-H2(11)	110(2)	C(1) -C(8) -H(8)	108.0(13)
H1(11)-C(11)-H3(11)	110(3)	C(7) -C(8) -H(8)	111.0(13)
H2(11)-C(11)-H3(11)	110(3)	C(81) -C(8) -H(8)	106.3(13)
C(2) -C(21)-H1(21)	107(2)	C(8) -C(81)-H1(81)	115(2)
C(2) -C(21)-H2(21)	109(2)	C(8) -C(81)-H2(81)	109(2)
C(2) -C(21)-H3(21)	113(2)	C(8) -C(81)-H3(81)	110(2)
H1(21)-C(21)-H2(21)	110(2)	H1(81)-C(81)-H2(81)	105(3)
H1(21)-C(21)-H3(21)	111(2)	H1(81)-C(81)-H3(81)	108(3)
H2(21)-C(21)-H3(21)	107(3)	H2(81)-C(81)-H3(81)	110(3)
C(3) -C(31)-H1(31)	115(2)	C(1) -C(9) -H1(9)	112.8(15)
C(3) -C(31)-H2(31)	108(2)	C(1) -C(9) -H2(9)	112.1(15)
C(3) -C(31)-H3(31)	110(2)	C(6) -C(9) -H1(9)	115.3(14)
H1(31)-C(31)-H2(31)	110(2)	C(6) -C(9) -H2(9)	110.6(15)
H1(31)-C(31)-H3(31)	110(2)	H1(9) -C(9) -H2(9)	106(2)
H2(31)-C(31)-H3(31)	104(2)	C(2) -C(10)-H1(10)	108.8(13)
O(1) -C(4) -H(4)	110.8(14)	C(2) -C(10)-H2(10)	112(2)
C(3) -C(4) -H(4)	109.3(14)	C(5) -C(10)-H1(10)	112.2(13)
C(5) -C(4) -H(4)	114.5(14)	C(5) -C(10)-H2(10)	116.8(15)
C(5) -C(51)-H1(51)	111(2)	H1(10)-C(10)-H2(10)	106(2)
C(5) -C(51)-H2(51)	113(2)		

same, however, cannot be said of the C(4)-O(1) bond whose length is 1.474(2) Å, approximately 0.05 Å longer than typical C-O distances in aliphatic ethers. This increased bond length is probably due to the mesyl group, which through S-O(1) $d\pi$-$p\pi$ bonding leaves O(1)-C(4) electron deficient resulting in the polarization of the O(1)-C(4) bonding electrons towards the oxygen and thereby weakening the bond. The sp^2 hybridization at the oxygen (C(4)-O(1)-S, 121.74°), in addition to any increased s-character at C(4) (and directed along the C(4)-O(1) bond), is insufficient to match the $d\pi$-$p\pi$ bonding effect between O(1) and S, and therefore the net result is lengthening of the C(4)-O(1) bond.

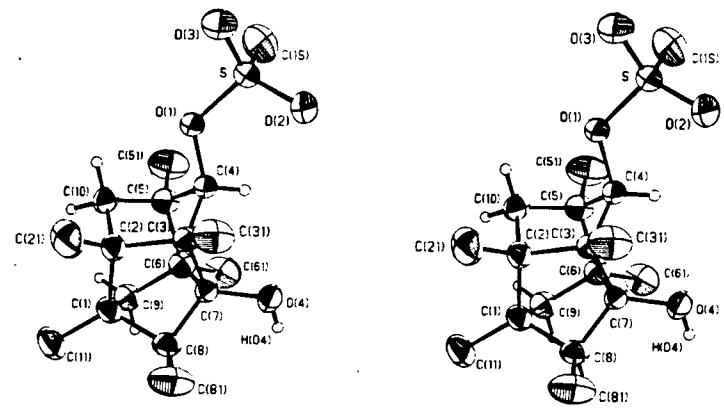


Figure 28

Stereo diagram of the mesyl derivative (XVII).

Notable intramolecular contacts are those between H1(9) and H2(10) and between H(4) and O(1). In the former case, the contact distance of 2.02(3) Å results from compression by the ring system, whereas the latter case, involving a 1.98(2) Å separation of oxygen and hydrogen, does not appear to arise from steric compression, although neighboring steric effects undoubtedly oppose an increase in the distance. On the basis of geometry considerations, hydrogen bonding between O(1) and H(4) does not seem probable – the C(4)-H...O(1) angle is 44(1)° and the oxygen lone pairs do not appear suitably positioned to interact with the hydrogen.

SUMMARY

The compounds described in the first three chapters followed reaction routes similar to those of previously studied naphthoquinols, both in the solid state and solution. Although the distances through which H-abstractions occurred were less than the van der Waals radii sum, proof is still lacking as to this being the upper limit for such processes.

The effects of substituents on conformation and reactivity have been illustrated throughout both Part I and Part II of this thesis, but the most notable were highlighted in the 6,7-dimethyl- (Chapter II), and heptamethyl-naphthoquinols (Chapter III). The occurrence of β-H abstraction by oxygen in the former derivative dispelled any notions that the change in chromophore from ene-dione to enone prohibited this reaction. It appears that subtle electronic effects arising from the substituents at the C(2) and C(3) positions play a key role in determining the photoreactivity in naphthoquinols. The heptamethyl derivative, on the other hand, showed the more obvious 'steric' effects of substituents on conformation which in turn determined the photochemical reactivity. Introduction of the methyl group at C(4) caused the less bulky OH group to assume the pseudo-axial position. The resulting conformation and reactivity was typical of previously studied OH anti derivatives despite the syn positioning of the hydroxyl group in this case.

The substitution process, when carried further to the replacement of the carbonyl oxygen by H and OH, forms the diol (Chapter IV). While the conformation typical of the 4α-ols was maintained, no photoreactivity was observed, for the chromophoric moiety had been lost.

The effect of hydrogen bonding on reactivity in the naphthoquinols is not apparent from this work since it was present in all structures. However, the type of H-bonding, be it O(4)...O(4) or O(1)...O(4), appears to be of no consequence in reactivity since structures with either have been observed to undergo similar reactions[1] (cf. Chapters II and III).

Some unusual reaction products have been observed in the course of this study, four of which have been described in Part II. The advent of these compounds serves to illustrate the complexity of these reactions and that all is not as clear and concise as the discussions in Part I may have the reader believe.

The intriguing results of internal irradiation (Chapters V and VI) may hinge on the presence of impurities; however, the consistent results of repeated experiments have decreased the likelihood of this as being a major factor. Whatever the cause, the ensuing products have prompted interesting discussions.

The last two chapters have documented the results of syntheses which have gone awry. Nevertheless, the structures have proved valuable, in one case showing that a 1,3-suprafacial shift of a bridging bond has occurred on photolysis (Chapter VII) and in the other, a novel entry into the rare tetracyclo[4.2.1.$1^{2,5}$.$0^{3,7}$]decane ring system.

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[1] Appel, Herbert, Jiang, Scheffer and Walsh (39) have shown that hydrogen bonding does not affect H(5)-abstraction by C(3), by their work on the acetate analog of 2,3,4aβ,6,7,8aβ-hexamethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol.

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SUPPLEMENTARY MATERIAL

2,3,6,7-tetramethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	1
-16	0	0	1.32*	0.89	3.21	16	0	6	10.12	10.00	2.46	6	0	14	1.09*	0.90	3.17	1	1	1	26.62	28.38	0.34	
-12	0	0	40.95	41.56	0.11	-16	0	8	1.41*	0.14	3.23	8	0	14	6.37	6.50	3.39	3	1	1	16.18	14.21	1.12	
-10	0	0	33.77	33.66	0.18	-14	0	8	5.03	4.77	3.53	10	0	14	3.00	2.80	3.46	5	1	1	52.05	52.08	0.06	
-8	0	0	6.87	6.36	3.30	-12	0	8	4.32	5.13	3.54	12	0	14	3.34	3.60	3.50	7	1	1	23.34	23.73	0.47	
-6	0	0	33.53	30.44	0.18	-10	0	8	14.31	13.65	1.44	-14	0	16	5.11	5.09	3.53	9	1	1	3.98	4.43	3.54	
-4	0	0	20.61	17.67	0.65	-8	0	8	16.58	17.04	1.06	-12	0	16	2.62*	0.73	3.42	11	1	1	18.00	17.70	0.89	
-2	0	0	67.77	75.59	0.03	-6	0	8	9.75	11.59	2.57	-10	0	16	12.12	11.60	1.92	13	1	1	1.31*	1.27	3.21	
14	0	0	1.06*	1.20	3.16	-4	0	8	15.58	16.02	1.21	-8	0	16	18.32	19.08	0.85	15	1	1	1.94*	2.01	3.32	
-16	0	2	4.47	4.70	3.54	-2	0	8	5.38	4.83	3.51	-6	0	16	1.37*	0.61	3.22	17	1	1	2.35*	2.69	3.38	
-14	0	2	1.40*	0.55	3.23	0	0	8	1.23*	2.83	3.20	-4	0	16	3.57	3.50	3.51	-17	1	2	1.48*	2.01	3.24	
-12	0	2	30.37	29.48	0.24	2	0	8	29.59	26.69	0.26	-2	0	16	4.38	3.99	3.54	-15	1	2	3.64	3.09	3.52	
-10	0	2	4.54	5.08	3.54	4	0	8	21.75	21.07	0.57	0	0	16	6.60	6.87	3.35	-13	1	2	11.30	10.61	2.14	
-8	0	2	7.23	6.70	3.23	6	0	8	4.43	3.70	3.54	2	0	16	29.17	28.84	0.27	-11	1	2	7.54	6.89	3.16	
-6	0	2	4.51	4.97	3.54	8	0	8	10.58	11.42	2.33	4	0	16	13.40	12.74	1.62	-9	1	2	1.70*	2.65	3.28	
-4	0	2	50.74	53.92	0.06	10	0	8	7.24	8.66	3.23	6	0	16	1.14*	0.19	3.18	-7	1	2	6.39	6.32	3.39	
-2	0	2	76.30	84.65	0.02	12	0	8	1.84*	1.22	3.30	8	0	16	1.19*	0.56	3.19	-5	1	2	4.49	4.11	3.54	
0	0	2	105.42	100.02	0.01	14	0	8	2.18*	2.62	3.36	10	0	16	3.12	2.78	3.48	-3	1	2	15.88	14.15	1.17	
2	0	2	47.34	40.17	0.07	-16	0	10	0.74*	2.01	3.10	-12	0	18	2.41*	2.83	3.39	-1	1	2	93.40	96.69	0.01	
4	0	2	16.75	17.91	1.04	-14	0	10	7.96	8.79	3.06	-10	0	18	1.68*	1.61	3.28	1	1	2	11.09	9.73	2.19	
6	0	2	7.74	7.57	3.11	-12	0	10	9.67	9.96	2.59	-8	0	18	3.80	3.15	3.53	3	1	2	32.44	32.89	0.20	
8	0	2	1.02*	1.40	3.16	-10	0	10	8.17	9.37	3.00	-6	0	18	4.27	4.68	3.54	5	1	2	15.32	14.47	1.26	
10	0	2	28.66	30.38	0.28	-8	0	10	1.12*	1.47	3.18	-4	0	18	3.14	3.87	3.48	7	1	2	10.56	10.29	2.34	
12	0	2	5.63	6.44	3.49	-6	0	10	8.61	8.10	2.89	-2	0	18	11.60	11.80	2.06	9	1	2	14.57	14.12	1.39	
14	0	2	2.25*	1.84	3.37	-4	0	10	3.96	3.73	3.54	0	0	18	1.18*	0.17	3.19	11	1	2	8.10	8.30	3.02	
16	0	2	1.62*	0.93	3.27	-2	0	10	40.22	40.21	0.11	2	0	18	3.49	3.75	3.51	13	1	2	0.52*	0.60	3.06	
-16	0	4	7.27	6.91	3.22	0	0	10	18.96	16.71	0.79	4	0	18	5.57	5.78	3.49	15	1	2	1.14*	1.26	3.18	
-14	0	4	6.47	6.23	3.37	2	0	10	5.49	5.32	3.50	6	0	18	2.53	2.37	3.41	17	1	2	2.57*	0.76	3.41	
-12	0	4	2.48	1.07	3.40	4	0	10	7.76	8.00	3.11	8	0	18	3.83	4.27.	3.53	-17	1	3	1.37*	2.18	3.22	
-10	0	4	0.53*	1.02	3.06	6	0	10	9.16	8.76	2.74	-10	0	20	6.41	6.63	3.38	-15	1	3	1.31*	0.03	3.21	
-8	0	4	20.28	21.64	0.67	8	0	10	4.94	5.47	3.53	-8	0	20	1.93*	1.95	3.32	-13	1	3	9.32	8.71	2.69	
-6	0	4	64.10	63.44	0.03	10	0	10	2.49	4.42	3.40	-6	0	20	2.36	1.86	3.38	-11	1	3	16.17	14.97	1.12	
-4	0	4	48.31	55.60	0.07	12	0	10	2.51	3.09	3.40	-4	0	20	11.14	11.12	2.18	-9	1	3	3.56	3.56	3.51	
-2	0	4	41.58	38.36	0.10	14	0	10	1.83*	1.87	3.30	-2	0	20	9.47	9.29	2.65	-7	1	3	37.07	32.87	0.14	
0	0	4	40.09	43.91	0.11	-16	0	12	2.90	2.46	3.45	0	0	20	4.88	4.78	3.54	-5	1	3	9.42	8.11	2.66	
2	0	4	21.17	24.58	0.60	-14	0	12	2.81	3.56	3.45	2.	0	20	8.45	8.44	2.93	-3	1	3	38.88	43.34	0.12	
4	0	4	76.13	74.29	0.02	-12	0	12	1.28*	0.40	3.21	4	0	20	1.27*	0.37	3.20	-1	1	3	133.39	137.20	0.00	
6	0	4	71.00	66.48	0.02	-10	0	12	12.50	13.11	1.83	6	0	20	2.00*	3.31	3.33	1	1	3	57.47	53.02	0.04	
8	0	4	9.64	9.45	2.60	-8	0	12	1.82*	1.11	3.30	-4	0	22	1.77*	2.46	3.29	3	1	3	8.04	8.16	3.04	
10	0	4	6.44	6.33	3.38	-6	0	12	4.32	4.06	3.54	-2	0	22	1.08*	0.54	3.17	5	1	3	46.92	40.90	0.07	
12	0	4	3.21	3.73	3.49	-4	0	12	19.00	19.91	0.78	0	0	22	3.82	3.81	3.53	7	1	3	5.13	4.89	3.52	
14	0	4	1.16*	1.87	3.18	-2	0	12	1.45*	0.65	3.24	-13	1	0	7.03	7.70	3.27	9	1	3	12.84	13.11	1.75	
16	0	4	9.64	10.15	2.60	0	0	12	0.42*	0.67	3.04	-11	1	0	30.51	30.13	0.24	11	1	3	24.29	24.93	0.43	
-16	0	6	2.11*	1.32	3.35	2	0	12	21.23	21.73	0.60	1	1	0	113.93	117.06	0.01	13	1	3	1.29*	1.93	3.21	
-14	0	6	10.30	10.98	2.41	4	0	12	9.20	9.71	2.73	3	1	0	17.20	15.67	0.98	15	1	3	1.22*	0.84	3.19	
-12	0	6	3.94	3.83	3.53	6	0	12	4.18	4.59	3.54	5	1	0	2.16	1.86	3.35	17	1	3	2.47*	2.55	3.40	
-10	0	6	3.19	3.49	3.48	8	0	12	6.75	7.45	3.32	7	1	0	15.40	16.15	1.24	-17	1	4	2.52*	2.11	3.41	
-8	0	6	28.31	22.83	0.29	10	0	12	1.78*	1.06	3.29	9	1	0	2.38	2.34	3.39	-15	1	4	3.53	3.22	3.51	
-6	0	6	40.01	35.32	0.11	12	0	12	1.24*	0.55	3.20	15	1	0	1.12*	0.07	3.18	-13	1	4	8.77	8.24	2.84	
-4	0	6	29.04	30.31	0.27	-14	0	14	6.88	6.01	3.30	17	1	0	2.52*	2.93	3.41	-11	1	4	12.43	12.36	1.85	
-2	0	6	46.42	43.22	0.08	-12	0	14	2.99	2.36	3.46	-17	1	1	1.45*	0.93	3.24	-9	1	4	4.51	4.74	3.54	
0	0	6	24.28	21.96	0.43	-10	0	14	1.13*	1.59	3.18	-15	1	1	5.72	5.12	3.48	-7	1	4	9.70	8.66	2.58	
2	0	6	26.98	24.86	0.33	-8	0	14	26.17	27.15	0.35	-13	1	1	1.84*	0.02	3.30	-5	1	4	18.22	19.72	0.86	
4	0	6	98.89	90.44	0.01	-6	0	14	10.75	11.04	2.29	-11	1	1	14.66	14.41	1.37	-3	1	4	8.28	8.17	2.98	
6	0	6	15.39	14.79	1.24	-4	0	14	10.18	10.80	2.45	-9	1	1	0.77*	1.13	3.11	-1	1	4	82.95	84.89	0.01	
8	0	6	1.00*	0.90	3.15	-2	0	14	22.42	22.57	0.52	-7	1	1	24.88	24.63	0.40	1	1	4	21.36	19.72	0.59	
10	0	6	1.25*	1.51	3.20	0	0	14	10.16	9.78	2.45	-5	1	1	28.95	32.30	0.27	3	1	4	6.76	7.08	3.32	
12	0	6	0.37*	2.13	3.03	2	0	14	11.00	11.52	2.22	-3	1	1	50.70	51.73	0.06	5	1	4	41.80	39.60	0.10	
14	0	6	1.33*	1.18	3.21	4	0	14	32.65	32.47	0.20	-1	1	1	31.19	29.02	0.22	7	1	4	3.03	3.45	3.47	

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	2
9	1	4	1.77*	1.30	3.29	-11	1	8	0.84*	2.33	3.12	9	1	11	2.93	2.42	3.46	11	1	15	2.33*	2.19	3.38	
11	1	4	13.05	13.68	1.70	-9	1	8	1.81*	1.83	3.30	11	1	11	1.95*	1.01	3.32	-13	1	16	1.43*	1.70	3.23	
13	1	4	1.00*	1.84	3.15	-7	1	8	2.03*	0.70	3.33	13	1	11	1.27*	0.85	3.20	-11	1	16	3.67	3.16	3.52	
15	1	4	1.65*	2.60	3.27	-5	1	8	10.02	10.98	2.49	-15	1	12	2.40*	3.41	3.39	-9	1	16	11.47	11.94	2.09	
-17	1	5	3.68	2.81	3.52	-3	1	8	14.85	14.62	1.34	-13	1	12	3.08	3.53	3.47	-7	1	16	4.89	5.09	3.54	
-15	1	5	1.35*	0.39	3.22	-1	1	8	34.23	32.36	0.17	-11	1	12	1.21*	0.64	3.19	-5	1	16	2.32	2.06	3.38	
-13	1	5	7.59	7.32	3.15	1	1	8	2.37	1.21	3.39	-9	1	12	9.26	9.06	2.71	-3	1	16	3.01	3.41	3.47	
-11	1	5	5.17	5.26	3.52	3	1	8	9.85	9.17	2.54	-7	1	12	2.92	3.64	3.46	-1	1	16	2.59	2.48	3.42	
-9	1	5	15.65	15.01	1.20	5	1	8	16.97	16.66	1.01	-5	1	12	0.89*	0.09	3.13	1	1	16	11.07	10.97	2.20	
-7	1	5	24.20	24.12	0.43	7	1	8	5.62	5.32	3.48	-3	1	12	7.45	7.53	3.18	3	1	16	14.50	14.19	1.40	
-5	1	5	11.46	11.70	2.09	9	1	8	1.59*	1.58	3.26	-1	1	12	1.28*	1.40	3.21	5	1	16	1.18*	0.15	3.19	
-3	1	5	5.70	2.95	3.48	11	1	8	3.28	3.98	3.49	1	1	12	6.26	6.02	3.41	7	1	16	1.16*	1.04	3.18	
-1	1	5	46.34	46.38	0.08	13	1	8	1.34*	1.16	3.22	3	1	12	13.09	12.69	1.69	9	1	16	1.86*	0.56	3.31	
1	1	5	18.16	17.14	0.87	15	1	8	1.33*	0.34	3.22	5	1	12	9.13	9.28	2.75	-13	1	17	5.15	4.26	3.52	
3	1	5	23.69	22.46	0.46	-17	1	9	2.86*	2.79	3.45	7	1	12	6.25	6.63	3.41	-11	1	17	2.25*	2.42	3.37	
5	1	5	16.18	15.74	1.12	-15	1	9	2.18*	2.85	3.36	9	1	12	1.86*	0.55	3.31	-9	1	17	1.62*	1.98	3.27	
7	1	5	4.01	3.73	3.54	-13	1	9	1.08*	1.49	3.17	11	1	12	1.23*	2.02	3.20	-7	1	17	4.89	5.06	3.54	
9	1	5	5.57	5.20	3.49	-11	1	9	1.20*	0.40	3.19	13	1	12	2.94	4.17	3.46	-5	1	17	5.05	4.47	3.53	
11	1	5	9.35	10.30	2.68	-9	1	9	2.12*	4.12	3.35	-15	1	13	1.48*	0.12	3.24	-3	1	17	16.00	16.87	1.15	
13	1	5	2.19*	1.23	3.36	-7	1	9	16.02	14.40	1.15	-13	1	13	1.32*	0.64	3.21	-1	1	17	9.65	9.05	2.60	
15	1	5	1.86*	1.73	3.31	-5	1	9	4.73	4.68	3.54	-11	1	13	1.01*	1.50	3.16	1	1	17	1.21*	0.59	3.19	
-17	1	6	1.49*	0.48	3.24	-3	1	9	3.98	2.76	3.54	-9	1	13	9.22	9.54	2.72	3	1	17	4.33	4.69	3.54	
-15	1	6	3.65	3.66	3.52	-1	1	9	8.33	7.50	2.96	-7	1	13	19.40	19.03	0.75	5	1	17	2.35	2.25	3.38	
-13	1	6	16.38	15.65	1.09	1	1	9	3.15	2.25	3.48	-5	1	13	5.07	5.53	3.53	7	1	17	4.41	4.30	3.54	
-11	1	6	4.56	4.18	3.54	3	1	9	13.51	13.05	1.60	-3	1	13	2.96	3.64	3.46	9	1	17	8.16	7.69	3.01	
-9	1	6	2.82	2.85	3.46	5	1	9	17.25	15.79	0.98	-1	1	13	5.02	4.77	3.53	-11	1	18	0.97*	0.37	3.15	
-7	1	6	25.60	23.90	0.37	7	1	9	6.53	6.13	3.36	1	1	13	1.64*	1.88	3.27	-9	1	18	2.46*	1.27	3.40	
-5	1	6	4.19	3.77	3.54	9	1	9	1.09*	0.79	3.17	3	1	13	19.92	19.89	0.70	-7	1	18	1.45*	1.65	3.24	
-3	1	6	42.10	41.41	0.10	11	1	9	1.42*	1.65	3.23	5	1	13	12.45	12.11	1.84	-5	1	18	1.17*	1.50	3.19	
-1	1	6	63.29	61.10	0.03	13	1	9	1.12*	0.07	3.18	7	1	13	2.05*	1.95	3.34	-3	1	18	4.45	4.46	3.54	
1	1	6	12.18	11.47	1.91	15	1	9	3.58	4.52	3.52	9	1	13	1.41*	0.76	3.23	-1	1	18	1.16*	1.55	3.18	
3	1	6	17.21	16.53	0.98	-15	1	10	2.65*	3.65	3.42	11	1	13	1.21*	0.17	3.19	1	1	18	3.91	3.85	3.53	
5	1	6	38.53	35.34	0.13	-13	1	10	9.04	9.84	2.77	-15	1	14	1.19*	1.27	3.19	3	1	18	5.21	5.08	3.52	
7	1	6	6.61	6.70	3.35	-11	1	10	1.21*	0.31	3.19	-13	1	14	1.32*	0.95	3.21	5	1	18	1.90*	0.34	3.31	
9	1	6	17.41	18.03	0.96	-9	1	10	12.40	12.62	1.85	-11	1	14	1.24*	1.28	3.20	7	1	18	1.25*	0.41	3.20	
11	1	6	2.95	3.38	3.46	-7	1	10	20.37	18.92	0.66	-9	1	14	9.35	9.33	2.68	-11	1	19	1.42*	0.98	3.23	
13	1	6	2.48	2.37	3.40	-5	1	10	1.89	1.48	3.31	-7	1	14	15.00	15.13	1.31	-9	1	19	1.36*	1.85	3.22	
15	1	6	5.98	6.19	3.45	-3	1	10	22.78	21.65	0.50	-5	1	14	1.76*	1.86	3.29	-7	1	19	1.44*	0.36	3.23	
-17	1	7	2.91*	3.17	3.45	-1	1	10	25.93	23.09	0.36	-3	1	14	5.62	5.97	3.49	-5	1	19	2.07*	0.34	3.34	
-15	1	7	2.60	2.09	3.42	1	1	10	1.93	0.77	3.32	-1	1	14	1.03*	0.89	3.16	-3	1	19	5.19	5.20	3.52	
-13	1	7	6.03	7.04	3.44	3	1	10	28.89	29.06	0.25	1	1	14	1.11*	0.88	3.17	-1	1	19	2.78	3.02	3.44	
-11	1	7	6.96	7.45	3.28	5	1	10	17.16	16.72	0.99	3	1	14	22.31	22.35	0.53	1	1	19	5.35	4.92	3.51	
-9	1	7	2.21	1.41	3.36	7	1	10	1.06*	0.89	3.16	5	1	14	8.10	7.54	3.02	3	1	19	4.22	4.16	3.54	
-7	1	7	29.56	27.65	0.26	9	1	10	6.94	8.06	3.29	7	1	14	2.01*	0.89	3.33	5	1	19	2.05*	0.17	3.34	
-5	1	7	15.74	17.82	1.19	11	1	10	1.15*	1.48	3.18	9	1	14	0.90*	0.24	3.13	7	1	19	2.06*	2.21	3.34	
-3	1	7	15.41	14.14	1.24	13	1	10	1.57*	0.36	3.26	11	1	14	1.66*	0.36	3.27	-9	1	20	6.75	6.79	3.32	
-1	1	7	34.78	28.57	0.17	-15	1	11	2.38*	3.48	3.39	-13	1	15	4.59	4.17	3.54	-7	1	20	1.48*	1.89	3.24	
1	1	7	15.10	15.83	1.29	-13	1	11	3.83*	3.25	3.53	-11	1	15	6.01	6.41	3.44	-5	1	20	0.59*	1.53	3.07	
3	1	7	22.27	20.16	0.53	-11	1	11	3.32	3.44	3.49	-9	1	15	0.54*	1.04	3.06	-3	1	20	4.97	5.13	3.53	
5	1	7	25.85	24.60	0.37	-9	1	11	4.28	4.72	3.54	-7	1	15	2.00*	0.90	3.33	-1	1	20	2.16*	1.37	3.35	
7	1	7	1.81*	0.43	3.30	-7	1	11	26.36	27.63	0.35	-5	1	15	9.04	9.35	2.77	1	1	20	8.43	8.44	2.94	
9	1	7	2.54	2.42	3.41	-5	1	11	6.80	6.79	3.32	-3	1	15	3.60	3.52	3.52	3	1	20	5.66	5.35	3.48	
11	1	7	1.11*	2.33	3.17	-3	1	11	15.65	16.84	1.20	-1	1	15	7.67	8.35	3.13	5	1	20	1.28*	0.30	3.21	
13	1	7	1.85*	0.36	3.31	-1	1	11	12.48	12.13	1.84	1	1	15	6.76	7.21	3.32	-7	1	21	2.50*	1.89	3.40	
15	1	7	4.43	4.44	3.54	1	1	11	13.46	13.78	1.61	3	1	15	0.72*	0.42	3.10	-5	1	21	0.61*	0.21	3.08	
-17	1	8	2.07*	2.29	3.34	3	1	11	16.32	16.82	1.10	5	1	15	3.19	3.23	3.48	-3	1	21	4.44	4.60	3.54	
-15	1	8	2.40*	1.76	3.39	5	1	11	20.38	20.74	0.66	7	1	15	3.88	4.01	3.53	-1	1	21	2.54*	2.19	3.41	
-13	1	8	1.89*	1.18	3.33	7	1	11	1.77*	1.27	3.29	9	1	15	3.86	3.57	3.53	1	1	21	2.09*	2.07	3.34	

h	k	l	Fo	Fc	weight
3	1	21	2.01*	2.05	3.33
-3	1	22	1.54*	0.90	3.25
-1	1	22	3.61	3.19	3.52
-10	2	0	2.17	2.05	3.36
-8	2	0	1.76*	1.70	3.29
-6	2	0	4.64	4.98	3.54
-4	2	0	2.18	1.72	3.36
-2	2	0	12.25	13.21	1.89
0	2	0	7.63	6.82	3.14
10	2	0	1.85*	2.05	3.31
12	2	0	1.36*	0.68	3.22
14	2	0	1.21*	0.96	3.19
16	2	0	1.76*	1.14	3.29
-16	2	1	1.37*	0.76	3.22
-14	2	1	4.19	4.02	3.54
-12	2	1	0.83*	0.83	3.12
-10	2	1	3.18	3.25	3.48
-8	2	1	1.95*	0.84	3.32
-6	2	1	11.32	11.92	2.13
-4	2	1	3.47	2.84	3.51
-2	2	1	5.91	5.77	3.45
0	2	1	1.63	0.44	3.27
2	2	1	27.46	27.96	0.31
4	2	1	7.34	7.84	3.20
6	2	1	21.20	20.24	0.60
8	2	1	4.90	5.23	3.54
10	2	1	5.01	4.71	3.53
12	2	1	2.41	2.36	3.39
14	2	1	4.51	5.20	3.54
16	2	1	1.36*	1.39	3.22
-16	2	2	1.30*	0.09	3.21
-14	2	2	2.69	3.19	3.43
-12	2	2	4.29	3.91	3.54
-10	2	2	2.83	3.13	3.45
-8	2	2	16.93	18.78	1.02
-6	2	2	1.40*	1.69	3.23
-4	2	2	11.84	12.88	2.00
-2	2	2	39.08	37.45	0.12
0	2	2	28.64	30.57	0.28
2	2	2	22.71	22.26	0.51
4	2	2	15.38	16.79	1.25
6	2	2	9.78	9.32	2.56
8	2	2	6.05	5.47	3.44
10	2	2	6.02	5.60	3.44
12	2	2	7.12	7.06	3.25
14	2	2	4.74	4.75	3.54
16	2	2	0.75*	1.15	3.10
-16	2	3	1.34*	0.20	3.22
-14	2	3	1.29*	1.17	3.21
-12	2	3	4.42	3.89	3.54
-10	2	3	1.90*	1.46	3.31
-8	2	3	11.48	10.51	2.09
-6	2	3	25.08	26.33	0.39
-4	2	3	3.75	3.85	3.53
-2	2	3	19.51	19.04	0.74
0	2	3	23.93	22.64	0.45
2	2	3	19.17	19.17	0.77
4	2	3	18.13	16.51	0.87
6	2	3	16.51	14.87	1.07
8	2	3	2.68	1.88	3.43
10	2	3	12.06	12.13	1.94
12	2	3	5.18	5.17	3.52
14	2	3	1.84*	1.59	3.30
16	2	3	2.18*	2.21	3.36
-16	2	4	1.37*	0.92	3.22
-14	2	4	1.76*	0.14	3.29
-12	2	4	24.93	24.31	0.40
-10	2	4	7.34	7.99	3.20
-8	2	4	5.15	5.40	3.52
-6	2	4	7.55	8.22	3.16
-4	2	4	12.95	14.76	1.73
-2	2	4	18.77	17.99	0.81
0	2	4	83.36	87.44	0.01
2	2	4	1.17*	1.11	3.19
4	2	4	19.17	20.18	0.77
6	2	4	6.14	5.40	3.42
8	2	4	6.86	6.75	3.30
10	2	4	16.92	17.45	1.02
12	2	4	8.59	8.71	2.89
14	2	4	2.06*	2.01	3.34
16	2	4	1.28*	0.29	3.21
-16	2	5	1.76*	1.58	3.29
-14	2	5	3.41	3.20	3.50
-12	2	5	9.46	9.36	2.65
-10	2	5	1.59*	0.28	3.26
-8	2	5	5.09	4.72	3.53
-6	2	5	3.60	3.17	3.52
-4	2	5	12.06	12.02	1.94
-2	2	5	26.14	26.46	0.35
0	2	5	40.81	38.37	0.11
2	2	5	2.85	2.81	3.45
4	2	5	5.70	5.25	3.48
6	2	5	8.65	8.54	2.88
8	2	5	6.52	6.48	3.36
10	2	5	7.27	7.27	3.22
12	2	5	2.82	3.51	3.44
14	2	5	1.25*	1.58	3.20
16	2	5	1.36*	0.80	3.22
-16	2	6	2.36*	1.32	3.38
-14	2	6	7.85	7.56	3.08
-12	2	6	20.24	19.25	0.67
-10	2	6	1.16*	0.16	3.18
-8	2	6	2.88	2.70	3.45
-6	2	6	2.81	1.75	3.44
-4	2	6	12.45	12.44	1.84
-2	2	6	67.57	67.90	0.03
0	2	6	46.57	43.99	0.07
2	2	6	3.15	2.79	3.48
4	2	6	0.86*	0.11	3.13
6	2	6	5.85	5.34	3.46
8	2	6	14.55	14.86	1.39
10	2	6	22.22	23.20	0.54
12	2	6	4.83	5.26	3.54
14	2	6	1.18*	1.44	3.19
-16	2	7	1.41*	0.58	3.23
-14	2	7	1.31*	1.10	3.21
-12	2	7	6.05	6.10	3.44
-10	2	7	1.63*	0.73	3.27
-8	2	7	5.66	5.75	3.48
-6	2	7	11.38	11.61	2.11
-4	2	7	1.21*	0.60	3.19
-2	2	7	1.64*	3.72	3.27
0	2	7	14.93	13.03	1.32
2	2	7	0.82*	0.11	3.12
4	2	7	6.58	5.59	3.36
6	2	7	11.05	12.39	2.20
8	2	7	1.33*	0.75	3.22
10	2	7	4.09	3.17	3.54
12	2	7	1.41*	0.29	3.23
14	2	7	1.64*	1.61	3.27
-16	2	8	2.11*	2.51	3.35
-14	2	8	2.14*	0.46	3.35
-12	2	8	2.27*	1.33	3.37
-10	2	8	5.76	5.02	3.47
-8	2	8	14.08	14.83	1.48
-6	2	8	32.89	33.47	0.19
-4	2	8	1.52*	1.87	3.25
-2	2	8	2.55	2.89	3.41
0	2	8	11.23	10.11	2.16
2	2	8	15.07	15.72	1.30
4	2	8	26.60	27.19	0.34
6	2	8	19.81	20.61	0.71
8	2	8	9.37	9.14	2.68
10	2	8	1.15*	0.94	3.18
12	2	8	1.06*	0.36	3.16
14	2	8	2.40*	1.30	3.39
-16	2	9	3.51	3.70	3.51
-14	2	9	5.67	5.06	3.48
-12	2	9	0.67*	1.41	3.09
-10	2	9	0.50*	0.41	3.05
-8	2	9	2.37	1.65	3.39
-6	2	9	7.02	7.85	3.27
-4	2	9	18.83	17.53	0.79
-2	2	9	19.60	20.57	0.73
0	2	9	0.86*	1.26	3.13
2	2	9	2.67	2.85	3.43
4	2	9	10.65	10.46	2.31
6	2	9	5.41	5.33	3.51
8	2	9	6.24	6.31	3.41
10	2	9	4.60	4.08	3.54
12	2	9	1.22*	0.59	3.19
14	2	9	2.59*	1.55	3.42
-16	2	10	2.56*	1.57	3.41
-14	2	10	5.49	5.33	3.50
-12	2	10	2.71	2.42	3.43
-10	2	10	1.52*	1.04	3.25
-8	2	10	33.47	32.44	0.18
-6	2	10	27.94	27.85	0.30
-4	2	10	4.37	4.75	3.54
-2	2	10	13.00	13.66	1.71
0	2	10	4.57	4.17	3.54
2	2	10	13.48	13.29	1.61
4	2	10	49.66	49.78	0.06
6	2	10	9.98	9.47	2.50
8	2	10	5.26	5.41	3.52
10	2	10	1.28*	1.58	3.21
12	2	10	1.10*	0.32	3.17
14	2	10	6.28	6.41	3.40
-14	2	11	1.73*	2.71	3.29
-12	2	11	1.31*	1.50	3.21
-10	2	11	0.82*	0.80	3.12
-8	2	11	12.38	12.96	1.86
-6	2	11	13.47	13.64	1.61
-4	2	11	3.51	4.10	3.51
-2	2	11	2.24	1.33	3.37
0	2	11	7.36	6.57	3.20
2	2	11	5.03	4.41	3.53
4	2	11	20.07	19.53	0.69
6	2	11	7.61	7.80	3.14
8	2	11	1.23*	1.36	3.20
10	2	11	3.26	3.08	3.49
12	2	11	1.75*	1.14	3.29
-14	2	12	4.54	4.93	3.54
-12	2	12	2.68*	3.55	3.43
-10	2	12	3.36	3.47	3.50
-8	2	12	10.93	11.08	2.24
-6	2	12	0.89*	1.20	3.13
-4	2	12	6.04	5.61	3.44
-2	2	12	6.33	6.49	3.40
0	2	12	5.03	4.67	3.53
2	2	12	10.09	9.90	2.47
4	2	12	9.33	8.78	2.69
6	2	12	3.43	3.70	3.50
8	2	12	3.16	3.23	3.48
10	2	12	2.87	2.38	3.45
12	2	12	1.31*	0.01	3.21
-14	2	13	1.30*	0.28	3.21
-12	2	13	2.08*	0.92	3.34
-10	2	13	2.75	3.10	3.44
-8	2	13	7.82	8.31	3.09
-6	2	13	1.48*	2.23	3.24
-4	2	13	6.22	6.11	3.41
-2	2	13	5.64	6.18	3.48
0	2	13	3.19	3.49	3.48
2	2	13	1.63*	1.60	3.27
4	2	13	7.56	7.42	3.16
6	2	13	0.98*	0.54	3.15
8	2	13	3.83	3.28	3.53
10	2	13	2.49	2.10	3.40
12	2	13	1.32*	0.81	3.21
-14	2	14	3.67	2.87	3.52
-12	2	14	3.91	3.43	3.53
-10	2	14	4.59	4.84	3.54
-8	2	14	1.95*	1.80	3.32
-6	2	14	2.52	2.29	3.41
-4	2	14	7.99	8.44	3.05
-2	2	14	13.26	14.12	1.65
0	2	14	6.70	6.96	3.33
2	2	14	3.53	3.72	3.51
4	2	14	3.65	3.15	3.52
6	2	14	3.63	3.18	3.52
8	2	14	4.25	4.16	3.54

h	k	l	Fo	Fc	weight
10	2	14	6.93	6.60	3.29
-12	2	15	3.30	3.38	3.49
-10	2	15	3.98	4.31	3.54
-8	2	15	2.08*	0.58	3.34
-6	2	15	1.14*	1.93	3.18
-4	2	15	1.31*	1.58	3.21
-2	2	15	4.29	5.01	3.54
0	2	15	6.27	6.86	3.40
2	2	15	2.85	2.78	3.45
4	2	15	1.14*	0.66	3.18
6	2	15	0.69*	2.33	3.09
8	2	15	1.56*	0.66	3.26
10	2	15	2.80	3.39	3.44
-12	2	16	1.95*	0.70	3.32
-10	2	16	4.08	4.78	3.54
-8	2	16	1.59*	0.64	3.26
-6	2	16	2.99	2.59	3.46
-4	2	16	2.98	2.91	3.46
-2	2	16	3.06	3.10	3.47
0	2	16	0.37*	0.75	3.03
2	2	16	5.97	5.96	3.45
4	2	16	4.46	4.38	3.54
6	2	16	1.22*	1.47	3.19
8	2	16	2.76	2.74	3.44
-12	2	17	1.05*	1.92	3.16
-10	2	17	1.35*	2.68	3.22
-8	2	17	0.58*	0.96	3.07
-6	2	17	1.67*	0.98	3.28
-4	2	17	4.31	4.71	3.54
-2	2	17	7.16	8.05	3.24
0	2	17	1.97*	1.15	3.33
2	2	17	1.14*	0.54	3.18
4	2	17	0.81*	0.07	3.12
6	2	17	0.42*	0.54	3.04
8	2	17	4.84	4.69	3.53
-10	2	18	2.33*	1.94	3.38
-8	2	18	3.36	3.04	3.50
-6	2	18	4.32	4.23	3.54
-4	2	18	1.24*	0.11	3.20
-2	2	18	4.55	3.77	3.54
0	2	18	7.19	6.98	3.24
2	2	18	1.20*	0.64	3.19
4	2	18	1.38*	2.00	3.22
6	2	18	2.38*	2.30	3.39
-8	2	19	1.44*	1.27	3.23
-6	2	19	1.25*	0.85	3.20
-4	2	19	4.79	5.14	3.54
-2	2	19	1.30*	2.17	3.21
0	2	19	2.16*	1.66	3.35
2	2	19	2.11*	1.44	3.35
4	2	19	1.94*	0.87	3.32
-8	2	20	5.71	5.72	3.48
-6	2	20	1.74*	0.87	3.29
-4	2	20	1.92*	2.49	3.32
-2	2	20	3.93	3.51	3.53
0	2	20	2.31*	2.26	3.38
2	2	20	7.84	7.83	3.09
4	2	20	2.36*	2.68	3.38
-4	2	21	1.36*	0.33	3.22
-2	2	21	2.07*	1.92	3.34
0	2	21	2.22*	1.27	3.36
-15	3	0	1.25*	0.48	3.20
-9	3	0	3.51	2.94	3.51
1	3	0	7.04	7.73	3.27
3	3	0	6.51	6.80	3.37
5	3	0	2.98	2.83	3.46
7	3	0	1.03*	1.15	3.16
11	3	0	3.90	3.69	3.53
13	3	0	1.71*	1.39	3.28
-15	3	1	1.31*	0.41	3.21
-13	3	1	4.54	4.37	3.54
-11	3	1	14.95	14.86	1.32
-9	3	1	7.33	7.22	3.21
-7	3	1	6.31	6.34	3.40
-5	3	1	5.77	5.13	3.47
-3	3	1	2.85	3.12	3.45
-1	3	1	21.90	22.26	0.56
1	3	1	28.25	29.02	0.29
3	3	1	9.33	8.47	2.69
5	3	1	2.00	2.33	3.33
7	3	1	5.81	5.14	3.47
9	3	1	1.77*	0.88	3.29
11	3	1	9.08	9.37	2.76
13	3	1	4.14	4.20	3.54
15	3	1	0.86*	0.20	3.13
-15	3	2	1.30*	0.40	3.21
-13	3	2	1.31*	1.45	3.21
-11	3	2	9.45	9.12	2.65
-9	3	2	4.09	3.65	3.54
-7	3	2	5.27	5.66	3.52
-5	3	2	10.79	10.17	2.28
-3	3	2	9.59	10.56	2.61
-1	3	2	2.67	3.09	3.43
1	3	2	21.81	21.36	0.56
3	3	2	8.22	7.93	2.99
5	3	2	2.13	0.78	3.35
7	3	2	13.76	13.91	1.55
9	3	2	5.86	6.04	3.46
11	3	2	1.19*	0.93	3.19
13	3	2	1.66*	0.55	3.27
15	3	2	1.28*	0.10	3.21
-15	3	3	2.58	2.28	3.41
-13	3	3	3.70	3.25	3.52
-11	3	3	9.95	9.67	2.51
-9	3	3	1.59*	1.08	3.26
-7	3	3	6.73	7.01	3.33
-5	3	3	11.18	10.53	2.17
-3	3	3	1.53*	1.37	3.25
-1	3	3	19.56	19.62	0.73
1	3	3	17.71	17.89	0.92
3	3	3	4.65	4.93	3.54
5	3	3	7.68	7.34	3.13
7	3	3	2.88	3.17	3.45
9	3	3	1.06*	0.63	3.16
11	3	3	5.66	6.02	3.48
13	3	3	2.34	2.25	3.38
15	3	3	1.96*	0.62	3.32
-15	3	4	1.31*	1.73	3.21
-13	3	4	3.92	4.41	3.53
-11	3	4	15.02	14.30	1.31
-9	3	4	2.99	3.05	3.46
-7	3	4	2.75	2.66	3.44
-5	3	4	15.91	16.72	1.16
-3	3	4	5.42	5.55	3.50
-1	3	4	31.75	30.71	0.21
1	3	4	15.39	13.85	1.25
3	3	4	1.38*	1.23	3.22
5	3	4	4.92	5.87	3.54
7	3	4	11.06	11.62	2.20
9	3	4	3.08	3.74	3.47
11	3	4	10.03	9.58	2.49
13	3	4	2.17*	1.70	3.36
15	3	4	1.88*	0.20	3.31
-15	3	5	5.07	4.57	3.53
-13	3	5	1.20*	0.97	3.19
-11	3	5	2.46	1.90	3.40
-9	3	5	8.63	8.17	2.88
-7	3	5	8.25	8.12	2.98
-5	3	5	17.61	18.26	0.93
-3	3	5	19.41	19.07	0.74
-1	3	5	3.07	1.62	3.47
1	3	5	11.19	11.03	2.17
3	3	5	12.46	12.51	1.84
5	3	5	12.50	13.18	1.83
7	3	5	11.36	11.89	2.12
9	3	5	4.57	4.34	3.54
11	3	5	2.28*	2.81	3.37
13	3	5	2.20*	2.13	3.36
-15	3	6	1.22*	1.43	3.20
-13	3	6	6.22	6.62	3.41
-11	3	6	7.32	6.86	3.21
-9	3	6	3.49	2.94	3.51
-7	3	6	7.00	7.35	3.28
-5	3	6	3.39	3.34	3.50
-3	3	6	9.24	9.04	2.71
-1	3	6	25.08	23.33	0.39
1	3	6	2.31	1.77	3.38
3	3	6	3.69	3.44	3.52
5	3	6	7.72	7.26	3.12
7	3	6	0.90*	1.44	3.13
9	3	6	12.35	12.33	1.87
11	3	6	6.39	6.64	3.39
13	3	6	1.33*	0.04	3.22
-15	3	7	1.38*	0.21	3.22
-13	3	7	4.04	3.70	3.54
-11	3	7	1.51*	1.52	3.25
-9	3	7	3.14	2.84	3.48
-7	3	7	29.01	29.54	0.27
-5	3	7	19.05	19.88	0.78
-3	3	7	4.16	3.15	3.54
-1	3	7	20.23	19.73	0.67
1	3	7	4.44	4.09	3.54
3	3	7	13.25	13.16	1.66
5	3	7	29.78	30.77	0.25
7	3	7	9.16	8.28	2.74
9	3	7	5.44	5.29	3.50
11	3	7	6.33	5.88	3.40
13	3	7	1.27*	1.16	3.20
15	3	8	2.52*	0.16	3.41
-13	3	8	1.34*	1.27	3.22
-11	3	8	0.86*	1.52	3.13
-9	3	8	4.71	4.84	3.54
-7	3	8	21.59	22.81	0.58
-5	3	8	7.88	9.01	3.08
-3	3	8	10.81	9.74	2.27
-1	3	8	9.63	9.91	2.60
1	3	8	4.48	4.13	3.54
3	3	8	9.60	9.47	2.61
5	3	8	24.64	24.06	0.41
7	3	8	1.81*	1.03	3.30
9	3	8	5.57	5.22	3.49
11	3	8	4.32	4.19	3.54
13	3	8	1.33*	0.97	3.22
-15	3	9	4.45	3.57	3.54
-13	3	9	5.31	5.01	3.51
-11	3	9	1.26*	1.13	3.20
-9	3	9	1.15*	0.64	3.18
-7	3	9	9.31	9.67	2.69
-5	3	9	10.89	10.71	2.25
-3	3	9	20.11	20.23	0.68
-1	3	9	16.20	16.41	1.12
1	3	9	3.82	3.85	3.53
3	3	9	4.81	5.32	3.54
5	3	9	4.44	4.81	3.54
7	3	9	10.53	10.89	2.35
9	3	9	10.29	10.50	2.42
11	3	9	1.17*	2.22	3.18
13	3	9	2.42*	1.04	3.39
-13	3	10	2.92	3.19	3.46
-11	3	10	1.37*	2.51	3.22
-9	3	10	2.43	2.27	3.39
-7	3	10	19.14	19.52	0.77
-5	3	10	3.66	3.56	3.52
-3	3	10	9.14	8.85	2.74
-1	3	10	1.63*	0.59	3.27
1	3	10	2.77	2.81	3.44
3	3	10	13.96	14.20	1.51
5	3	10	13.49	13.16	1.61
7	3	10	1.78*	0.58	3.29
9	3	10	4.54	4.29	3.54
11	3	10	1.63*	0.89	3.27
-13	3	11	2.21*	1.03	3.36
-11	3	11	4.08	3.59	3.54
-9	3	11	1.12*	0.49	3.18
-7	3	11	1.87*	1.94	3.31
-5	3	11	4.21	4.20	3.54
-3	3	11	3.88	4.17	3.54
-1	3	11	9.43	10.99	2.66
1	3	11	7.92	8.51	3.07
3	3	11	1.05*	1.62	3.16
5	3	11	1.78*	0.47	3.29
7	3	11	4.16	4.25	3.54

h	k	l	Fo	Fc	weight
9	3	11	3.20	2.69	3.48
11	3	11	4.65	4.36	3.54
-13	3	12	1.89*	2.86	3.31
-11	3	12	2.52*	3.62	3.41
-9	3	12	2.22*	0.76	3.36
-7	3	12	5.61	6.12	3.49
-5	3	12	7.41	6.91	3.19
-3	3	12	14.75	15.54	1.36
-1	3	12	4.90	5.67	3.54
1	3	12	1.02*	0.68	3.16
3	3	12	9.89	9.96	2.53
5	3	12	1.15*	0.92	3.18
7	3	12	5.78	5.41	3.47
9	3	12	5.78	5.60	3.47
11	3	12	2.01*	2.60	3.33
-13	3	13	2.33*	2.22	3.38
-11	3	13	2.08*	1.20	3.34
-9	3	13	4.93	4.17	3.53
-7	3	13	6.26	6.19	3.41
-5	3	13	2.29*	2.18	3.37
-3	3	13	7.87	8.77	3.08
-1	3	13	3.04	3.33	3.47
1	3	13	6.31	6.53	3.40
3	3	13	9.16	9.34	2.74
5	3	13	6.46	6.33	3.38
7	3	13	3.03	2.36	3.47
9	3	13	5.80	5.58	3.47
-11	3	14	1.77*	2.62	3.29
-9	3	14	4.84	4.31	3.54
-7	3	14	1.95*	2.14	3.32
-5	3	14	1.56*	1.85	3.26
-3	3	14	5.12	6.17	3.53
-1	3	14	2.09*	4.28	3.34
1	3	14	0.84*	0.19	3.12
3	3	14	3.55	2.99	3.51
5	3	14	1.53*	0.13	3.25
7	3	14	1.66*	1.90	3.27
9	3	14	4.53	4.23	3.54
-11	3	15	1.37*	0.28	3.22
-9	3	15	3.88	3.56	3.53
-7	3	15	6.23	6.41	3.41
-5	3	15	1.94*	1.84	3.32
-3	3	15	5.12	5.11	3.53
-1	3	15	1.10*	0.77	3.17
1	3	15	0.70*	1.58	3.10
3	3	15	6.13	5.68	3.42
5	3	15	3.73	3.43	3.52
7	3	15	1.95*	1.77	3.32
9	3	15	0.89*	1.06	3.13
-11	3	16	2.47*	3.16	3.40
-9	3	16	5.27	4.64	3.52
-7	3	16	2.09*	0.57	3.34
-5	3	16	2.79	3.35	3.44
-3	3	16	2.34*	3.21	3.38
-1	3	16	2.41	2.54	3.39
1	3	16	7.25	6.86	3.22
3	3	16	3.15	3.21	3.48
5	3	16	2.34*	0.54	3.38
7	3	16	1.85*	0.34	3.31
9	3	16	5.71	5.21	3.48
-9	3	17	5.70	4.84	3.48
-7	3	17	6.27	5.98	3.41
-5	3	17	2.06*	2.02	3.34
-3	3	17	2.19*	1.78	3.36
-1	3	17	1.20*	0.99	3.19
1	3	17	1.64*	0.66	3.27
3	3	17	5.71	5.21	3.48
5	3	17	3.18	3.22	3.48
-9	3	18	2.64*	1.77	3.42
-7	3	18	2.10*	1.64	3.34
-5	3	18	1.99*	2.64	3.33
-3	3	18	1.24*	0.39	3.20
-1	3	18	1.51*	1.14	3.25
1	3	18	1.41*	3.03	3.23
3	3	18	3.63	3.44	3.52
5	3	18	1.27*	0.05	3.20
-7	3	19	1.54*	1.63	3.25
-5	3	19	3.68	3.74	3.52
-3	3	19	1.31*	0.41	3.21
-1	3	19	2.40	2.48	3.39
1	3	19	1.29*	0.27	3.21
3	3	19	1.27*	0.13	3.20
-3	3	20	1.37*	0.39	3.22
-1	3	20	1.61*	0.37	3.26
-12	4	0	9.07	8.41	2.76
-2	4	0	8.37	8.30	2.95
0	4	0	28.85	29.03	0.27
4	4	0	3.78	3.55	3.53
6	4	0	1.03*	0.76	3.16
8	4	0	1.13*	1.21	3.18
10	4	0	8.02	8.00	3.04
14	4	0	1.31*	0.01	3.21
-14	4	1	1.46*	0.49	3.24
-12	4	1	7.16	6.75	3.24
-10	4	1	10.20	10.06	2.44
-8	4	1	6.60	6.80	3.35
-6	4	1	4.71	4.77	3.54
-4	4	1	13.90	14.36	1.52
-2	4	1	9.16	9.09	2.74
0	4	1	22.22	22.14	0.54
2	4	1	7.57	7.28	3.15
4	4	1	6.55	6.44	3.36
6	4	1	6.74	7.04	3.33
8	4	1	8.32	8.72	2.96
10	4	1	8.49	8.61	2.92
12	4	1	5.53	5.73	3.50
14	4	1	1.93*	0.56	3.32
-14	4	2	2.48*	0.03	3.40
-12	4	2	5.19	4.63	3.52
-10	4	2	2.07*	1.39	3.34
-8	4	2	4.24	4.05	3.54
-6	4	2	9.31	9.64	2.70
-4	4	2	8.93	9.33	2.80
-2	4	2	9.57	9.83	2.62
0	4	2	9.21	10.05	2.72
2	4	2	4.54	3.87	3.54
4	4	2	3.71	4.03	3.52
6	4	2	8.80	8.88	2.84
8	4	2	2.66	2.62	3.42
10	4	2	9.09	8.31	2.76
12	4	2	4.19	4.41	3.54
14	4	2	1.28*	0.09	3.21
-14	4	3	3.96	3.51	3.54
-12	4	3	3.61	3.85	3.53
-10	4	3	2.31	2.80	3.38
-8	4	3	1.11*	0.54	3.17
-6	4	3	2.03*	2.28	3.33
-4	4	3	2.47	2.87	3.40
-2	4	3	3.32	4.51	3.49
0	4	3	10.40	10.25	2.38
2	4	3	4.10	4.19	3.54
4	4	3	2.86	2.56	3.45
6	4	3	1.26*	1.40	3.20
8	4	3	3.57	3.29	3.51
10	4	3	1.24*	0.21	3.20
12	4	3	2.22*	2.75	3.36
-14	4	4	1.37*	1.08	3.22
-12	4	4	2.30	1.80	3.38
-10	4	4	1.18*	0.24	3.19
-8	4	4	7.54	7.09	3.16
-6	4	4	18.42	18.95	0.84
-4	4	4	9.34	9.74	2.68
-2	4	4	4.00	4.09	3.54
0	4	4	5.82	6.21	3.46
2	4	4	4.48	3.98	3.54
4	4	4	11.17	11.44	2.17
6	4	4	16.88	16.99	1.02
8	4	4	2.49	2.34	3.40
10	4	4	2.72	2.52	3.43
12	4	4	3.03	2.92	3.47
-14	4	5	3.07	3.14	3.47
-12	4	5	2.19*	2.72	3.36
-10	4	5	1.70*	1.95	3.28
-8	4	5	2.28	1.13	3.37
-6	4	5	14.31	14.73	1.44
-4	4	5	14.67	16.16	1.37
-2	4	5	3.33	3.98	3.50
0	4	5	8.53	10.11	2.63
2	4	5	4.64	3.98	3.54
4	4	5	7.00	7.13	3.28
6	4	5	11.79	12.02	2.01
8	4	5	7.71	7.64	3.12
10	4	5	1.17*	0.59	3.19
12	4	5	2.18*	2.43	3.36
-14	4	6	1.37*	0.35	3.22
-12	4	6	1.38*	1.23	3.22
-10	4	6	3.28	3.06	3.49
-8	4	6	1.18*	2.03	3.19
-6	4	6	1.90*	1.64	3.31
-4	4	6	3.98	3.75	3.54
-2	4	6	1.45*	0.82	3.24
0	4	6	5.64	5.82	3.48
2	4	6	4.06	3.96	3.54
4	4	6	2.82	3.15	3.44
6	4	6	1.21*	0.28	3.19
8	4	6	1.16*	0.78	3.18
10	4	6	1.19*	0.15	3.19
12	4	6	1.44*	0.73	3.23
-14	4	7	1.39*	0.14	3.23
-12	4	7	3.55	3.59	3.51
-10	4	7	2.51	3.15	3.41
-8	4	7	5.65	5.53	3.48
-6	4	7	15.27	15.89	1.27
-4	4	7	4.60	4.96	3.54
-2	4	7	6.41	6.39	3.38
0	4	7	8.74	9.19	2.85
2	4	7	3.10	2.69	3.48
4	4	7	13.58	13.63	1.59
6	4	7	8.00	7.84	3.05
8	4	7	1.51*	1.34	3.25
10	4	7	4.86	4.69	3.54
12	4	7	1.30*	0.91	3.21
-12	4	8	1.34*	0.28	3.22
-10	4	8	5.79	5.06	3.47
-8	4	8	1.90*	2.47	3.31
-6	4	8	2.25	2.30	3.37
-4	4	8	4.86	4.72	3.54
-2	4	8	5.55	6.56	3.49
0	4	8	6.50	6.85	3.37
2	4	8	8.09	8.20	3.03
4	4	8	1.70*	1.65	3.28
6	4	8	0.92*	1.47	3.14
8	4	8	3.46	3.22	3.51
10	4	8	1.30*	1.83	3.21
12	4	8	3.18	2.80	3.48
-12	4	9	2.46*	2.69	3.40
-10	4	9	1.52*	2.24	3.25
-8	4	9	5.80	6.21	3.46
-6	4	9	2.82	3.68	3.44
-4	4	9	5.11	5.11	3.53
-2	4	9	4.48	4.64	3.54
0	4	9	0.79*	0.67	3.11
2	4	9	1.14*	0.09	3.18
4	4	9	10.29	10.63	2.42
6	4	9	2.19	2.05	3.36
8	4	9	5.80	5.80	3.47
10	4	9	2.06*	2.06	3.34
-12	4	10	0.61*	1.66	3.08
-10	4	10	1.09*	1.37	3.17
-8	4	10	5.01	3.86	3.53
-6	4	10	2.33*	3.03	3.38
-4	4	10	2.05*	1.85	3.34
-2	4	10	6.07	5.18	3.43
0	4	10	1.81*	2.28	3.30
2	4	10	3.96	3.33	3.54
4	4	10	4.51	4.67	3.54
6	4	10	4.53	4.24	3.54
8	4	10	2.18*	2.11	3.36
10	4	10	1.32*	0.86	3.21
-12	4	11	2.06*	0.11	3.34
-10	4	11	1.57*	1.20	3.26
-8	4	11	2.19*	2.18	3.36
-6	4	11	4.56	3.88	3.54

h	k	l	Fo	Fc	weight
-4	4	11	4.37	4.22	3.54
-2	4	11	2.06*	3.07	3.34
0	4	11	0.64*	3.11	3.08
2	4	11	2.45	1.89	3.40
4	4	11	3.34	3.50	3.50
6	4	11	4.48	4.39	3.54
8	4	11	2.16*	1.61	3.35
10	4	11	2.22*	2.60	3.36
-12	4	12	1.39*	0.85	3.23
-10	4	12	1.95*	1.04	3.32
-8	4	12	4.87	4.78	3.53
-6	4	12	2.40*	1.46	3.39
-4	4	12	9.45	8.64	2.66
-2	4	12	5.82	6.34	3.47
0	4	12	2.30	2.55	3.38
2	4	12	1.12*	0.49	3.18
4	4	12	5.27	5.01	3.52
6	4	12	1.16*	1.40	3.18
8	4	12	5.85	5.63	3.46
-10	4	13	1.79*	1.32	3.29
-8	4	13	1.61*	2.20	3.27
-6	4	13	2.31*	1.81	3.38
-4	4	13	4.49	4.76	3.54
-2	4	13	8.17	8.70	3.00
0	4	13	1.46*	1.55	3.24
2	4	13	1.16*	0.72	3.18
4	4	13	2.80	3.25	3.44
6	4	13	1.63*	1.05	3.27
8	4	13	4.22	4.57	3.54
-10	4	14	1.25*	2.14	3.20
-8	4	14	9.45	8.57	2.65
-6	4	14	3.83	3.69	3.53
-4	4	14	3.40	0.21	3.50
-2	4	14	1.23*	1.32	3.20
0	4	14	1.66*	1.19	3.27
2	4	14	4.35	3.61	3.54
4	4	14	7.63	7.32	3.14
6	4	14	1.30*	0.29	3.21
-8	4	15	7.01	6.67	3.27
-6	4	15	7.41	6.81	3.19
-4	4	15	5.74	6.26	3.47
-2	4	15	1.48*	2.15	3.24
0	4	15	2.27*	2.73	3.37
2	4	15	2.25*	3.03	3.37
4	4	15	7.06	6.41	3.26
6	4	15	4.34	4.22	3.54
-8	4	16	4.21	4.32	3.54
-6	4	16	1.32*	1.24	3.21
-4	4	16	1.28*	1.99	3.21
-2	4	16	2.50*	2.17	3.40
0	4	16	1.59*	1.38	3.26
2	4	16	7.32	6.77	3.21
4	4	16	2.63	3.13	3.42
-6	4	17	2.30*	1.26	3.38
-4	4	17	1.32*	0.67	3.21
-2	4	17	2.45	1.98	3.40
0	4	17	2.26*	0.41	3.37
2	4	17	2.46*	1.30	3.40
-2	4	18	7.37	6.60	3.20
0	4	18	6.22	6.13	3.41
-7	5	0	2.09*	2.14	3.34
-5	5	0	1.34*	0.97	3.22
1	5	0	9.69	9.51	2.59
3	5	0	1.73*	2.20	3.29
9	5	0	1.01*	1.34	3.16
-11	5	1	2.56*	0.61	3.41
-9	5	1	4.70	4.74	3.54
-7	5	1	1.22*	1.16	3.19
-5	5	1	10.92	10.72	2.24
-3	5	1	9.44	9.21	2.66
-1	5	1	1.49*	1.43	3.24
1	5	1	1.45*	0.44	3.24
3	5	1	6.16	6.24	3.42
5	5	1	1.97*	1.57	3.32
7	5	1	8.46	8.51	2.93
9	5	1	3.90	4.19	3.53
11	5	1	1.31*	1.29	3.21
-11	5	2	6.00	5.61	3.44
-9	5	2	3.88	4.06	3.53
-7	5	2	10.10	10.13	2.47
-5	5	2	9.16	9.47	2.74
-3	5	2	4.51	4.82	3.54
-1	5	2	12.36	12.55	1.86
1	5	2	10.11	10.49	2.47
3	5	2	8.21	8.31	2.99
5	5	2	11.43	11.55	2.10
7	5	2	4.59	4.86	3.54
9	5	2	2.84	3.07	3.45
11	5	2	6.65	6.62	3.34
-11	5	3	2.49*	2.11	3.40
-9	5	3	1.98*	0.85	3.33
-7	5	3	2.97	2.62	3.46
-5	5	3	1.47*	1.81	3.24
-3	5	3	7.24	7.15	3.23
-1	5	3	10.82	10.63	2.27
1	5	3	4.00	4.12	3.54
3	5	3	1.71*	1.36	3.28
5	5	3	4.90	4.91	3.54
7	5	3	1.44*	0.27	3.23
9	5	3	5.35	5.32	3.51
11	5	3	4.04	3.89	3.54
-11	5	4	4.23	4.15	3.54
-9	5	4	1.75*	2.21	3.29
-7	5	4	7.58	7.79	3.15
-5	5	4	5.57	6.83	3.49
-3	5	4	1.53*	0.01	3.25
-1	5	4	8.46	9.13	2.93
1	5	4	7.15	7.51	3.24
3	5	4	5.68	5.55	3.48
5	5	4	9.68	10.05	2.58
7	5	4	1.66*	1.19	3.27
9	5	4	3.54	3.81	3.51
11	5	4	4.57	4.52	3.54
-11	5	5	1.28*	1.08	3.21
-9	5	5	2.12*	1.25	3.35
-7	5	5	1.87*	1.18	3.31
-5	5	5	5.89	5.78	3.46
-3	5	5	7.65	8.02	3.13
-1	5	5	3.19	3.09	3.48
1	5	5	1.18*	1.87	3.19
3	5	5	1.12*	0.55	3.18
5	5	5	1.20*	0.23	3.19
7	5	5	5.40	5.35	3.51
9	5	5	4.87	5.32	3.54
-11	5	6	1.32*	1.19	3.21
-9	5	6	1.30*	2.42	3.21
-7	5	6	3.72	3.58	3.52
-5	5	6	1.03*	1.48	3.16
-3	5	6	3.14	3.47	3.48
-1	5	6	1.72*	0.83	3.28
1	5	6	1.51*	1.92	3.25
3	5	6	1.13*	0.08	3.18
5	5	6	5.12	5.21	3.53
7	5	6	1.21*	0.59	3.19
9	5	6	1.31*	0.71	3.21
-11	5	7	1.25*	1.27	3.20
-9	5	7	3.28	3.18	3.49
-7	5	7	1.94*	1.83	3.32
-5	5	7	1.21*	1.67	3.19
-3	5	7	1.72*	2.25	3.28
-1	5	7	0.85*	1.29	3.12
1	5	7	1.43*	2.36	3.23
3	5	7	3.54	3.09	3.51
5	5	7	0.88*	1.43	3.15
7	5	7	0.59*	0.16	3.07
9	5	7	1.29*	0.39	3.21
-11	5	8	1.61*	1.08	3.26
-9	5	8	2.09*	2.68	3.34
-7	5	8	2.17*	2.31	3.36
-5	5	8	1.44*	0.74	3.23
-3	5	8	3.16	4.11	3.48
-1	5	8	1.19*	0.79	3.19
1	5	8	3.57	4.25	3.51
3	5	8	1.37*	1.03	3.22
5	5	8	2.56	2.89	3.41
7	5	8	2.08*	1.13	3.34
9	5	8	2.39	1.84	3.39
-9	5	9	1.98*	0.21	3.33
-7	5	9	3.24	2.47	3.49
-5	5	9	3.45	3.42	3.51
-3	5	9	0.56*	0.40	3.07
-1	5	9	2.33*	2.00	3.38
1	5	9	0.69*	1.69	3.09
3	5	9	2.10*	0.27	3.35
5	5	9	3.08	2.79	3.47
7	5	9	2.37	2.80	3.39
-9	5	10	1.32*	0.32	3.21
-7	5	10	3.61	4.31	3.52
-5	5	10	1.59*	1.89	3.26
-3	5	10	1.17*	0.59	3.19
-1	5	10	1.24*	0.02	3.20
1	5	10	2.06*	1.39	3.34
3	5	10	1.22*	2.25	3.19
5	5	10	3.19	3.72	3.48
7	5	10	1.24*	0.45	3.20
-9	5	11	1.40*	1.35	3.23
-7	5	11	8.39	7.31	2.95
-5	5	11	6.85	6.92	3.31
-3	5	11	1.97*	2.19	3.33
-1	5	11	1.18*	0.70	3.19
1	5	11	0.71*	0.65	3.10
3	5	11	3.13	2.33	3.48
5	5	11	6.88	6.24	3.30
7	5	11	3.52	3.27	3.51
-7	5	12	7.46	7.19	3.18
-5	5	12	1.35*	1.04	3.22
-3	5	12	1.51*	1.26	3.25
-1	5	12	3.01	2.66	3.47
1	5	12	1.52*	2.18	3.25
3	5	12	5.13	5.08	3.52
5	5	12	4.32	4.44	3.54
-7	5	13	3.63	3.39	3.52
-5	5	13	1.91*	1.02	3.31
-3	5	13	3.46	3.57	3.51
-1	5	13	1.28*	1.40	3.21
1	5	13	1.72*	0.71	3.28
3	5	13	5.04	4.28	3.53
-5	5	14	1.40*	1.37	3.23
-3	5	14	1.33*	0.61	3.21
-1	5	14	2.35*	1.81	3.38
1	5	14	1.91*	1.36	3.32
3	5	14	5.12	4.50	3.53
-3	5	15	1.00*	0.11	3.15
-1	5	15	5.73	4.83	3.47
-4	6	0	1.27*	0.04	3.20
-2	6	0	1.36*	2.88	3.22
0	6	0	3.97	3.34	3.54
2	6	0	2.49	2.88	3.40
4	6	0	1.29*	0.82	3.21
6	6	0	1.31*	0.43	3.21
-8	6	1	2.04*	2.08	3.34
-6	6	1	0.74*	0.95	3.10
-4	6	1	1.27*	2.79	3.20
-2	6	1	2.08*	2.15	3.34
0	6	1	7.27	7.85	3.22
2	6	1	0.71*	1.48	3.10
4	6	1	1.33*	2.06	3.21
6	6	1	1.30*	1.74	3.21
8	6	1	1.73*	0.84	3.29
-8	6	2	4.97	4.73	3.53
-6	6	2	4.30	4.70	3.54
-4	6	2	3.68	3.95	3.52
-2	6	2	3.20	2.49	3.48
0	6	2	1.20*	1.23	3.19
2	6	2	6.26	6.83	3.41
4	6	2	7.65	7.40	3.13
6	6	2	2.89	3.41	3.45
-6	6	3	1.36*	1.20	3.22
-4	6	3	3.68	3.55	3.52
-2	6	3	1.52*	0.03	3.25
0	6	3	4.16	4.18	3.54
2	6	3	5.31	5.32	3.51

h	k	l	Fo	Fc	weight
2	6	3	1.38*	1.18	3.22
4	6	3	3.26	3.17	3.49
6	6	3	1.73*	2.40	3.29
-8	6	4	1.84*	1.60	3.30
-6	6	4	1.28*	0.32	3.21
-4	6	4	1.19*	0.01	3.19
-2	6	4	1.00*	0.91	3.15
0	6	4	0.42*	1.04	3.04
2	6	4	2.85*	3.48	3.41
4	6	4	1.65*	2.43	3.27
6	6	4	0.88*	0.52	3.13
-6	6	5	1.48*	2.26	3.24
-4	6	5	3.18	3.09	3.48
-2	6	5	4.89	4.66	3.54
0	6	5	5.37	4.83	3.51
2	6	5	3.03	2.68	3.47
4	6	5	6.14	5.82	3.42
6	6	5	1.98*	0.31	3.33
-6	6	6	2.44*	2.39	3.40
-4	6	6	1.48*	0.27	3.24
-2	6	6	4.53	4.35	3.54
0	6	6	3.34	3.22	3.50
2	6	6	0.95*	2.42	3.14
4	6	6	1.84*	1.67	3.30
6	6	6	2.80	1.85	3.44
-6	6	7	1.17*	1.69	3.19
-4	6	7	0.43*	0.35	3.04
-2	6	7	1.86*	1.32	3.31
0	6	7	3.71	3.09	3.52
2	6	7	2.98	2.41	3.46
4	6	7	4.11	3.59	3.54
-6	6	8	4.11	3.35	3.54
-4	6	8	0.91*	0.45	3.14
-2	6	8	2.63*	3.01	3.42
0	6	8	2.14*	2.96	3.35
2	6	8	2.54*	2.91	3.41
4	6	8	1.94*	2.62	3.32
-4	6	9	4.65	4.70	3.54
-2	6	9	0.44*	1.35	3.04
0	6	9	3.03	2.21	3.47
2	6	9	0.77*	1.62	3.11
-2	6	10	2.22*	1.82	3.36
0	6	10	1.48*	1.29	3.24

1435 reflections

2,3-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

h	k	l	Fo	Fc	weight
0	0	2	42.64	44.69	1.27
0	0	4	38.21	39.11	1.47
0	0	6	12.13	11.85	9.97
0	0	8	32.17	30.89	1.81
0	0	10	8.35	8.87	12.57
0	0	12	14.98	15.02	7.10
0	0	14	24.85	26.06	2.21
0	0	16	2.08*	1.15	0.23
0	0	18	4.04*	2.08	0.83
0	0	20	4.83	5.24	3.22
0	1	21	3.32*	4.81	0.21
0	1	20	1.71*	1.76	0.10
0	1	19	1.17*	1.83	0.04
0	1	18	2.09*	1.15	0.23
0	1	17	5.60	5.53	5.85
0	1	16	2.54*	4.21	0.26
0	1	15	8.44	8.85	8.62
0	1	14	8.31	8.11	8.69
0	1	13	0.91*	0.16	0.08
0	1	12	9.88	10.25	10.19
0	1	11	0.82*	2.33	0.07
0	1	10	2.06*	3.96	0.38
0	1	9	12.22	11.06	9.54
0	1	8	44.39	43.17	1.06
0	1	7	12.15	12.60	8.94
0	1	6	13.84	14.34	7.03
0	1	5	11.41	11.78	10.38
0	1	4	13.33	13.19	7.02
0	1	3	19.50	19.18	4.19
0	1	2	60.47	64.39	0.48
0	1	1	43.09	45.82	1.26
0	2	0	20.91	21.24	4.03
0	2	1	46.02	49.08	1.10
0	2	2	10.88	10.91	9.39
0	2	3	4.57	4.42	11.90
0	2	4	12.27	12.02	8.43
0	2	5	22.86	22.84	3.15
0	2	6	51.93	51.01	0.83
0	2	7	33.55	32.98	1.73
0	2	8	2.23*	1.71	0.58
0	2	9	14.89	15.22	6.10
0	2	10	4.80	4.80	12.19
0	2	11	2.20*	2.50	0.41
0	2	12	14.48	14.48	7.04
0	2	13	7.35	7.22	10.69
0	2	14	8.51	8.36	9.48
0	2	15	1.00*	1.52	0.06
0	2	16	1.91*	0.10	0.27
0	2	17	2.66*	0.51	0.42
0	2	18	2.09*	2.27	0.23
0	2	19	2.62*	2.66	0.35
0	2	20	3.44*	5.87	0.18
0	2	21	3.33*	4.27	0.24
0	3	20	2.54*	0.21	0.16
0	3	19	2.37*	2.19	0.18
0	3	18	3.01*	3.00	0.39
0	3	17	2.45*	1.76	0.21
0	3	16	3.65*	4.73	0.44
0	3	15	2.86*	2.56	0.36
0	3	14	11.70	12.00	7.77
0	3	13	6.52	7.27	7.56
0	3	12	1.99*	0.27	0.38
0	3	11	12.52	11.93	8.62
0	3	10	1.93*	0.87	0.27
0	3	9	9.15	9.21	12.85
0	3	8	21.78	20.75	3.24
0	3	7	19.16	19.35	3.98
0	3	6	1.12*	0.52	0.21
0	3	5	16.21	16.15	6.14
0	3	4	43.65	45.07	1.16
0	3	3	10.85	10.96	10.49
0	3	2	5.28	5.32	12.87
0	3	1	25.63	24.82	2.83
0	4	0	60.81	60.98	0.63
0	4	1	24.21	24.07	2.94
0	4	2	13.01	13.05	8.14
0	4	3	14.64	15.04	6.86
0	4	4	36.90	36.94	1.51
0	4	5	7.06	6.59	16.63
0	4	6	11.73	11.78	10.48
0	4	7	14.73	14.08	6.35
0	4	8	11.01	11.44	10.85
0	4	9	2.87*	3.85	0.73
0	4	10	11.43	11.17	9.73
0	4	11	1.97*	2.05	0.26
0	4	12	9.45	9.42	10.35
0	4	13	17.45	17.64	4.50
0	4	14	15.78	16.11	5.59
0	4	15	2.91*	2.04	0.44
0	4	16	2.21*	1.09	0.21
0	4	17	2.01*	0.50	0.25
0	4	18	2.31*	0.15	0.30
0	4	19	2.48*	0.66	0.16
0	4	20	2.12*	1.61	0.86
0	5	20	2.81*	1.46	0.27
0	5	19	2.43*	1.21	0.17
0	5	18	3.71*	0.13	0.55
0	5	17	2.16*	0.20	0.21
0	5	16	1.54*	2.15	0.13
0	5	15	2.12*	1.47	0.22
0	5	14	2.26*	4.13	0.19
0	5	13	10.48	10.37	8.96
0	5	12	12.09	12.02	8.09
0	5	11	7.66	7.91	11.29
0	5	10	3.49	3.15	6.69
0	5	9	16.93	16.77	4.81
0	5	8	7.82	7.75	12.63
0	5	7	1.78*	1.51	0.31
0	5	6	5.61	6.14	12.94
0	5	5	21.92	21.26	3.27
0	5	4	23.08	21.82	3.20
0	5	3	18.74	18.14	4.20
0	5	2	10.82	10.80	11.98
0	5	1	23.94	24.52	2.82
0	6	0	9.00	8.98	14.44
0	6	1	8.34	8.33	14.45
0	6	2	4.50	4.41	11.75
0	6	3	16.60	16.48	5.35
0	6	4	21.87	20.71	3.27
0	6	5	5.12	5.44	11.99
0	6	6	10.71	10.01	10.54
0	6	7	29.45	27.78	1.87
0	6	8	3.91*	3.18	0.89
0	6	9	1.93*	1.60	0.29
0	6	10	10.67	10.43	10.04
0	6	11	3.72*	4.06	1.03
0	6	12	3.06*	1.17	0.66
0	6	13	6.31	6.60	7.12
0	6	14	3.45*	2.28	0.52
0	6	15	2.30*	1.07	0.19
0	6	16	1.58*	0.84	0.13
0	6	17	2.31*	1.06	0.19
0	6	18	2.72*	0.27	1.99
0	6	19	3.71*	4.65	0.29
0	7	19	2.49*	0.85	0.16
0	7	18	2.34*	1.10	0.18
0	7	17	2.29*	0.48	0.19
0	7	16	2.29*	2.08	0.21
0	7	15	4.69*	4.82	0.63
0	7	14	5.23	4.91	5.85
0	7	13	2.20*	1.76	0.21
0	7	12	8.53	8.76	8.63
0	7	11	0.97*	1.98	0.06
0	7	10	17.61	17.85	4.59
0	7	9	10.55	10.55	9.14
0	7	8	11.89	12.20	9.58
0	7	7	4.84	4.83	8.66
0	7	6	15.49	15.31	5.63
0	7	5	4.31	3.70	9.51
0	7	4	8.29	8.06	12.42
0	7	3	3.60*	4.07	1.05
0	7	2	12.25	11.95	9.14
0	7	1	7.99	8.29	13.22
0	8	0	16.51	16.82	5.72
0	8	1	12.54	12.54	9.16
0	8	2	3.03	3.99	5.01
0	8	3	7.42	7.17	10.92
0	8	4	7.78	7.89	12.30
0	8	5	4.90	5.40	8.09
0	8	6	1.97*	2.78	0.26
0	8	7	4.39	4.11	7.25
0	8	8	4.28	4.36	5.56
0	8	9	10.69	10.17	8.95
0	8	10	8.92	8.64	9.13
0	8	11	10.82	11.25	7.62
0	8	12	2.98*	3.96	2.60
0	8	13	7.06	6.34	8.44
0	8	14	3.31*	5.26	0.25
0	8	15	2.55*	1.90	0.23
0	8	16	2.35*	0.44	0.14
0	8	17	2.17*	0.35	0.21
0	8	18	6.98	5.84	4.80
0	9	17	3.94*	2.93	0.33
0	9	16	4.84*	5.08	0.48
0	9	15	3.52*	2.99	0.32
0	9	14	2.03*	0.98	0.24
0	9	13	5.26	5.28	5.07
0	9	12	5.02	4.68	5.78
0	9	11	5.92	5.98	6.97
0	9	10	2.16*	2.65	0.21
0	9	9	14.23	14.60	6.55
0	9	8	1.98*	2.44	0.25
0	9	7	2.84*	2.66	0.49
0	9	6	2.13*	2.75	0.22
0	9	5	1.92*	1.20	1.95
0	9	4	13.14	13.26	8.25
0	9	3	2.04*	2.87	0.24
0	9	2	3.59*	3.71	0.86
0	9	1	10.86	10.81	8.83
0	10	0	1.92*	0.60	0.27
0	10	1	8.52	8.48	9.46
0	10	2	1.99*	2.02	0.25
0	10	3	9.66	9.32	9.60
0	10	4	6.55	6.38	7.72
0	10	5	2.54*	2.68	0.33
0	10	6	7.97	8.15	8.99
0	10	7	10.23	9.82	8.47
0	10	8	5.52	5.13	6.10
0	10	9	4.80	4.92	5.11
0	10	10	12.11	12.20	7.24
0	10	11	2.39*	3.00	0.18
0	10	12	1.96*	2.34	1.15
0	10	13	3.63*	3.04	0.51
0	10	14	2.04*	0.49	0.26
0	10	15	3.43*	2.61	0.34
0	10	16	2.16*	2.16	0.11
0	11	15	3.32*	3.26	0.32
0	11	14	4.73*	2.20	0.62
0	11	13	3.58*	0.39	0.76
0	11	12	2.24*	2.86	0.20
0	11	11	7.06	7.34	6.40
0	11	10	4.01*	4.01	0.56
0	11	9	4.49*	3.26	0.67
0	11	8	2.08*	1.38	0.23
0	11	7	2.77*	2.01	0.37
0	11	6	2.30*	4.12	0.21
0	11	5	2.03*	1.34	0.22
0	11	4	9.77	10.23	8.19
0	11	3	15.65	15.28	6.22
0	11	2	1.97*	0.10	0.25
0	11	1	5.31	5.54	6.13
0	12	0	2.93*	0.06	0.52
0	12	1	1.35*	0.96	0.55
0	12	2	9.68	9.81	7.91
0	12	3	12.13	12.49	6.95
0	12	4	2.33*	1.62	0.18
0	12	5	6.89	6.10	6.95
0	12	6	5.99	5.82	7.16
0	12	7	3.81*	1.73	0.59
0	12	8	2.38*	0.48	0.18
0	12	9	3.60*	1.99	0.58
0	12	10	2.84*	1.83	0.37

h	k	l	Fo	Fc	weight
0	12	11	3.83*	2.96	0.58
0	12	12	2.46*	1.21	0.16
0	12	13	3.03*	0.44	0.32
0	12	14	2.54*	1.62	0.15
0	13	12	3.35*	4.19	1.56
0	13	11	2.39*	1.27	0.17
0	13	10	2.97*	1.31	0.30
0	13	9	6.74	6.32	6.04
0	13	8	2.34*	1.43	0.20
0	13	7	4.50	4.53	3.52
0	13	6	3.40*	3.62	2.18
0	13	5	9.13	8.65	6.96
0	13	4	7.83	8.08	6.40
0	13	3	6.41	6.27	7.12
0	13	2	2.39*	3.82	0.17
0	13	1	3.29*	3.65	0.47
0	14	0	4.00*	4.27	0.34
0	14	1	2.25*	2.76	0.20
0	14	2	2.32*	1.32	0.35
0	14	3	2.60*	4.10	0.17
0	14	4	2.40*	0.54	0.17
0	14	5	2.37*	2.35	0.25
0	14	6	2.48*	0.22	0.16
0	14	7	2.96*	2.11	0.34
0	14	8	3.88*	2.54	0.45
0	14	9	2.60*	1.33	0.15
0	14	10	5.22	5.35	3.54
0	15	7	1.27*	1.58	0.04
0	15	6	1.25*	0.12	0.04
0	15	5	1.01*	2.80	0.17
0	15	4	2.35*	0.66	0.18
0	15	3	2.73*	2.72	0.20
0	15	2	2.72*	0.89	0.23
0	15	1	2.10*	1.13	0.16
1	15	0	1.22*	1.63	0.05
1	15	1	1.73*	1.17	0.08
1	15	2	5.07	4.57	3.84
1	15	3	2.48*	1.42	0.16
1	15	4	2.44*	2.36	0.17
1	15	5	3.31*	0.31	0.29
1	15	6	5.05*	3.68	0.48
1	14	9	2.46*	0.35	0.17
1	14	8	2.45*	1.07	0.17
1	14	7	4.73*	4.21	0.52
1	14	6	3.19*	2.11	0.28
1	14	5	4.14*	3.55	0.46
1	14	4	4.74*	3.96	0.64
1	14	3	2.29*	1.96	0.19
1	14	2	3.88*	2.58	0.59
1	14	1	2.34*	1.03	0.18
1	14	0	2.25*	1.22	0.20
1	13	0	4.96*	5.47	0.61
1	13	1	2.30*	1.23	0.19
1	13	2	2.35*	1.50	0.18
1	13	3	6.89	6.33	7.11
1	13	4	8.85	8.73	7.88
1	13	5	1.97*	5.81	0.12
1	13	6	5.42	5.06	5.28
1	13	7	2.21*	0.97	0.21
1	13	8	4.65	4.50	3.28
1	13	9	2.69*	3.19	0.26
1	13	10	5.79	5.84	4.11
1	13	11	3.30*	2.08	0.29
1	12	13	2.53*	2.36	0.16
1	12	12	5.77	6.09	3.85
1	12	11	2.39*	2.33	0.19
1	12	10	4.39*	4.21	0.64
1	12	9	2.36*	0.93	0.18
1	12	8	3.58*	3.79	0.48
1	12	7	2.23*	0.51	0.32
1	12	6	2.69*	3.45	0.36
1	12	5	4.33*	4.32	0.76
1	12	4	1.52*	2.09	0.14
1	12	3	6.48	6.94	6.04
1	12	2	5.27	5.27	5.69
1	12	1	5.89	5.83	6.43
1	12	0	1.88*	1.62	0.28
1	11	0	8.74	8.38	8.85
1	11	1	5.67	6.27	6.56
1	11	2	10.69	10.66	8.05
1	11	3	7.92	8.08	7.58
1	11	4	5.88	6.33	6.34
1	11	5	5.71	6.15	6.39
1	11	6	3.87	4.51	3.57
1	11	7	5.09	5.38	5.56
1	11	8	4.26	4.13	5.17
1	11	9	3.09*	3.52	2.46
1	11	10	2.50*	3.47	0.16
1	11	11	4.14*	3.01	0.63
1	11	12	3.33*	3.89	0.31
1	11	13	1.70*	3.64	0.07
1	11	14	2.47*	1.80	0.20
1	11	15	2.53*	1.60	0.17
1	10	16	1.78*	2.12	0.11
1	10	15	2.59*	2.01	0.15
1	10	14	2.38*	1.45	0.24
1	10	13	2.28*	2.61	0.18
1	10	12	1.13*	1.96	0.04
1	10	11	4.68	5.27	4.23
1	10	10	2.13*	1.55	0.22
1	10	9	4.48	4.17	4.72
1	10	8	7.41	7.38	8.43
1	10	7	1.43*	2.43	0.11
1	10	6	2.14*	1.63	0.22
1	10	5	7.62	7.79	8.59
1	10	4	7.63	7.15	8.93
1	10	3	10.59	10.27	8.88
1	10	2	8.54	8.50	8.65
1	10	1	9.58	9.91	8.51
1	10	0	2.30*	3.19	0.22
1	9	0	1.87*	1.57	0.26
1	9	1	2.65*	3.57	0.45
1	9	2	3.77*	3.77	0.92
1	9	3	8.03	8.16	10.88
1	9	4	14.18	14.46	7.58
1	9	5	3.06*	1.94	0.86
1	9	6	5.16	4.82	6.55
1	9	7	7.31	7.02	8.67
1	9	8	8.61	9.12	8.72
1	9	9	7.94	7.90	8.71
1	9	10	9.77	9.61	8.12
1	9	11	1.84*	1.45	0.12
1	9	12	2.18*	1.00	0.21
1	9	13	3.17*	1.54	0.57
1	9	14	3.99*	2.88	0.84
1	9	15	3.75*	0.40	0.48
1	9	16	2.11*	1.76	0.20
1	9	17	3.97*	3.69	0.33
1	8	18	1.26*	2.18	0.04
1	8	17	2.58*	3.18	0.15
1	8	16	3.14*	2.29	0.32
1	8	15	2.43*	3.01	0.17
1	8	14	2.42*	2.63	0.17
1	8	13	5.15	4.75	6.11
1	8	12	7.06	7.64	6.70
1	8	11	2.10*	2.76	0.23
1	8	10	10.52	10.68	8.46
1	8	9	7.15	7.36	7.99
1	8	8	3.24*	4.72	0.47
1	8	7	2.42*	0.53	0.45
1	8	6	2.05*	3.45	0.24
1	8	5	8.49	8.37	11.67
1	8	4	15.11	15.19	6.43
1	8	3	9.48	9.42	10.81
1	8	2	12.96	13.27	7.44
1	8	1	6.65	6.62	11.53
1	8	0	0.83*	1.30	0.07
1	7	0	10.81	10.49	11.09
1	7	1	17.81	16.83	4.40
1	7	2	2.46*	1.57	0.68
1	7	3	23.43	23.27	2.88
1	7	4	16.51	16.23	5.06
1	7	5	3.19*	2.92	1.25
1	7	6	5.09	5.14	10.25
1	7	7	9.84	9.46	10.29
1	7	8	5.59	5.44	10.34
1	7	9	8.98	8.59	9.58
1	7	10	3.43*	3.68	0.58
1	7	11	9.84	10.41	8.54
1	7	12	7.71	7.53	8.80
1	7	13	7.88	8.01	8.16
1	7	14	4.19*	4.86	0.50
1	7	15	4.80	4.83	4.40
1	7	16	2.58*	0.60	0.28
1	7	17	3.96*	2.66	0.51
1	7	18	2.66*	2.09	0.14
1	6	19	2.57*	1.89	0.15
1	6	18	2.57*	2.96	0.15
1	6	17	3.56*	3.43	2.65
1	6	16	2.21*	0.92	0.20
1	6	15	6.00	5.50	6.92
1	6	14	2.35*	2.06	0.27
1	6	13	6.88	6.79	8.18
1	6	12	5.48	5.64	6.63
1	6	11	3.90	4.50	4.10
1	6	10	17.96	18.43	4.42
1	6	9	10.31	10.26	9.66
1	6	8	6.11	6.58	10.25
1	6	7	6.03	6.13	11.40
1	6	6	7.24	7.14	12.74
1	6	5	26.47	26.47	2.24
1	6	4	16.93	15.95	5.05
1	6	3	13.86	12.87	6.97
1	6	2	6.27	5.67	14.80
1	6	1	9.12	9.58	13.04
1	6	0	16.15	15.82	5.48
1	5	0	9.20	9.12	14.56
1	5	1	27.29	25.91	2.33
1	5	2	25.03	25.94	2.54
1	5	3	11.22	10.84	10.70
1	5	4	14.93	14.72	6.67
1	5	5	18.33	19.10	3.72
1	5	6	16.65	15.96	5.30
1	5	7	4.89	4.61	12.06
1	5	8	2.94*	3.51	0.74
1	5	9	13.97	14.47	7.12
1	5	10	10.20	10.19	8.58
1	5	11	11.57	11.77	8.77
1	5	12	4.64	5.30	5.96
1	5	13	10.72	10.69	8.53
1	5	14	1.78*	2.84	0.18
1	5	15	2.38*	0.62	0.37
1	5	16	4.25	4.19	4.85
1	5	17	4.28*	2.19	0.61
1	5	18	3.74*	2.79	0.48
1	5	19	2.50*	0.29	0.16
1	5	20	2.69*	1.68	0.14
1	4	20	4.50*	2.12	0.67
1	4	19	2.41*	2.03	0.27
1	4	18	2.19*	1.35	0.21
1	4	17	2.35*	1.87	0.18
1	4	16	2.18*	1.81	0.21
1	4	15	2.31*	1.91	0.19
1	4	14	5.51	5.55	6.59
1	4	13	8.88	8.80	9.19
1	4	12	8.96	9.19	8.93
1	4	11	11.00	11.87	8.65
1	4	10	11.65	11.71	8.98
1	4	9	15.58	15.79	5.96
1	4	8	13.50	13.33	7.74
1	4	7	14.26	14.21	6.59
1	4	6	21.18	20.56	3.46
1	4	5	12.69	12.56	8.46
1	4	4	24.15	23.60	2.75
1	4	3	12.44	12.27	8.06
1	4	2	15.34	15.12	6.44
1	4	1	13.90	12.91	7.18
1	4	0	21.24	20.01	3.38
1	3	0	54.33	55.82	0.79
1	3	1	73.41	75.69	0.44
1	3	2	18.22	18.67	4.60
1	3	3	21.02	20.76	3.39

h	k	l	Fo	Fc	weight
1	3	4	17.75	17.24	4.72
1	3	5	12.54	12.29	8.52
1	3	6	10.71	10.46	12.15
1	3	7	29.63	29.33	2.02
1	3	8	19.58	19.99	3.45
1	3	9	10.17	10.14	11.99
1	3	10	6.84	6.53	12.84
1	3	11	17.96	17.90	4.38
1	3	12	16.00	15.94	5.37
1	3	13	12.87	12.93	7.52
1	3	14	6.75	7.13	8.95
1	3	15	3.70*	4.21	0.50
1	3	16	0.87*	2.03	0.25
1	3	17	2.32*	2.40	0.19
1	3	18	2.85*	2.29	2.00
1	3	19	1.19*	1.45	0.04
1	3	20	2.64*	1.42	0.14
1	2	20	1.23*	4.87	0.04
1	2	19	3.69	3.45	2.73
1	2	18	1.97*	2.60	0.14
1	2	17	2.21*	0.12	0.21
1	2	16	4.09*	3.87	0.76
1	2	15	6.12	6.14	8.24
1	2	14	4.35*	5.87	0.78
1	2	13	14.12	13.91	6.67
1	2	12	11.34	11.62	9.43
1	2	11	6.56	7.01	11.71
1	2	10	11.22	10.95	10.33
1	2	9	12.83	12.46	8.90
1	2	8	19.49	18.28	3.97
1	2	7	29.38	28.93	2.03
1	2	6	26.33	26.69	2.46
1	2	5	4.87	4.88	13.53
1	2	4	8.44	8.57	15.32
1	2	3	7.94	7.93	14.39
1	2	2	41.23	43.08	1.30
1	2	1	52.07	53.30	0.86
1	2	0	77.85	82.38	0.40
1	1	0	28.58	28.71	2.43
1	1	1	45.24	45.91	1.11
1	1	2	28.37	28.25	2.49
1	1	3	48.97	49.30	0.95
1	1	4	7.33	7.41	15.83
1	1	5	26.81	27.20	2.52
1	1	6	16.79	16.74	4.84
1	1	7	18.05	17.61	5.00
1	1	8	7.70	7.83	14.74
1	1	9	1.07*	0.96	0.17
1	1	10	2.65*	2.09	0.75
1	1	11	13.75	13.24	8.02
1	1	12	3.64*	4.66	0.75
1	1	13	3.06*	3.82	0.36
1	1	14	8.72	8.70	9.01
1	1	15	10.39	10.73	8.53
1	1	16	5.11	5.61	4.41
1	1	17	3.93*	2.18	0.87
1	1	18	2.29*	0.49	0.19
1	1	19	2.36*	3.32	0.18
1	1	20	4.59	3.38	4.01
1	1	21	1.79*	1.62	0.05
1	0	21	2.39*	1.51	0.18
1	0	20	2.46*	2.67	0.16
1	0	19	5.39	4.57	4.43
1	0	18	1.60*	1.19	0.10
1	0	17	2.15*	0.75	0.22
1	0	16	3.77*	0.10	0.85
1	0	15	7.64	8.39	7.79
1	0	14	7.56	7.67	9.47
1	0	13	8.72	8.46	10.69
1	0	12	3.43	3.45	6.07
1	0	11	1.80*	2.15	0.31
1	0	10	5.33	5.69	11.44
1	0	9	20.40	19.49	3.29
1	0	8	13.60	14.16	6.87
1	0	7	28.40	28.13	2.15
1	0	6	17.46	17.13	4.57
1	0	5	26.88	26.23	2.45
1	0	4	5.80	6.05	14.53
1	0	3	12.13	12.29	8.99
1	0	2	4.57	4.47	11.77
1	0	1	81.75	89.78	0.28
2	0	0	33.40	32.57	1.78
2	0	1	23.14	23.14	3.01
2	0	2	16.49	16.85	5.71
2	0	3	17.18	17.20	4.71
2	0	4	12.91	12.91	8.01
2	0	5	10.39	10.40	13.14
2	0	6	25.39	24.70	2.74
2	0	7	9.04	8.97	13.45
2	0	8	20.04	19.82	3.46
2	0	9	1.16*	0.14	0.16
2	0	10	1.61*	0.41	0.31
2	0	11	8.48	8.55	10.23
2	0	12	12.05	12.07	8.23
2	0	13	11.08	11.76	8.15
2	0	14	3.16*	3.68	3.50
2	0	15	8.19	7.70	8.44
2	0	16	2.66*	1.50	0.28
2	0	17	2.24*	0.77	0.20
2	0	18	6.82	6.42	5.66
2	0	19	5.53	5.40	4.25
2	0	20	2.55*	0.54	0.15
2	1	20	2.89*	4.02	0.12
2	1	19	4.53*	2.90	0.75
2	1	18	3.31*	1.19	0.52
2	1	17	4.22*	5.88	0.44
2	1	16	5.62	5.68	6.85
2	1	15	2.10*	5.07	0.17
2	1	14	4.72	4.95	5.67
2	1	13	7.24	7.07	9.12
2	1	12	8.10	8.22	9.43
2	1	11	13.01	13.39	7.85
2	1	10	1.49*	1.35	0.21
2	1	9	4.92	5.21	10.47
2	1	8	5.81	6.11	12.15
2	1	7	7.91	8.23	13.90
2	1	6	7.58	7.85	14.45
2	1	5	17.41	17.43	4.73
2	1	4	9.09	8.82	15.31
2	1	3	14.22	14.18	7.23
2	1	2	23.66	24.53	2.88
2	1	1	15.86	15.48	6.39
2	1	0	5.04	5.02	16.22
2	2	0	41.14	41.05	1.26
2	2	1	27.81	27.59	2.33
2	2	2	27.74	27.94	2.27
2	2	3	17.20	17.12	5.03
2	2	4	16.69	16.90	5.32
2	2	5	10.27	10.18	12.79
2	2	6	6.05	6.07	14.18
2	2	7	2.97*	3.15	1.32
2	2	8	7.44	7.93	13.26
2	2	9	1.83*	1.92	0.27
2	2	10	9.12	8.72	10.55
2	2	11	12.81	12.82	7.20
2	2	12	7.75	7.35	8.03
2	2	13	11.98	11.80	7.91
2	2	14	8.19	8.45	7.64
2	2	15	5.77	5.39	6.36
2	2	16	4.38	3.85	4.53
2	2	17	2.36*	1.80	0.18
2	2	18	4.07*	2.18	0.63
2	2	19	1.22*	1.78	0.05
2	2	20	2.62*	0.56	0.15
2	3	19	2.42*	2.00	0.17
2	3	18	3.35*	2.93	0.33
2	3	17	2.29*	1.29	0.23
2	3	16	2.55*	3.16	1.75
2	3	15	3.54*	3.16	0.58
2	3	14	2.72*	3.85	0.43
2	3	13	6.38	7.00	7.46
2	3	12	4.89	4.91	6.14
2	3	11	14.92	14.70	6.06
2	3	10	6.36	6.52	10.11
2	3	9	8.58	8.46	12.38
2	3	8	7.00	6.48	12.64
2	3	7	9.58	9.40	12.16
2	3	6	6.47	6.71	14.62
2	3	5	8.36	7.68	14.74
2	3	4	16.04	15.14	5.58
2	3	3	31.36	31.11	1.87
2	3	2	28.51	28.45	2.15
2	3	1	27.50	27.39	2.23
2	3	0	17.76	16.92	4.84
2	4	0	15.92	15.85	5.71
2	4	1	29.19	28.61	2.07
2	4	2	34.37	33.86	1.60
2	4	3	23.79	22.86	2.99
2	4	4	19.71	19.60	3.89
2	4	5	17.68	17.18	4.88
2	4	6	9.49	8.64	12.07
2	4	7	9.18	8.31	12.01
2	4	8	13.82	14.16	6.22
2	4	9	2.89*	2.54	0.63
2	4	10	9.19	8.93	9.60
2	4	11	12.63	12.44	7.73
2	4	12	6.57	6.83	7.52
2	4	13	2.01*	1.44	0.25
2	4	14	8.88	8.59	8.31
2	4	15	2.65*	1.78	0.42
2	4	16	3.72*	4.21	0.38
2	4	17	2.54*	1.13	0.16
2	4	18	2.96*	3.12	0.18
2	4	19	2.44*	2.33	0.17
2	5	19	2.53*	1.24	0.16
2	5	18	2.50*	2.05	0.16
2	5	17	4.25*	4.56	0.35
2	5	16	3.78*	2.39	0.81
2	5	15	3.66*	3.69	0.60
2	5	14	4.97	4.91	6.23
2	5	13	4.68	4.17	5.99
2	5	12	11.19	11.39	7.89
2	5	11	6.38	6.64	8.86
2	5	10	15.91	16.16	5.51
2	5	9	15.81	15.83	5.23
2	5	8	9.89	10.18	10.21
2	5	7	13.51	13.35	7.98
2	5	6	7.93	7.73	12.06
2	5	5	1.73*	0.46	0.34
2	5	4	6.91	6.91	13.49
2	5	3	4.83	5.26	11.37
2	5	2	19.22	19.15	4.22
2	5	1	23.58	23.84	2.92
2	5	0	14.44	13.85	6.83
2	6	0	1.36*	5.40	0.17
2	6	1	8.17	8.25	14.74
2	6	2	12.80	13.08	8.19
2	6	3	10.79	10.54	11.16
2	6	4	7.23	7.26	12.11
2	6	5	11.19	11.49	10.02
2	6	6	2.71*	3.41	0.57
2	6	7	21.68	21.24	3.38
2	6	8	6.35	6.30	9.46
2	6	9	14.41	14.42	7.03
2	6	10	7.25	7.26	9.64
2	6	11	12.95	13.14	7.42
2	6	12	7.07	6.94	8.52
2	6	13	2.33*	3.31	0.18
2	6	14	2.67*	3.10	0.37
2	6	15	4.37*	2.52	0.81
2	6	16	3.68*	2.13	0.45
2	6	17	1.70*	2.56	0.11
2	6	18	1.24*	2.68	0.06
2	7	18	4.73*	3.93	0.46
2	7	17	3.88*	1.25	0.45
2	7	16	2.37*	1.33	0.18
2	7	15	4.16*	1.31	0.89
2	7	14	2.36*	3.28	0.18
2	7	13	6.35	6.36	6.41
2	7	12	5.18	5.77	5.44
2	7	11	8.55	8.58	8.49
2	7	10	4.52	5.08	5.27

h	k	l	Fo	Fc	weight
2	7	9	6.75	7.56	8.47
2	7	8	6.97	7.00	8.91
2	7	7	2.25*	4.02	0.24
2	7	6	3.73	3.88	5.56
2	7	5	10.78	11.05	9.54
2	7	4	10.97	11.14	10.15
2	7	3	1.20*	3.32	0.10
2	7	2	6.51	6.23	11.35
2	7	1	14.48	14.01	6.57
2	7	0	9.47	9.46	10.74
2	8	0	9.60	9.44	11.27
2	8	1	5.63	6.04	8.70
2	8	2	7.52	7.68	11.80
2	8	3	20.93	21.26	3.48
2	8	4	3.01	3.72	4.23
2	8	5	14.98	15.22	5.73
2	8	6	13.62	13.60	7.53
2	8	7	3.96*	3.84	0.75
2	8	8	3.54*	2.82	0.79
2	8	9	3.18*	5.88	0.33
2	8	10	8.83	9.00	8.83
2	8	11	6.36	6.28	7.44
2	8	12	2.35*	1.65	0.18
2	8	13	3.54	4.17	2.92
2	8	14	2.39*	1.48	0.18
2	8	15	2.80*	3.02	0.31
2	8	16	2.53*	1.14	0.16
2	8	17	6.28	5.67	4.68
2	9	16	3.31*	0.67	0.36
2	9	15	3.86*	2.34	0.66
2	9	14	2.06*	0.85	0.19
2	9	13	2.83*	1.93	0.42
2	9	12	2.33*	2.60	0.18
2	9	11	4.87	4.66	5.16
2	9	10	4.01*	4.58	0.48
2	9	9	3.31*	4.47	0.38
2	9	8	3.08*	3.69	0.45
2	9	7	2.01*	3.45	0.19
2	9	6	9.54	9.57	9.04
2	9	5	8.53	8.28	8.54
2	9	4	10.74	10.97	8.75
2	9	3	6.82	6.65	8.83
2	9	2	15.56	16.22	5.85
2	9	1	9.93	10.50	8.49
2	9	0	3.73*	1.43	1.02
2	10	0	1.97*	0.64	0.21
2	10	1	1.71*	1.60	0.18
2	10	2	9.32	9.77	9.26
2	10	3	4.60	4.89	5.41
2	10	4	11.91	11.86	8.09
2	10	5	1.97*	2.20	0.26
2	10	6	6.02	5.91	7.26
2	10	7	5.77	6.64	6.22
2	10	8	5.13	6.11	4.73
2	10	9	6.03	5.77	6.28
2	10	10	4.02*	0.96	0.61
2	10	11	5.17	5.15	4.88
2	10	12	5.43	5.19	5.56
2	10	13	2.52*	1.66	0.16
2	10	14	2.53*	2.61	0.16
2	10	15	3.87*	3.70	2.17
2	11	14	5.73	5.21	4.05
2	11	13	2.61*	1.78	0.15
2	11	12	2.44*	0.83	0.17
2	11	11	1.67*	4.16	0.07
2	11	10	3.47*	3.16	2.62
2	11	9	2.55*	3.03	0.23
2	11	8	1.58*	1.97	0.20
2	11	7	2.81*	1.52	0.37
2	11	6	1.08*	1.81	0.04
2	11	5	5.31	5.83	5.79
2	11	4	3.81*	3.87	0.62
2	11	3	2.05*	2.91	0.24
2	11	2	3.61*	4.21	0.66
2	11	1	3.85	3.78	4.59
2	11	0	2.15*	1.04	0.22
2	12	0	2.33*	1.80	0.18
2	12	1	3.62*	4.65	0.47
2	12	2	1.10*	1.97	0.05
2	12	3	6.38	6.23	6.21
2	12	4	3.33*	3.56	0.38
2	12	5	3.54*	2.53	0.68
2	12	6	4.88	4.89	4.91
2	12	7	4.14*	2.78	0.63
2	12	8	3.69*	3.54	0.72
2	12	9	2.54*	4.10	0.15
2	12	10	4.52*	2.92	0.67
2	12	11	3.89*	4.63	0.41
2	12	12	1.77*	2.65	0.08
2	13	10	2.41*	0.32	0.17
2	13	9	4.78*	3.65	0.61
2	13	8	4.22*	3.14	0.66
2	13	7	2.47*	1.03	0.16
2	13	6	2.45*	2.23	0.17
2	13	5	2.35*	2.34	0.22
2	13	4	2.60*	3.12	0.19
2	13	3	3.27*	1.75	0.54
2	13	2	1.15*	1.00	0.12
2	13	1	2.56*	4.07	0.17
2	13	0	1.98*	1.24	0.16
2	14	0	2.32*	1.71	0.19
2	14	1	2.42*	0.85	0.17
2	14	2	3.41*	4.01	0.29
2	14	3	2.50*	2.28	0.16
2	14	4	2.23*	2.06	0.20
2	14	5	3.25*	1.04	0.59
2	14	6	3.28*	3.89	1.73
2	14	7	4.32	3.89	3.14
2	15	3	4.56*	2.30	0.74
2	15	2	4.88*	0.53	0.65
2	15	1	4.87*	4.27	0.46
2	15	0	2.80*	3.33	0.13
3	14	3	2.61*	2.28	1.19
3	14	2	2.42*	1.23	0.17
3	14	1	3.70*	3.11	2.40
3	14	0	2.39*	0.72	0.18
3	13	0	2.58*	4.68	0.15
3	13	1	6.46	5.73	6.24
3	13	2	2.58*	1.51	0.15
3	13	3	2.38*	0.86	0.18
3	13	4	4.86	4.25	3.71
3	13	5	2.13*	1.88	0.20
3	13	6	3.29*	4.06	0.37
3	13	7	4.16*	3.46	0.38
3	12	10	2.65*	2.62	0.14
3	12	9	2.31*	1.32	1.27
3	12	8	1.73*	0.80	0.09
3	12	7	3.62*	3.72	0.54
3	12	6	2.39*	1.31	0.16
3	12	5	2.26*	1.58	0.20
3	12	4	2.03*	2.63	0.17
3	12	3	2.01*	2.34	0.15
3	12	2	3.66*	4.41	0.39
3	12	1	5.95	6.49	4.86
3	12	0	2.34*	1.81	0.18
3	11	0	2.45*	3.62	0.17
3	11	1	2.17*	3.27	0.21
3	11	2	2.47*	2.60	0.39
3	11	3	5.50	5.15	5.64
3	11	4	2.24*	3.78	0.20
3	11	5	6.31	6.77	5.94
3	11	6	2.40*	3.70	1.21
3	11	7	1.38*	2.14	0.53
3	11	8	3.33*	1.50	0.33
3	11	9	1.69*	2.82	0.07
3	11	10	2.60*	3.85	0.15
3	11	11	4.47*	1.79	0.77
3	11	12	3.34*	2.95	0.31
3	10	13	2.50*	2.37	0.25
3	10	12	3.46*	1.71	0.55
3	10	11	3.79*	3.01	0.33
3	10	10	2.35*	2.24	0.22
3	10	9	2.24*	2.03	0.20
3	10	8	2.40*	1.46	0.17
3	10	7	1.12*	3.33	0.04
3	10	6	2.91*	3.20	0.31
3	10	5	5.61	5.43	6.59
3	10	4	3.04*	3.08	0.44
3	10	3	3.84*	4.54	0.61
3	10	2	3.67*	1.12	1.00
3	10	1	3.17*	4.78	0.46
3	10	0	2.02*	0.30	0.24
3	9	0	12.12	13.08	7.29
3	9	1	8.80	9.10	8.88
3	9	2	6.32	6.65	8.09
3	9	3	2.20*	2.59	1.85
3	9	4	6.17	6.33	7.36
3	9	5	4.55	4.68	5.24
3	9	6	2.89*	3.53	0.45
3	9	7	3.87*	4.77	0.48
3	9	8	2.30*	1.64	0.19
3	9	9	2.49*	2.09	0.24
3	9	10	2.32*	3.50	0.19
3	9	11	2.69*	2.30	0.23
3	9	12	2.67*	2.31	1.85
3	9	13	3.84*	3.30	2.43
3	9	14	4.76	3.79	3.85
3	9	15	3.93*	0.72	0.40
3	8	14	3.83*	3.17	0.42
3	8	13	2.48*	3.79	0.16
3	8	12	3.82*	4.20	0.32
3	8	11	2.47*	3.03	0.16
3	8	10	2.15*	1.56	0.22
3	8	9	4.60	5.00	4.89
3	8	8	4.54	4.63	5.43
3	8	7	2.34*	4.27	0.18
3	8	6	7.31	7.86	8.07
3	8	5	6.18	6.36	7.71
3	8	4	9.57	9.78	8.14
3	8	3	4.15*	3.97	0.81
3	8	2	18.66	18.52	4.22
3	8	1	9.39	9.51	9.11
3	8	0	6.96	7.28	9.03
3	7	0	4.84	4.55	8.79
3	7	1	6.32	6.72	9.32
3	7	2	14.01	14.18	6.50
3	7	3	17.52	17.70	4.64
3	7	4	6.50	6.64	8.80
3	7	5	10.42	10.16	8.83
3	7	6	4.15*	6.58	0.50
3	7	7	11.08	11.40	8.49
3	7	8	2.08*	0.14	0.23
3	7	9	4.65*	5.84	0.51
3	7	10	9.19	9.32	7.74
3	7	11	6.85	7.18	7.10
3	7	12	3.17*	3.94	0.34
3	7	13	2.21*	1.16	0.20
3	7	14	2.64*	4.22	0.35
3	7	15	2.71*	1.24	0.21
3	7	16	2.58*	0.30	0.15
3	7	17	3.08*	1.37	0.28
3	6	16	2.62*	3.03	0.15
3	6	15	2.39*	0.84	0.18
3	6	14	4.60	4.16	4.19
3	6	13	2.08*	0.98	0.23
3	6	12	2.10*	2.30	0.23
3	6	11	5.33	5.22	7.00
3	6	10	7.35	7.26	7.97
3	6	9	9.33	9.73	8.45
3	6	8	10.41	10.55	8.47
3	6	7	2.12*	3.47	0.22
3	6	6	14.26	14.85	6.99
3	6	5	4.84	4.67	7.74
3	6	4	10.12	10.20	10.26
3	6	3	9.31	9.64	10.04
3	6	2	14.42	14.60	6.28
3	6	1	8.12	8.20	12.18
3	6	0	3.19*	0.82	0.89
3	5	0	15.21	14.72	5.76
3	5	1	7.40	7.33	12.41
3	5	2	9.34	9.04	11.85
3	5	3	3.38	2.95	5.82

h	k	l	Fo	Fc	weight
3	5	4	9.94	9.84	10.36
3	5	5	7.54	7.56	10.26
3	5	6	5.83	5.70	9.93
3	5	7	12.45	12.72	8.19
3	5	8	7.36	7.02	10.08
3	5	9	4.04*	4.14	0.77
3	5	10	8.87	8.53	9.37
3	5	11	2.12*	0.64	0.22
3	5	12	2.13*	3.12	0.24
3	5	13	2.46*	4.17	0.18
3	5	14	4.38*	1.64	0.80
3	5	15	3.68*	2.62	0.56
3	5	16	2.40*	0.61	0.17
3	5	17	3.03*	1.89	0.37
3	4	18	2.34*	1.39	0.18
3	4	17	4.39*	2.48	0.70
3	4	16	2.36*	3.65	0.18
3	4	15	4.93	5.30	4.21
3	4	14	7.08	7.13	6.34
3	4	13	6.43	6.11	7.05
3	4	12	1.71*	1.61	1.25
3	4	11	10.00	10.06	8.21
3	4	10	2.19*	2.94	0.21
3	4	9	6.01	6.30	7.86
3	4	8	9.92	10.09	9.06
3	4	7	14.07	14.15	7.42
3	4	6	12.63	12.97	8.54
3	4	5	3.51	3.09	7.02
3	4	4	4.61	4.65	7.95
3	4	3	10.15	10.36	10.58
3	4	2	14.90	14.60	6.54
3	4	1	15.69	15.22	5.75
3	4	0	21.22	20.40	3.17
3	3	0	3.27*	3.00	0.98
3	3	1	10.75	10.50	10.09
3	3	2	6.74	6.62	14.15
3	3	3	14.04	13.99	7.37
3	3	4	15.80	15.46	5.84
3	3	5	6.05	5.86	12.22
3	3	6	8.45	8.69	11.01
3	3	7	14.56	14.46	6.74
3	3	8	13.95	14.27	7.27
3	3	9	6.65	6.75	9.99
3	3	10	7.84	7.62	9.64
3	3	11	8.58	8.69	7.56
3	3	12	2.02*	1.27	0.25
3	3	13	4.25*	4.81	0.79
3	3	14	2.19*	1.54	0.29
3	3	15	2.99*	4.23	0.29
3	3	16	3.69*	2.27	0.63
3	3	17	2.95*	3.16	0.19
3	3	18	4.42	3.26	3.31
3	2	18	3.57*	2.53	2.50
3	2	17	2.43*	3.10	1.27
3	2	16	4.72	4.26	4.42
3	2	15	1.94*	4.00	0.15
3	2	14	5.95	5.27	7.04
3	2	13	5.57	5.60	7.38
3	2	12	11.24	10.86	7.73
3	2	11	10.01	10.35	8.00
3	2	10	6.56	6.48	9.33
3	2	9	5.37	5.77	8.56
3	2	8	2.37*	1.09	0.38
3	2	7	10.74	10.52	9.44
3	2	6	9.10	9.09	10.77
3	2	5	11.03	10.31	10.25
3	2	4	3.02*	3.51	0.85
3	2	3	8.60	8.17	13.73
3	2	2	1.75*	0.53	0.42
3	2	1	17.18	17.19	4.93
3	2	0	15.69	15.60	6.18
3	1	0	13.19	12.84	8.68
3	1	1	6.67	6.74	14.21
3	1	2	18.33	18.45	4.23
3	1	3	22.33	21.84	3.04
3	1	4	14.40	14.04	7.47
3	1	5	3.15*	0.97	1.01
3	1	6	9.11	8.88	11.63
3	1	7	10.24	10.16	10.33
3	1	8	5.61	5.30	11.10
3	1	9	3.03*	5.51	0.45
3	1	10	8.02	8.30	9.52
3	1	11	14.68	14.85	6.42
3	1	12	2.25*	5.42	0.17
3	1	13	3.46*	4.46	0.39
3	1	14	6.66	6.08	7.06
3	1	15	3.07*	2.57	2.59
3	1	16	2.57*	1.21	0.25
3	1	17	4.28*	2.44	0.54
3	1	18	2.74*	1.37	0.22
3	1	19	2.19*	0.99	0.12
3	0	19	3.57*	0.94	0.35
3	0	18	2.45*	2.06	0.18
3	0	17	1.19*	1.36	0.07
3	0	16	3.04*	2.63	0.38
3	0	15	2.07*	0.06	0.23
3	0	14	1.86*	3.15	0.15
3	0	13	14.04	14.35	5.69
3	0	12	12.63	12.66	7.12
3	0	11	9.63	9.90	8.72
3	0	10	1.80*	0.87	0.31
3	0	9	1.29*	1.98	0.12
3	0	8	5.73	5.91	10.62
3	0	7	13.68	14.45	7.32
3	0	6	2.50*	2.88	0.55
3	0	5	11.26	11.06	10.84
3	0	4	2.50*	2.83	0.76
3	0	3	10.81	10.87	11.01
3	0	2	7.73	7.88	14.13
3	0	1	16.14	15.85	5.72
4	0	0	5.45	5.50	9.44
4	0	1	13.01	13.02	8.55
4	0	2	11.65	11.62	8.93
4	0	3	1.93*	1.56	0.27
4	0	4	16.31	16.22	5.55
4	0	5	2.09*	0.08	0.23
4	0	6	13.13	13.36	7.68
4	0	7	4.15	4.37	4.91
4	0	8	8.06	7.20	9.28
4	0	9	3.05*	1.81	0.67
4	0	10	12.76	12.74	7.07
4	0	11	5.33	5.01	5.96
4	0	12	2.69*	5.41	0.13
4	0	13	1.60*	0.56	0.11
4	0	14	2.34*	1.67	0.18
4	0	15	1.69*	1.26	0.08
4	0	16	1.23*	1.96	0.04
4	0	17	2.19*	2.28	0.15
4	1	17	3.58*	3.60	2.31
4	1	16	4.61*	4.94	0.37
4	1	15	2.68*	4.78	0.18
4	1	14	2.37*	1.61	0.18
4	1	13	4.86	4.63	5.34
4	1	12	7.98	7.88	8.61
4	1	11	4.59	4.87	4.81
4	1	10	2.00*	0.97	0.25
4	1	9	2.50*	4.05	0.21
4	1	8	4.69	4.31	6.89
4	1	7	4.27	4.77	5.95
4	1	6	3.45*	1.05	1.01
4	1	5	8.72	8.98	9.56
4	1	4	9.24	9.15	10.28
4	1	3	13.32	13.45	8.09
4	1	2	19.25	19.22	4.03
4	1	1	2.70*	1.47	0.69
4	1	0	3.68	3.34	6.71
4	2	0	2.11*	2.67	0.22
4	2	1	12.48	12.39	8.43
4	2	2	2.05*	3.23	0.24
4	2	3	6.49	6.67	9.90
4	2	4	1.45*	1.94	0.90
4	2	5	3.41*	4.68	0.66
4	2	6	8.93	9.05	9.21
4	2	7	2.01*	1.00	0.25
4	2	8	9.56	9.19	8.34
4	2	9	1.03*	0.92	0.07
4	2	10	9.20	8.79	8.24
4	2	11	2.86*	3.47	0.30
4	2	12	9.56	9.28	7.61
4	2	13	5.33	4.44	6.18
4	2	14	2.32*	1.84	0.19
4	2	15	3.40*	3.23	0.35
4	2	16	4.28*	2.87	0.43
4	3	16	2.49*	2.64	0.20
4	3	15	4.54*	3.98	0.46
4	3	14	0.86*	2.01	0.19
4	3	13	2.12*	0.43	0.22
4	3	12	7.22	7.20	6.71
4	3	11	2.47*	1.82	0.16
4	3	10	5.63	5.61	6.11
4	3	9	5.76	5.13	7.20
4	3	8	3.95	4.56	4.11
4	3	7	3.45	3.63	4.16
4	3	6	1.93*	1.40	0.27
4	3	5	4.71	4.84	6.99
4	3	4	9.48	9.77	8.82
4	3	3	12.04	11.62	8.18
4	3	2	2.08*	3.12	0.21
4	3	1	2.61*	4.14	0.37
4	3	0	12.23	12.20	8.13
4	4	0	1.88*	2.71	0.23
4	4	1	7.43	7.08	9.73
4	4	2	7.83	7.58	9.72
4	4	3	6.38	6.40	9.11
4	4	4	10.41	10.21	8.85
4	4	5	10.86	10.66	8.92
4	4	6	11.42	11.76	8.01
4	4	7	8.01	8.34	9.62
4	4	8	7.84	7.60	9.28
4	4	9	5.72	5.64	6.84
4	4	10	11.41	11.47	7.24
4	4	11	9.18	9.35	7.58
4	4	12	1.61*	2.87	0.12
4	4	13	4.03*	2.26	0.52
4	4	14	2.93*	4.16	0.28
4	4	15	5.38	4.96	4.01
4	4	16	3.78*	1.79	0.44
4	5	15	3.05*	0.36	0.43
4	5	14	2.17*	2.20	1.12
4	5	13	2.99*	3.25	1.83
4	5	12	4.47*	4.29	0.50
4	5	11	2.25*	3.29	0.24
4	5	10	2.70*	1.33	0.36
4	5	9	10.87	10.71	8.48
4	5	8	3.17*	3.09	0.62
4	5	7	2.07*	1.28	0.28
4	5	6	10.69	10.90	8.38
4	5	5	7.89	7.82	9.69
4	5	4	3.43*	5.09	0.57
4	5	3	9.19	9.35	8.21
4	5	2	8.40	9.06	8.89
4	5	1	8.11	7.86	8.64
4	5	0	8.67	8.73	8.97
4	6	0	10.17	10.29	9.24
4	6	1	6.46	6.77	8.16
4	6	2	3.88*	5.95	0.55
4	6	3	9.86	10.34	8.32
4	6	4	2.06*	3.32	0.24
4	6	5	2.30*	3.51	0.35
4	6	6	2.16*	0.18	0.21
4	6	7	3.87*	1.90	0.87
4	6	8	6.54	7.29	6.72
4	6	9	3.82*	3.07	0.49
4	6	10	2.25*	2.62	0.24
4	6	11	2.33*	2.53	0.18
4	6	12	4.67	4.51	4.27
4	6	13	5.15	5.42	3.38
4	6	14	3.90*	4.01	0.44
4	6	15	2.22*	1.60	0.20
4	7	14	2.18*	1.55	0.15
4	7	13	2.45*	1.63	0.17
4	7	12	2.95*	4.51	0.27
4	7	11	2.04*	2.81	0.15
4	7	10	1.15*	2.83	0.04
4	7	9	4.85	4.67	5.22
4	7	8	2.22*	1.04	0.20
4	7	7	5.20	4.95	6.67
4	7	6	1.52*	4.27	0.10
4	7	5	2.17*	0.69	0.21
4	7	4	2.97*	3.43	0.51
4	7	3	1.80*	0.66	0.17
4	7	2	7.72	7.96	7.34
4	7	1	7.90	8.11	8.56
4	7	0	2.81*	1.54	0.48
4	8	0	2.38*	3.78	0.23
4	8	1	4.83	4.63	5.41
4	8	2	1.07*	1.91	0.06
4	8	3	2.24*	1.36	0.20
4	8	4	3.74	3.47	3.44
4	8	5	3.29*	2.79	0.52
4	8	6	4.15*	3.37	0.89
4	8	7	6.94	7.09	6.19
4	8	8	3.79*	5.17	0.32
4	8	9	1.16*	0.68	0.06
4	8	10	3.55*	2.78	0.44
4	8	11	3.20*	0.99	0.44
4	8	12	0.64*	2.86	0.07
4	8	13	4.18*	3.27	0.58
4	9	12	2.53*	1.22	0.15
4	9	11	1.24*	3.19	0.06
4	9	10	4.39*	3.07	0.51
4	9	9	4.48*	3.40	0.68
4	9	8	4.08	5.01	2.81
4	9	7	1.16*	1.77	0.05
4	9	6	2.26*	2.35	0.20
4	9	5	6.66	6.97	5.93
4	9	4	3.72*	4.14	0.58
4	9	3	5.65	5.41	6.58
4	9	2	1.11*	3.17	0.05
4	9	1	2.92*	2.28	0.46
4	9	0	4.57	5.06	4.63
4	10	0	4.72*	7.34	0.66
4	10	1	3.24*	3.32	2.31
4	10	2	4.14*	5.38	0.45
4	10	3	4.32*	2.42	0.73
4	10	4	2.23*	3.32	0.20
4	10	5	4.23*	2.70	0.61
4	10	6	6.41	6.49	4.99
4	10	7	2.36*	1.95	0.18
4	10	8	1.09*	0.10	0.28
4	10	9	2.55*	3.06	0.15
4	10	10	3.32*	1.25	0.36
4	11	8	2.58*	2.48	0.15
4	11	7	1.76*	1.27	0.08
4	11	6	3.47*	4.87	0.37
4	11	5	4.55*	3.41	0.60
4	11	4	2.31*	1.98	0.19
4	11	3	2.57*	3.73	0.15
4	11	2	5.33	5.84	3.60
4	11	1	5.32*	7.07	0.50
4	11	0	2.36*	0.01	0.18
4	12	0	10.24	10.02	6.27
4	12	1	2.76*	3.29	0.24
4	12	2	3.27*	2.06	0.29
4	12	3	2.40*	2.09	0.17
4	12	4	2.17*	3.83	0.13
4	12	5	2.34*	1.82	0.18
5	10	4	4.19*	1.97	0.77
5	10	3	3.97*	3.31	0.43
5	10	2	3.31*	1.01	0.32
5	10	1	2.68*	1.66	0.14
5	10	0	9.62	9.34	6.12
5	9	0	7.83	6.88	6.42
5	9	1	2.36*	3.06	0.18
5	9	2	4.03*	5.12	0.41
5	9	3	2.41*	0.15	0.17
5	9	4	2.41*	2.34	0.17
5	9	5	1.24*	3.76	0.03
5	9	6	2.39*	2.53	0.18
5	9	7	2.70*	3.57	0.14
5	8	8	3.57*	1.50	0.62
5	8	8	2.49*	2.91	0.18
5	8	7	2.38*	2.60	1.08
5	8	6	7.52	7.10	6.21
5	8	5	2.09*	2.38	0.14
5	8	4	5.73	5.77	4.75
5	8	3	2.60*	2.73	1.54
5	8	2	4.80	4.47	3.98
5	8	1	2.35*	2.78	0.20
5	8	0	1.66*	2.33	0.10
5	7	0	3.24*	1.62	0.75
5	7	1	2.81*	2.19	0.25
5	7	2	2.30*	1.07	0.19
5	7	3	3.27*	2.45	0.47
5	7	4	3.08*	2.04	0.47
5	7	5	6.53	5.97	6.02
5	7	6	2.53*	1.83	0.16
5	7	7	4.16*	4.77	0.45
5	7	8	2.42*	2.00	0.17
5	7	9	3.49*	2.87	0.41
5	7	10	2.64*	3.77	0.14
5	6	11	2.17*	1.52	0.11
5	6	10	4.52	4.48	3.56
5	6	9	4.19*	2.11	0.67
5	6	8	3.57*	3.32	0.36
5	6	7	4.84*	4.46	0.62
5	6	6	0.60*	1.69	0.08
5	6	5	1.52*	0.64	0.14
5	6	4	5.98	5.80	5.83
5	6	3	3.38*	1.22	0.48
5	6	2	2.32*	3.23	0.19
5	6	1	1.58*	2.78	0.13
5	6	0	2.95*	1.99	0.33
5	5	0	5.55	5.99	6.43
5	5	1	4.69	4.34	5.33
5	5	2	2.45*	0.53	0.25
5	5	3	6.21	5.92	6.75
5	5	4	2.30*	2.29	0.18
5	5	5	2.24*	1.73	0.24
5	5	6	2.78*	2.66	2.01
5	5	7	3.64*	3.03	0.42
5	5	8	6.06	5.51	6.17
5	5	8	1.68*	2.35	0.11
5	5	10	3.63*	2.78	0.54
5	5	11	4.93*	5.05	0.44
5	5	12	2.34*	0.48	0.18
5	4	13	3.10*	2.70	0.31
5	4	12	3.92*	4.13	0.48
5	4	11	2.26*	0.76	0.20
5	4	10	5.18	5.29	3.83
5	4	9	4.68*	5.76	0.56
5	4	8	3.98*	4.47	0.54
5	4	7	2.26*	1.83	0.31
5	4	6	3.16*	1.94	0.51
5	4	5	4.68*	6.72	0.48
5	4	4	4.08*	5.26	0.57
5	4	3	1.72*	2.79	0.88
5	4	2	8.62	9.23	7.33
5	4	1	2.84*	3.06	0.28
5	4	0	3.03*	4.60	0.34
5	3	0	7.94	7.60	8.00
5	3	1	2.08*	2.53	0.23
5	3	2	3.51*	5.13	0.43
5	3	3	7.20	7.89	7.71
5	3	4	1.86*	3.16	0.14
5	3	5	5.37	5.81	6.44
5	3	6	1.56*	2.68	0.09
5	3	7	4.58	4.40	4.83
5	3	8	2.38*	2.73	0.18
5	3	9	9.05	8.84	7.46
5	3	10	7.24	7.33	6.00
5	3	11	2.33*	0.87	0.18
5	3	12	2.60*	2.28	0.15
5	3	13	2.31*	1.64	0.19
5	2	13	3.28*	2.18	0.24
5	2	12	3.44*	2.17	0.43
5	2	11	7.27	8.02	5.20
5	2	10	2.02*	1.42	0.14
5	2	9	5.57	5.78	4.95
5	2	8	5.86	5.27	7.09
5	2	7	5.31	5.43	5.43
5	2	6	5.26	5.63	5.81
5	2	5	9.97	9.82	7.44
5	2	4	2.31*	2.93	0.19
5	2	3	6.63	6.46	8.05
5	2	2	10.36	10.35	7.45
5	2	1	7.12	6.75	7.40
5	2	0	6.69	6.71	7.60
5	1	0	11.75	11.69	7.76
5	1	1	1.73*	3.23	0.96
5	1	2	4.03*	3.46	0.86
5	1	3	10.32	10.05	8.14
5	1	4	14.38	14.62	6.45
5	1	5	6.99	6.51	8.08
5	1	6	2.29*	1.14	0.19
5	1	7	6.64	6.47	6.79
5	1	8	4.18*	3.63	0.78
5	1	9	4.62	5.15	3.80
5	1	10	6.67	5.74	6.51
5	1	11	2.05*	1.69	0.19
5	1	12	2.67*	3.15	0.14
5	1	13	2.48*	1.81	0.16
5	1	14	1.79*	1.82	0.09
5	0	14	2.38*	0.37	0.18
5	0	13	2.55*	0.97	0.15
5	0	12	2.96*	2.44	0.30
5	0	11	2.64*	2.09	0.24
5	0	10	3.68	4.49	2.70
5	0	9	2.44*	1.69	0.17
5	0	8	5.56	5.70	5.57
5	0	7	2.45*	1.48	0.31
5	0	6	3.89*	1.30	0.79
5	0	5	6.13	6.36	6.77
5	0	4	2.35*	0.59	0.18
5	0	3	10.00	10.12	8.28
5	0	2	3.60*	2.70	0.91
5	0	1	8.34	8.31	7.96
6	0	0	3.70*	5.41	0.35
6	0	1	8.42	8.30	6.27
6	0	2	7.67	7.88	6.03
6	0	3	2.36*	1.94	0.22
6	0	4	4.60	4.85	3.66
6	0	5	3.17*	1.25	0.39
6	0	6	1.21*	0.02	0.06
6	0	7	4.25*	5.03	0.47
6	0	8	6.40	6.00	4.92
6	0	9	4.54*	3.87	0.48
6	1	9	3.99*	3.34	0.38
6	1	8	2.49*	2.81	0.15
6	1	7	1.23*	2.39	0.05
6	1	6	4.38*	2.42	0.71
6	1	5	2.69*	4.76	0.18
6	1	4	4.98	5.75	3.78
6	1	3	4.10*	4.41	0.56
6	1	2	5.41	5.27	4.59
6	1	1	7.58	7.72	5.39
6	1	0	4.07*	2.94	0.44
6	2	0	2.36*	3.29	0.18
6	2	1	2.60*	1.34	0.15
6	2	2	2.65*	2.65	0.24
6	2	3	5.83	5.60	5.45
6	2	4	3.97*	5.59	0.34
6	2	5	2.18*	0.58	0.21
6	2	6	3.23*	1.75	0.43
6	2	7	3.27*	2.95	0.37
6	2	8	1.25*	2.03	0.04
6	3	8	3.33*	1.73	0.40
6	3	7	1.24*	1.02	0.05
6	3	6	3.25*	3.13	0.25
6	3	5	3.22*	3.60	0.34
6	3	4	2.70*	3.06	0.21
6	3	3	4.16*	3.17	0.68
6	3	2	4.47*	3.01	0.68
6	3	1	4.31	5.25	3.02

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	7
6	3	0	2.43*	1.50	0.17																			
6	4	0	2.09*	1.19	0.16																			
6	4	1	5.81	5.54	4.93																			
6	4	2	2.36*	1.03	0.18																			
6	4	3	5.04	5.97	3.86																			
6	4	4	3.19*	3.76	2.17																			
6	4	5	6.79	6.90	4.79																			
6	4	6	2.80*	2.56	1.35																			
6	4	7	2.64*	2.27	0.14																			
6	5	6	6.73	6.55	4.57																			
6	5	5	3.06*	1.99	0.25																			
6	5	4	2.50*	1.58	0.16																			
6	5	3	3.26*	2.57	0.37																			
6	5	2	2.44*	1.38	0.17																			
6	5	1	2.27*	1.64	0.19																			
6	5	0	2.99*	2.26	0.33																			
6	6	0	2.78*	4.33	0.16																			
6	6	1	2.37*	1.15	0.18																			
6	6	2	2.66*	4.23	0.14																			
6	6	3	2.55*	1.08	0.15																			
6	6	4	4.37*	2.53	0.62																			

1413 reflections

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4α-ol

h	k	l	Fo	Fc	weight
1	0	0	64.91	68.74	0.57
2	0	0	59.72	61.76	0.63
3	0	0	28.63	28.43	2.00
4	0	0	48.26	46.64	0.83
5	0	0	12.46	13.21	6.74
6	0	0	14.90	14.17	5.52
7	0	0	2.86*	2.44	0.12
8	0	0	3.01*	2.07	0.11
9	0	0	2.26*	1.57	0.05
10	0	0	3.11*	0.60	0.10
-10	0	2	3.49*	4.13	0.08
-9	0	2	3.32*	2.99	0.68
-8	0	2	11.70	12.02	3.87
-7	0	2	32.02	31.77	1.61
-6	0	2	16.29	15.51	3.86
-5	0	2	4.98*	0.46	0.61
-4	0	2	10.62	11.37	4.63
-3	0	2	34.30	31.86	1.44
-2	0	2	2.79*	3.92	0.13
-1	0	2	4.05*	1.94	0.31
0	0	2	20.52	19.89	3.32
1	0	2	9.81	10.01	4.78
2	0	2	9.59	9.42	5.64
3	0	2	10.74	10.48	5.76
4	0	2	23.55	24.24	2.89
5	0	2	20.92	20.78	3.28
6	0	2	2.82*	1.23	0.13
7	0	2	7.52	7.72	3.46
8	0	2	1.89*	0.28	0.28
9	0	2	3.34*	2.55	0.09
-9	0	4	4.71*	4.14	0.12
-8	0	4	4.12*	4.49	0.71
-7	0	4	2.23*	3.97	0.03
-6	0	4	5.95	5.58	1.37
-5	0	4	3.65*	3.73	0.08
-4	0	4	8.46	8.82	1.44
-3	0	4	17.75	17.94	2.18
-2	0	4	7.37*	8.37	0.25
-1	0	4	0.62*	0.45	0.01
0	0	4	9.76	9.13	1.97
1	0	4	7.32	7.02	1.59
2	0	4	6.23	7.04	1.48
3	0	4	18.63	18.00	3.21
4	0	4	3.44*	3.64	0.09
5	0	4	5.14*	5.75	1.29
6	0	4	3.58*	0.95	0.08
-4	0	6	6.22*	5.63	0.13
-3	0	6	3.56*	2.49	0.05
-2	0	6	5.99*	2.58	0.17
-1	0	6	5.06*	5.13	0.10
1	1	0	44.99	46.53	1.10
2	1	0	31.71	32.32	1.88
3	1	0	31.71	31.65	1.76
4	1	0	44.71	45.15	0.95
5	1	0	26.54	26.15	2.52
6	1	0	12.95	12.60	5.83
7	1	0	7.59	7.27	3.93
8	1	0	2.83*	2.43	0.12
9	1	0	3.08*	3.35	0.11
10	1	0	5.24*	0.22	0.45
-10	1	1	3.29*	2.67	0.09
-9	1	1	4.05*	2.06	0.19
-8	1	1	6.50	6.63	2.72
-7	1	1	2.89*	2.51	0.09
-6	1	1	6.12	6.24	3.90
-5	1	1	2.02*	0.06	0.11
-4	1	1	5.39	5.87	3.52
-3	1	1	17.05	17.49	4.63
-2	1	1	20.23	21.13	3.40
-1	1	1	38.63	41.37	1.26
0	1	1	84.03	88.09	0.33
1	1	1	2.27*	0.94	0.19
2	1	1	12.04	11.95	6.90
3	1	1	17.93	16.96	4.55
4	1	1	37.43	35.77	1.26
5	1	1	3.10*	2.33	0.22
6	1	1	5.37*	5.20	0.40
7	1	1	2.33*	0.68	0.08
8	1	1	2.98*	1.07	0.11
9	1	1	3.16*	0.93	0.84
10	1	1	2.91*	2.00	0.06
-10	1	2	5.61	4.06	1.87
-9	1	2	3.24*	0.69	0.10
-8	1	2	6.72*	7.54	0.31
-7	1	2	25.61	26.07	2.27
-6	1	2	5.20*	2.72	0.38
-5	1	2	17.29	16.82	4.09
-4	1	2	2.35*	1.55	0.10
-3	1	2	19.41	19.21	3.39
-2	1	2	17.47	17.09	3.70
-1	1	2	3.37*	4.61	0.16
0	1	2	2.79*	2.11	0.13
1	1	2	14.24	14.48	4.72
2	1	2	11.36	10.89	5.65
3	1	2	3.71*	4.65	0.25
4	1	2	21.44	21.49	3.26
5	1	2	3.44*	5.24	0.14
6	1	2	3.10*	3.33	0.10
7	1	2	4.54*	0.22	0.26
8	1	2	5.04*	5.07	0.29
9	1	2	2.50*	1.46	0.07
-10	1	3	3.48*	1.91	0.08
-9	1	3	3.39*	0.78	0.09
-8	1	3	3.36*	1.37	0.09
-7	1	3	15.79	16.39	3.21
-6	1	3	5.94*	6.16	0.28
-5	1	3	2.82*	3.57	0.39
-4	1	3	3.81*	1.40	0.18
-3	1	3	24.69	24.18	2.37
-2	1	3	9.88	8.98	2.02
-1	1	3	16.22	16.67	3.42
0	1	3	22.32	21.96	2.80
1	1	3	3.00*	0.40	0.11
2	1	3	3.56*	2.46	0.14
3	1	3	22.57	21.56	2.68
4	1	3	29.93	29.66	1.79
5	1	3	10.13	9.94	4.09
6	1	3	1.29*	3.92	0.02
7	1	3	6.67	5.90	2.23
8	1	3	5.46*	4.35	0.26
-9	1	4	4.50*	1.41	0.14
-8	1	4	2.34*	2.73	0.04
-7	1	4	5.47*	5.14	0.23
-6	1	4	3.40*	1.05	0.09
-5	1	4	5.81*	4.24	0.18
-4	1	4	5.77*	6.10	0.85
-3	1	4	23.91	23.76	1.95
-2	1	4	18.67	19.65	2.20
-1	1	4	3.34*	4.95	0.06
0	1	4	5.31*	4.81	0.88
1	1	4	3.42*	2.01	0.09
2	1	4	8.97	9.90	2.39
3	1	4	6.97	7.10	2.11
4	1	4	5.81*	3.59	0.27
5	1	4	6.40	6.25	1.89
6	1	4	4.63*	4.54	1.08
-8	1	5	3.93*	0.43	0.06
-7	1	5	5.47*	4.95	0.14
-6	1	5	3.93*	2.48	0.06
-5	1	5	3.76*	6.86	0.05
-4	1	5	4.12*	2.53	0.08
-3	1	5	5.90*	5.17	0.14
-2	1	5	4.25*	3.72	0.09
-1	1	5	5.14*	2.89	0.14
0	1	5	4.87*	2.32	0.13
1	1	5	3.55*	1.58	0.08
2	1	5	3.62*	2.12	0.08
3	1	5	3.60*	2.09	0.08
4	1	5	9.11	8.72	2.21
-4	1	6	7.62*	7.41	0.22
-3	1	6	6.17*	2.70	0.12
-2	1	6	5.63*	5.72	0.09
-1	1	6	3.58*	4.50	0.05
0	2	0	14.33	14.17	6.11
1	2	0	1.75*	0.13	0.33
2	2	0	23.86	23.85	2.90
3	2	0	6.39	6.31	7.10
4	2	0	34.39	35.11	1.48
5	2	0	6.04	6.12	5.25
6	2	0	4.87*	4.43	0.53
7	2	0	17.73	17.48	4.07
8	2	0	5.27*	4.50	0.33
9	2	0	3.08*	0.31	0.11
10	2	0	3.36*	0.90	0.09
-10	2	1	2.39*	1.31	0.06
-9	2	1	3.20*	1.42	0.10
-8	2	1	3.36*	0.10	0.13
-7	2	1	31.30	31.77	1.70
-6	2	1	5.12	5.09	3.03
-5	2	1	23.60	23.15	2.75
-4	2	1	6.85	7.10	4.89
-3	2	1	3.53*	2.25	0.38
-2	2	1	13.15	13.74	5.45
-1	2	1	72.74	75.56	0.43
0	2	1	21.66	22.47	3.06
1	2	1	2.31*	0.49	0.19
2	2	1	15.73	15.88	5.61
3	2	1	10.54	10.50	6.37
4	2	1	36.36	35.71	1.37
5	2	1	2.66*	2.31	0.14
6	2	1	2.49*	1.83	0.75
7	2	1	7.75	8.45	3.60
8	2	1	4.73*	4.34	0.29
9	2	1	3.27*	1.36	0.09
10	2	1	5.25*	2.11	0.33
-10	2	2	5.20*	3.99	0.27
-9	2	2	6.97	6.96	2.41
-8	2	2	4.99*	5.16	0.27
-7	2	2	7.03	6.27	2.63
-6	2	2	8.51	8.49	3.56
-5	2	2	5.28*	6.58	0.43
-4	2	2	9.30	8.20	4.75
-3	2	2	22.26	21.92	2.76
-2	2	2	26.45	26.44	2.21
-1	2	2	35.17	35.46	1.38
0	2	2	65.73	65.90	0.49
1	2	2	9.37	9.45	5.07
2	2	2	7.72	8.24	4.69
3	2	2	4.38*	4.67	0.37
4	2	2	8.55	8.98	4.68
5	2	2	6.57	6.25	2.93
6	2	2	3.13*	2.77	0.10
7	2	2	3.18*	2.57	0.10
8	2	2	3.23*	2.65	0.10
9	2	2	2.04*	0.53	0.04
-10	2	3	3.40*	1.40	0.09
-9	2	3	3.49*	1.73	0.08
-8	2	3	11.34	11.22	3.65
-7	2	3	13.10	12.57	3.56
-6	2	3	1.12*	4.04	0.01
-5	2	3	4.99*	6.46	0.18
-4	2	3	9.32	8.93	3.04
-3	2	3	16.89	16.59	3.44
-2	2	3	26.03	26.37	2.17
-1	2	3	20.25	19.26	2.87
0	2	3	5.66*	2.26	0.44
1	2	3	13.63	13.21	3.96
2	2	3	5.12	5.48	1.48
3	2	3	9.37	9.13	3.53
4	2	3	5.39*	1.39	0.31
5	2	3	1.73*	1.63	0.05
6	2	3	4.87	4.17	1.62
7	2	3	3.27*	2.87	0.09
8	2	3	2.07*	4.09	0.22
-9	2	4	1.42*	3.39	0.01
-8	2	4	3.59*	3.13	0.08
-7	2	4	6.20*	6.11	0.22
-6	2	4	4.10*	6.53	0.10
-5	2	4	3.52*	4.43	0.08
-4	2	4	3.61*	1.60	0.08
-3	2	4	1.13*	4.26	0.01
-2	2	4	3.34*	0.21	0.06

h	k	l	Fo	Fc	weight
-1	2	4	6.70*	3.34	0.23
0	2	4	3.79*	6.32	0.07
1	2	4	13.58	12.85	2.95
2	2	4	3.49*	3.11	0.08
3	2	4	3.29*	3.17	0.08
4	2	4	3.31*	2.66	0.09
5	2	4	3.30*	1.41	0.09
6	2	4	3.49*	3.33	0.08
-6	2	5	4.02*	5.68	0.06
-7	2	5	3.46*	4.30	0.06
-6	2	5	2.37*	4.43	0.02
-5	2	5	2.46*	0.72	0.16
-4	2	5	11.88	12.14	1.99
-3	2	5	12.06	13.07	2.13
-2	2	5	9.15	9.33	1.83
-1	2	5	4.65*	2.92	0.13
0	2	5	7.15*	7.80	0.27
1	2	5	7.41*	5.71	0.27
2	2	5	2.21*	3.37	0.20
3	2	5	3.73*	4.08	0.07
4	2	5	4.14*	1.19	0.14
-4	2	6	2.84*	1.27	0.03
-3	2	6	6.35*	4.98	0.14
-2	2	6	4.05*	0.93	0.06
-1	2	6	6.87*	2.40	0.21
1	3	0	42.19	44.60	1.20
2	3	0	22.54	23.46	3.22
3	3	0	14.34	15.11	6.13
4	3	0	18.34	18.33	4.39
5	3	0	16.87	16.47	5.12
6	3	0	6.95	5.94	5.72
7	3	0	2.90*	0.42	0.12
8	3	0	5.43*	5.22	0.34
9	3	0	2.96*	2.63	0.11
10	3	0	4.45*	1.48	0.24
-10	3	1	3.66*	3.16	0.11
-9	3	1	1.82*	0.56	0.04
-8	3	1	8.53	8.63	3.54
-7	3	1	19.63	19.96	3.42
-6	3	1	18.21	18.02	4.21
-5	3	1	12.15	12.34	6.09
-4	3	1	2.57*	2.53	0.15
-3	3	1	36.77	37.93	1.35
-2	3	1	63.18	63.91	0.55
-1	3	1	30.36	31.41	1.87
0	3	1	80.40	84.44	0.36
1	3	1	26.65	26.35	2.34
2	3	1	22.29	22.06	3.15
3	3	1	17.84	17.91	4.58
4	3	1	14.17	13.61	5.89
5	3	1	21.16	21.53	3.65
6	3	1	5.73	5.76	2.92
7	3	1	3.12*	1.98	0.10
8	3	1	3.00*	2.58	0.11
9	3	1	3.33*	0.10	0.09
10	3	1	3.14*	1.53	0.10
-10	3	2	3.94*	1.98	0.11
-9	3	2	3.19*	2.17	0.09
-8	3	2	2.86*	2.42	0.12
-7	3	2	6.49*	8.63	0.34
-6	3	2	8.33	9.60	3.96
-5	3	2	8.13	7.66	4.39
-4	3	2	16.63	17.28	4.32
-3	3	2	49.02	47.82	0.77
-2	3	2	6.34	6.07	2.97
-1	3	2	13.62	14.37	4.15
0	3	2	17.97	18.10	3.77
1	3	2	15.64	15.63	4.89
2	3	2	17.07	17.07	4.50
3	3	2	16.60	16.53	4.65
4	3	2	8.61	8.50	5.16
5	3	2	25.43	25.03	2.48
6	3	2	8.82	9.42	3.59
7	3	2	5.81	5.50	2.61
8	3	2	3.23*	1.50	0.10
9	3	2	4.57*	2.31	0.15
-10	3	3	2.87*	5.77	0.05
-9	3	3	8.58	8.96	2.29
-8	3	3	1.80*	1.06	0.03
-7	3	3	6.88*	9.09	0.28
-6	3	3	4.89*	4.10	1.16
-5	3	3	4.78*	8.38	0.16
-4	3	3	2.70*	5.59	0.06
-3	3	3	11.45	11.73	3.38
-2	3	3	9.00	10.18	2.90
-1	3	3	5.78*	7.20	0.38
0	3	3	16.61	15.49	3.67
1	3	3	9.54	9.99	3.58
2	3	3	3.12*	0.38	0.10
3	3	3	3.22*	1.09	0.10
4	3	3	2.83*	1.80	0.08
5	3	3	12.72	12.53	4.22
6	3	3	3.31*	3.68	0.09
7	3	3	3.15*	2.76	0.10
8	3	3	2.93*	0.76	0.09
-9	3	4	3.77*	1.86	0.07
-8	3	4	3.58*	2.80	0.54
-7	3	4	6.61*	7.20	0.26
-6	3	4	3.46*	0.86	0.08
-5	3	4	4.47*	4.85	0.12
-4	3	4	4.12*	2.92	0.54
-3	3	4	11.56	11.03	2.04
-2	3	4	3.76*	4.54	0.07
-1	3	4	4.29*	5.39	0.54
0	3	4	3.59*	1.91	0.08
1	3	4	3.61*	0.86	0.08
2	3	4	9.98	10.19	3.02
3	3	4	1.77*	3.23	0.03
4	3	4	4.13*	6.06	0.10
5	3	4	3.40*	6.08	0.09
6	3	4	3.53*	1.39	0.09
-7	3	5	4.00*	4.81	0.06
-6	3	5	2.38*	6.96	0.02
-5	3	5	3.85*	0.07	0.07
-4	3	5	1.31*	2.30	0.01
-3	3	5	4.07*	4.71	0.06
-2	3	5	6.04*	6.21	0.18
-1	3	5	3.88*	6.74	0.07
0	3	5	3.70*	5.27	0.07
1	3	5	8.53	8.10	1.90
2	3	5	7.41	7.09	1.76
3	3	5	3.07*	5.29	0.36
4	3	5	3.60*	1.69	0.09
-3	3	6	4.13*	3.30	0.06
-2	3	6	4.10*	0.04	0.06
-1	3	6	4.01*	0.75	0.06
0	4	0	64.08	66.92	0.57
1	4	0	21.80	21.10	3.56
2	4	0	9.03	8.79	7.75
3	4	0	4.37*	2.18	0.73
4	4	0	18.36	17.33	4.62
5	4	0	8.77	9.00	6.50
6	4	0	8.54	9.14	4.86
7	4	0	3.56*	4.64	0.17
8	4	0	4.40*	4.38	0.24
9	4	0	3.09*	3.44	0.81
10	4	0	3.07*	3.59	0.11
-10	4	1	4.81*	3.83	0.22
-9	4	1	6.07*	5.61	0.39
-8	4	1	9.59	9.91	4.34
-7	4	1	2.67*	2.89	0.56
-6	4	1	2.80*	2.95	0.13
-5	4	1	2.71*	4.53	0.14
-4	4	1	19.07	18.88	3.95
-3	4	1	45.68	45.43	0.91
-2	4	1	49.03	50.47	0.84
-1	4	1	61.28	64.85	0.58
0	4	1	34.68	35.75	1.50
1	4	1	69.97	71.80	0.46
2	4	1	24.26	24.35	2.86
3	4	1	23.78	23.55	2.87
4	4	1	23.16	23.16	3.06
5	4	1	9.67	9.23	5.74
6	4	1	4.22*	3.14	0.32
7	4	1	9.85	11.28	3.94
8	4	1	2.21*	2.01	0.07
9	4	1	3.22*	0.20	0.10
10	4	1	3.35*	1.27	0.09
-10	4	2	1.98*	1.34	0.03
-9	4	2	1.91*	0.94	0.27
-8	4	2	10.17	10.52	3.62
-7	4	2	5.09*	5.17	0.22
-6	4	2	4.09*	2.61	0.23
-5	4	2	2.94*	3.42	0.15
-4	4	2	12.61	11.91	5.07
-3	4	2	24.58	23.66	2.66
-2	4	2	2.75*	4.61	0.13
-1	4	2	5.06*	6.24	0.41
0	4	2	18.31	18.59	3.74
1	4	2	40.10	40.21	1.12
2	4	2	31.08	30.12	1.78
3	4	2	17.98	17.61	4.42
4	4	2	9.26	9.64	4.63
5	4	2	19.12	18.18	3.58
6	4	2	17.67	18.07	3.71
7	4	2	4.59*	6.39	0.26
8	4	2	2.72*	2.27	0.07
9	4	2	6.33*	2.39	0.32
-10	4	3	1.44*	3.56	0.01
-9	4	3	3.84*	3.60	0.76
-8	4	3	3.35*	3.60	0.09
-7	4	3	13.55	13.11	3.53
-6	4	3	5.34*	6.36	0.20
-5	4	3	2.85*	3.58	0.07
-4	4	3	3.18*	1.82	0.10
-3	4	3	11.83	12.20	3.68
-2	4	3	3.11*	3.47	0.10
-1	4	3	8.11	7.07	3.29
0	4	3	7.09	6.46	2.79
1	4	3	11.95	11.16	4.17
2	4	3	3.12*	1.97	0.10
3	4	3	1.10*	4.88	0.01
4	4	3	15.13	15.79	3.61
5	4	3	9.88	9.83	3.68
6	4	3	4.89*	2.01	0.37
7	4	3	5.00*	0.49	0.24
8	4	3	4.97*	3.08	0.16
-8	4	4	3.64*	1.78	0.08
-7	4	4	3.63*	2.75	0.08
-6	4	4	5.98*	4.71	0.25
-5	4	4	6.32	6.52	1.33
-4	4	4	3.68*	3.42	0.07
-3	4	4	3.60*	4.06	0.07
-2	4	4	15.59	15.46	2.33
-1	4	4	15.94	15.14	2.66
0	4	4	3.53*	2.83	0.08
1	4	4	6.62	5.70	1.74
2	4	4	9.22	9.63	2.93
3	4	4	11.43	11.67	3.62
4	4	4	3.15*	0.27	0.10
5	4	4	4.35*	0.03	0.17
6	4	4	3.70*	3.08	0.07
-7	4	5	5.10*	5.18	0.80
-6	4	5	3.73*	2.14	0.07
-5	4	5	3.28*	3.29	0.05
-4	4	5	3.81*	0.62	0.07
-3	4	5	3.84*	4.12	0.07
-2	4	5	14.85	14.63	2.47
-1	4	5	5.03*	0.67	0.15
0	4	5	3.55*	0.73	0.08
1	4	5	4.65*	3.71	0.13
2	4	5	6.60*	2.17	0.31
3	4	5	3.54*	0.30	0.08
4	4	6	7.76*	3.32	0.22
-6	4	6	7.03*	3.10	0.21
-5	4	6	2.90*	0.36	0.49
-4	5	0	25.93	26.33	2.47
-3	5	0	13.83	13.21	6.08
-2	5	0	21.49	20.61	3.62
-1	5	0	11.65	11.63	6.40
0	5	0	14.23	13.96	8.16
1	5	0	2.27*	3.60	0.06

h	k	l	Fo	Fc	weight
8	5	0	2.15*	2.24	0.54
9	5	0	5.12*	4.63	0.30
10	5	0	3.76*	0.26	0.15
-10	5	1	2.79*	2.74	0.57
-9	5	1	3.26*	4.68	0.09
-8	5	1	2.71*	4.49	0.08
-7	5	1	14.82	15.51	3.75
-6	5	1	9.88	9.47	5.00
-5	5	1	3.40*	2.01	0.28
-4	5	1	20.01	19.02	3.77
-3	5	1	23.20	21.68	2.94
-2	5	1	27.98	28.53	2.14
-1	5	1	27.91	27.55	2.21
0	5	1	39.79	40.25	1.22
1	5	1	60.29	60.78	0.59
2	5	1	36.54	36.55	1.42
3	5	1	20.35	19.60	3.77
4	5	1	12.62	12.67	6.20
5	5	1	7.98	8.14	5.43
6	5	1	4.16*	3.21	1.80
7	5	1	5.46*	5.32	0.37
8	5	1	2.87*	4.96	0.09
9	5	1	3.08*	1.73	0.11
-10	5	2	4.44*	2.85	0.18
-9	5	2	3.14*	2.10	0.10
-8	5	2	3.69*	4.73	0.17
-7	5	2	9.09	9.70	3.15
-6	5	2	3.08*	2.54	0.11
-5	5	2	5.26*	4.25	0.43
-4	5	2	18.27	18.45	4.02
-3	5	2	3.48*	3.95	0.21
-2	5	2	3.10*	1.28	1.08
-1	5	2	8.96	9.26	4.39
0	5	2	18.10	17.77	4.05
1	5	2	43.78	41.80	1.00
2	5	2	5.25*	5.97	0.50
3	5	2	5.60	5.31	3.70
4	5	2	2.87*	3.78	0.12
5	5	2	13.06	13.01	4.37
6	5	2	2.07*	2.38	0.06
7	5	2	3.21*	3.92	0.10
8	5	2	2.74*	3.76	0.10
9	5	2	3.35*	1.16	0.09
-10	5	3	3.52*	1.66	0.08
-9	5	3	3.21*	0.35	0.10
-8	5	3	3.46*	1.91	0.08
-7	5	3	3.13*	0.01	0.10
-6	5	3	12.86	12.39	3.24
-5	5	3	3.32*	4.13	0.09
-4	5	3	8.66	8.36	2.53
-3	5	3	9.43	9.80	3.23
-2	5	3	15.09	14.80	3.82
-1	5	3	8.53	8.85	3.12
0	5	3	18.72	17.83	3.54
1	5	3	3.06*	1.38	0.11
2	5	3	3.66*	4.30	0.14
3	5	3	5.87*	3.93	0.41
4	5	3	12.34	12.43	3.80
5	5	3	5.94*	6.82	0.38
6	5	3	5.58*	6.34	0.27
7	5	3	3.45*	0.31	0.08
-9	5	4	3.42*	0.44	0.09
-8	5	4	3.45*	0.23	0.08
-7	5	4	2.62*	0.69	0.05
-6	5	4	14.41	14.47	3.06
-5	5	4	3.74*	7.05	0.07
-4	5	4	1.17*	5.50	0.01
-3	5	4	3.80*	2.98	0.07
-2	5	4	10.98	11.17	2.11
-1	5	4	5.22*	5.68	0.14
0	5	4	6.81*	5.44	0.28
1	5	4	7.31	7.73	1.81
2	5	4	8.93	9.02	2.95
3	5	4	3.58*	7.49	0.08
4	5	4	2.64*	1.42	0.08
5	5	4	5.87*	3.59	0.41
6	5	4	3.25*	4.43	0.08
-7	5	5	5.35*	2.96	0.16
-6	5	5	6.65*	7.06	0.18
-5	5	5	5.40*	5.18	0.13
-4	5	5	2.96*	5.57	0.04
-3	5	5	8.12	8.01	1.46
-2	5	5	2.05*	0.73	0.14
-1	5	5	6.08	5.45	1.13
0	5	5	5.61*	3.89	0.20
1	5	5	4.47*	3.35	0.11
2	5	5	3.91*	0.59	0.12
3	5	5	4.28*	1.32	0.12
4	5	5	2.46*	1.43	0.36
5	6	0	3.79*	3.96	0.59
6	6	0	21.66	21.49	3.46
7	6	0	34.05	33.66	1.52
8	6	0	3.97	2.98	3.19
9	6	0	5.87	5.70	4.99
10	6	0	15.06	15.23	4.96
-10	6	1	4.75	4.73	2.14
-9	6	1	18.87	18.94	3.73
-8	6	1	2.97*	2.60	0.11
-7	6	1	3.06*	1.12	0.11
-6	6	1	3.25*	3.00	0.09
-5	6	1	5.41*	3.88	0.32
-4	6	1	5.98*	5.60	0.39
-3	6	1	1.96*	0.79	0.06
-2	6	1	5.57	5.36	2.81
-1	6	1	3.59*	3.90	1.96
0	6	1	8.13	8.19	5.42
1	6	1	31.68	30.19	1.74
2	6	1	27.45	27.09	2.28
3	6	1	2.17*	0.20	0.21
4	6	1	20.15	20.06	3.95
5	6	1	2.38*	1.37	0.18
6	6	1	3.23*	0.60	0.30
7	6	1	4.21*	2.51	0.60
8	6	1	3.76*	0.25	0.51
9	6	1	2.71*	4.95	0.11
10	6	1	5.67*	4.63	0.40
-10	6	2	3.52*	1.52	0.08
-9	6	2	7.68	6.86	2.95
-8	6	2	8.95	8.85	3.61
-7	6	2	8.31	8.20	3.17
-6	6	2	4.46*	6.33	0.20
-5	6	2	16.61	15.68	4.39
-4	6	2	26.33	25.44	2.28
-3	6	2	22.66	22.34	3.07
-2	6	2	5.37*	3.78	0.49
-1	6	2	25.43	25.93	2.47
0	6	2	29.25	28.61	1.99
1	6	2	2.66*	4.11	0.14
2	6	2	9.60	9.91	5.44
3	6	2	14.96	14.83	4.92
4	6	2	7.63	7.06	4.07
5	6	2	9.48	8.99	4.03
6	6	2	2.09*	1.09	0.05
7	6	2	1.29*	3.41	0.02
8	6	2	4.77*	1.78	0.20
9	6	2	3.47*	1.40	0.08
-10	6	3	7.77	8.94	1.79
-9	6	3	4.34*	2.07	0.15
-8	6	3	4.10*	3.77	0.14
-7	6	3	3.35*	2.83	0.09
-6	6	3	5.31*	7.16	0.20
-5	6	3	11.34	10.61	3.36
-4	6	3	14.31	14.65	3.28
-3	6	3	16.11	15.65	3.60
-2	6	3	7.88	8.26	2.82
-1	6	3	3.04*	0.33	0.11
0	6	3	20.55	20.40	3.27
1	6	3	8.30	7.45	3.29
2	6	3	12.72	12.35	4.08
3	6	3	8.92	8.97	3.14
4	6	3	3.16*	4.01	0.71
5	6	3	6.25*	6.25	0.36
6	6	3	3.74*	2.97	0.14
7	6	3	2.80*	3.35	0.06
-9	6	4	3.54*	0.50	0.08
-8	6	4	4.47*	5.47	0.82
-7	6	4	6.05*	2.87	0.27
-6	6	4	8.19	9.28	2.04
-5	6	4	2.99*	2.28	0.05
-4	6	4	13.47	13.69	2.74
-3	6	4	3.52*	2.05	0.08
-2	6	4	3.76*	3.40	0.07
-1	6	4	5.27*	4.47	0.18
0	6	4	3.60*	3.24	0.08
1	6	4	4.76*	4.52	0.21
2	6	4	6.61*	5.93	0.34
3	6	4	2.55*	4.24	0.06
4	6	4	4.97*	4.94	0.13
5	6	4	13.20	13.14	3.45
6	6	4	3.46*	2.02	0.08
-7	6	5	4.32*	5.16	0.08
-6	6	5	3.88*	4.67	0.07
-5	6	5	2.72*	1.40	0.04
-4	6	5	1.88*	1.47	0.02
-3	6	5	2.28*	1.17	0.03
-2	6	5	3.62*	2.60	0.08
-1	6	5	5.10*	0.87	0.17
0	6	5	3.72*	2.52	0.07
1	6	5	3.55*	2.68	0.08
2	6	5	3.58*	2.90	0.08
3	6	5	2.03*	3.21	0.03
1	7	0	40.36	40.17	1.19
2	7	0	34.07	34.29	1.56
3	7	0	7.14	7.89	5.81
4	7	0	9.35	8.47	7.43
5	7	0	3.54*	0.81	0.36
6	7	0	2.70*	1.25	0.14
7	7	0	4.18*	3.68	0.33
8	7	0	11.96	11.32	4.76
9	7	0	3.00*	0.83	0.11
10	7	0	3.02*	2.74	0.11
-10	7	1	3.36*	1.33	0.09
-9	7	1	3.07*	3.10	0.11
-8	7	1	2.90*	1.71	0.12
-7	7	1	8.00	8.53	3.47
-6	7	1	1.06*	1.52	0.02
-5	7	1	13.65	13.32	5.40
-4	7	1	25.67	24.67	2.59
-3	7	1	17.98	17.03	4.45
-2	7	1	23.12	22.11	2.99
-1	7	1	23.44	24.52	2.85
0	7	1	5.54	6.42	4.07
1	7	1	2.84*	2.27	0.26
2	7	1	2.42*	0.40	0.17
3	7	1	4.67*	4.99	0.50
4	7	1	2.60*	1.16	0.15
5	7	1	2.88*	0.42	0.12
6	7	1	9.76	9.50	4.10
7	7	1	15.27	15.61	4.23
8	7	1	14.19	15.11	3.93
9	7	1	2.99*	3.54	0.11
-10	7	2	3.21*	0.22	0.10
-9	7	2	1.89*	3.70	0.03
-8	7	2	4.61*	5.05	1.47
-7	7	2	5.97*	5.27	0.32
-6	7	2	4.38*	5.77	0.19
-5	7	2	5.37	5.31	2.22
-4	7	2	5.44*	6.88	0.40
-3	7	2	23.62	23.14	2.84
-2	7	2	5.56	5.08	3.17
-1	7	2	9.96	10.38	5.11
0	7	2	26.79	26.92	2.30
1	7	2	12.89	12.60	5.41
2	7	2	7.84	7.56	5.03
3	7	2	7.09	6.92	4.45
4	7	2	1.06*	2.80	0.02
5	7	2	3.01*	0.06	0.13
6	7	2	5.58*	6.44	0.33
7	7	2	3.94*	4.98	1.10

h	k	l	Fo	Fc	weight
8	7	2	3.21*	1.10	0.10
-10	7	3	5.48*	2.35	0.22
-9	7	3	4.15*	4.54	0.15
-8	7	3	3.19*	0.49	0.10
-7	7	3	1.24*	0.31	0.02
-6	7	3	3.10*	0.05	0.10
-5	7	3	12.80	12.48	3.41
-4	7	3	13.40	11.97	3.54
-3	7	3	8.98	8.33	3.42
-2	7	3	3.06*	3.42	0.11
-1	7	3	11.67	11.98	3.71
0	7	3	9.15	9.82	3.29
1	7	3	25.89	26.14	2.31
2	7	3	3.09*	2.69	0.10
3	7	3	3.24*	0.82	0.10
4	7	3	2.66*	4.57	0.52
5	7	3	12.08	12.08	4.19
6	7	3	4.62*	1.20	0.26
7	7	3	3.28*	2.36	0.09
-9	7	4	2.92*	3.53	0.04
-8	7	4	4.82*	5.12	0.13
-7	7	4	6.23	7.66	1.35
-6	7	4	4.04*	0.61	0.15
-5	7	4	6.04*	2.96	0.30
-4	7	4	1.69*	0.78	0.02
-3	7	4	3.49*	0.99	0.08
-2	7	4	8.61	9.14	1.90
-1	7	4	3.29*	3.94	0.07
0	7	4	6.83	6.36	1.68
1	7	4	4.33*	6.55	0.10
2	7	4	1.24*	2.84	0.02
3	7	4	1.88*	2.42	0.28
4	7	4	3.79*	4.29	0.12
5	7	4	3.42*	3.94	0.09
-7	7	5	3.55*	3.56	0.06
-6	7	5	2.43*	1.87	0.03
-5	7	5	8.19	9.14	1.49
-4	7	5	11.89	13.30	2.07
-3	7	5	4.40*	1.88	0.11
-2	7	5	5.45*	4.77	0.12
-1	7	5	5.14*	2.38	0.17
0	7	5	3.77*	6.30	0.07
1	7	5	6.12*	2.56	0.26
2	7	5	3.64*	2.71	0.08
3	7	5	3.69*	4.69	0.07
0	8	0	38.50	38.84	1.33
1	8	0	17.41	17.68	4.64
2	8	0	5.40	5.65	4.80
3	8	0	6.92	7.48	5.88
4	8	0	24.65	24.35	2.83
5	8	0	3.33*	2.80	0.24
6	8	0	2.82*	1.56	0.13
7	8	0	7.42	7.85	3.40
8	8	0	6.67	6.74	3.02
9	8	0	3.59*	0.53	0.15
10	8	0	2.51*	0.65	0.05
-10	8	1	3.15*	1.35	0.10
-9	8	1	2.99*	1.11	0.10
-8	8	1	6.43	7.13	2.78
-7	8	1	1.64*	1.78	0.03
-6	8	1	4.93*	3.59	0.37
-5	8	1	2.99*	2.86	0.15
-4	8	1	4.69	4.02	3.45
-3	8	1	7.31	7.24	5.42
-2	8	1	2.43*	2.77	0.17
-1	8	1	3.85*	2.14	0.47
0	8	1	24.29	23.90	2.81
1	8	1	37.38	36.22	1.31
2	8	1	15.94	15.88	5.25
3	8	1	26.25	25.41	2.51
4	8	1	16.92	17.42	4.73
5	8	1	7.21	7.78	4.00
6	8	1	3.94*	3.16	1.56
7	8	1	14.24	14.35	4.33
8	8	1	4.75*	3.45	0.30
9	8	1	1.99*	1.18	0.05
-10	8	2	3.48*	2.02	0.79
-9	8	2	9.82	9.78	3.26
-8	8	2	15.73	15.73	3.81
-7	8	2	3.18*	1.80	0.10
-6	8	2	3.12*	0.85	0.10
-5	8	2	14.03	13.72	4.32
-4	8	2	12.56	12.28	5.00
-3	8	2	30.80	30.68	1.85
-2	8	2	6.91	7.51	4.16
-1	8	2	2.79*	0.60	0.18
0	8	2	3.88*	0.83	0.37
1	8	2	19.80	19.10	3.86
2	8	2	6.33	6.72	3.87
3	8	2	2.85*	2.36	0.12
4	8	2	2.95*	2.90	0.11
5	8	2	10.61	10.18	3.93
6	8	2	3.02*	2.67	0.11
7	8	2	5.87*	4.99	0.33
8	8	2	3.17*	0.70	0.10
-9	8	3	4.41*	2.64	0.17
-8	8	3	2.04*	1.09	0.24
-7	8	3	8.10	8.33	3.06
-6	8	3	6.60*	5.49	0.33
-5	8	3	4.08*	3.81	0.14
-4	8	3	4.34*	6.68	0.14
-3	8	3	11.08	11.28	3.25
-2	8	3	6.70	7.27	2.22
-1	8	3	3.08*	4.71	0.11
0	8	3	4.97*	7.71	0.18
1	8	3	8.23	8.09	3.01
2	8	3	3.15*	4.04	0.10
3	8	3	6.22	6.51	2.24
4	8	3	3.63*	5.10	0.14
5	8	3	3.12*	2.58	0.13
6	8	3	8.01	7.41	2.94
7	8	3	3.37*	1.21	0.09
8	8	3	4.21*	4.12	0.16
-8	8	4	3.74*	2.44	0.07
-7	8	4	3.65*	4.39	0.10
-6	8	4	5.60	5.59	1.31
-5	8	4	3.64*	5.37	0.08
-4	8	4	7.14	6.57	2.00
-3	8	4	12.28	12.49	2.78
-2	8	4	5.40*	4.65	0.19
-1	8	4	3.41*	2.01	0.09
0	8	4	3.36*	1.18	0.09
1	8	4	3.96*	1.65	0.15
2	8	4	3.16*	1.54	0.10
3	8	4	3.36*	0.21	0.09
4	8	4	3.28*	1.95	0.09
5	8	4	3.68*	0.24	0.07
6	8	5	4.48*	3.61	0.11
7	8	5	3.38*	3.19	0.05
8	8	5	3.59*	0.25	0.07
9	8	5	3.78*	3.93	0.07
-10	8	5	10.57	10.93	2.30
-9	8	5	3.28*	1.21	0.06
-8	8	5	6.64*	6.09	0.28
-7	8	5	3.65*	3.85	0.09
-6	8	5	2.45*	2.07	0.04
-5	8	5	2.15*	2.43	0.22
-4	8	5	7.32	7.58	6.22
-3	8	5	8.06	8.06	6.40
-2	8	5	13.20	12.80	6.51
-1	8	5	0.95*	4.26	0.02
0	8	5	4.35*	3.10	0.32
1	8	5	3.99*	5.22	0.18
2	8	5	1.19*	2.07	0.02
3	8	5	7.90	7.37	4.10
4	8	5	3.21*	2.83	0.10
5	8	5	2.53*	0.14	0.05
-10	9	1	4.32*	1.47	0.16
-9	9	1	3.02*	6.14	0.07
-8	9	1	9.83	10.65	3.72
-7	9	1	4.08*	0.91	0.21
-6	9	1	4.55*	3.84	1.71
-5	9	1	12.73	12.22	5.59
-4	9	1	9.31	9.06	6.06
-3	9	1	12.03	12.87	8.85
-2	9	1	4.81*	4.66	0.60
-1	9	1	2.55*	3.89	0.15
0	9	1	8.70	8.28	5.88
1	9	1	8.47	8.12	6.19
2	9	1	8.18	8.80	6.13
3	9	1	13.32	12.95	6.02
4	9	1	2.84*	1.32	0.17
5	9	1	16.99	17.01	4.04
6	9	1	3.12*	5.32	0.10
7	9	1	9.26	9.48	3.98
8	9	1	1.88*	1.96	0.28
9	9	1	3.76*	2.46	0.15
-10	9	2	3.34*	4.63	0.09
-9	9	2	4.31*	2.67	0.17
-8	9	2	5.56	4.74	2.41
-7	9	2	3.18*	0.72	0.14
-6	9	2	7.86	7.51	2.87
-5	9	2	5.82*	7.02	0.31
-4	9	2	10.99	11.51	4.68
-3	9	2	5.16*	6.05	0.45
-2	9	2	11.93	11.81	5.62
-1	9	2	9.60	10.08	5.22
0	9	2	4.49	4.49	2.38
1	9	2	7.40	8.14	5.11
2	9	2	8.41	8.10	4.92
3	9	2	3.60*	2.53	0.26
4	9	2	9.00	9.22	3.72
5	9	2	11.99	12.23	4.23
6	9	2	1.76*	3.47	0.05
7	9	2	8.21	9.30	3.01
8	9	2	3.19*	0.65	0.10
-9	9	3	3.43*	1.95	0.09
-8	9	3	4.81*	3.39	0.21
-7	9	3	3.92*	1.85	0.09
-6	9	3	5.10*	2.52	0.23
-5	9	3	3.41*	2.60	0.09
-4	9	3	12.26	12.48	3.54
-3	9	3	4.54*	4.02	0.19
-2	9	3	12.43	12.73	3.56
-1	9	3	18.25	17.93	3.49
0	9	3	9.27	9.61	3.15
1	9	3	3.09*	0.94	0.10
2	9	3	1.94*	2.21	0.04
3	9	3	4.21*	2.50	0.18
4	9	3	3.21*	4.28	0.10
5	9	3	11.97	12.74	3.97
6	9	3	5.61*	3.28	0.35
7	9	3	4.98*	5.19	0.25
-8	9	4	4.91*	1.30	0.19
-7	9	4	3.42*	0.45	0.09
-6	9	4	3.55*	4.57	0.08
-5	9	4	2.82*	0.19	0.05
-4	9	4	3.47*	3.64	0.08
-3	9	4	13.31	13.00	3.16
-2	9	4	3.51*	4.47	0.08
-1	9	4	3.56*	4.60	0.09
0	9	4	11.81	12.11	3.15
1	9	4	5.78*	3.77	0.30
2	9	4	3.80*	1.93	0.15
3	9	4	3.29*	0.38	0.09
4	9	4	5.63*	6.18	0.21
5	9	4	4.51*	3.66	0.14
-6	9	5	3.72*	0.61	0.07
-5	9	5	5.56*	6.17	0.15
-4	9	5	3.63*	2.21	0.08
-3	9	5	3.77*	2.15	0.07
-2	9	5	10.85	10.86	2.37
-1	9	5	9.64	9.74	2.09
0	9	5	5.64*	8.21	0.16
1	9	5	3.76*	3.61	0.59
2	9	5	2.85*	4.88	0.05
0	10	0	16.28	16.48	5.27
1	10	0	25.21	24.52	2.56
2	10	0	3.72*	2.90	0.42
3	10	0	17.57	17.78	4.92
4	10	0	8.01	8.44	6.26
5	10	0	9.68	9.18	5.68

h	k	l	Fo	Fc	weight
6	10	0	3.19*	5.35	0.17
7	10	0	5.92*	8.02	0.39
8	10	0	3.08*	3.97	0.11
9	10	0	3.22*	1.82	0.10
-10	10	1	3.17*	2.90	0.10
-9	10	1	3.86*	4.19	0.12
-8	10	1	8.38	8.58	3.43
-7	10	1	17.17	16.86	3.88
-6	10	1	3.53*	0.28	0.15
-5	10	1	12.89	12.36	4.63
-4	10	1	26.45	26.91	2.36
-3	10	1	17.61	17.59	4.65
-2	10	1	31.96	30.85	1.75
-1	10	1	4.32*	5.23	0.47
0	10	1	26.72	26.31	2.37
1	10	1	21.46	20.94	3.49
2	10	1	6.82	6.36	5.84
3	10	1	4.51*	3.67	0.51
4	10	1	14.45	13.64	5.21
5	10	1	3.65*	0.20	0.18
6	10	1	5.00*	5.80	0.28
7	10	1	8.27	7.43	4.21
8	10	1	3.30*	5.36	0.11
9	10	1	3.14*	2.66	0.10
-10	10	2	3.47*	1.70	0.08
-9	10	2	3.22*	1.03	0.10
-8	10	2	3.23*	0.26	0.10
-7	10	2	3.02*	0.41	0.11
-6	10	2	8.17	7.81	3.56
-5	10	2	2.66*	0.81	0.10
-4	10	2	12.24	12.04	4.52
-3	10	2	2.78*	0.31	0.14
-2	10	2	15.84	15.92	4.75
-1	10	2	2.77*	1.70	0.13
0	10	2	17.88	18.15	4.27
1	10	2	2.66*	0.07	0.14
2	10	2	4.76	4.29	2.65
3	10	2	7.11	7.32	3.41
4	10	2	3.06*	3.52	0.11
5	10	2	12.62	13.42	4.07
6	10	2	3.07*	1.82	0.11
7	10	2	3.10*	0.51	0.10
8	10	2	3.12*	1.83	0.10
-9	10	3	3.42*	1.60	0.09
-8	10	3	3.44*	1.75	0.08
-7	10	3	3.33*	0.58	0.86
-6	10	3	1.94*	2.83	0.27
-5	10	3	3.31*	1.30	0.09
-4	10	3	3.89*	3.91	0.16
-3	10	3	11.97	11.25	3.65
-2	10	3	11.56	11.73	3.40
-1	10	3	3.15*	2.76	0.10
0	10	3	7.74	7.82	2.50
1	10	3	16.01	14.87	3.80
2	10	3	6.36	4.93	2.52
3	10	3	5.30*	4.11	0.30
4	10	3	1.24*	2.20	0.02
5	10	3	4.08*	5.76	1.00
6	10	3	3.43*	3.56	0.09
7	10	3	3.55*	0.51	0.12
-8	10	4	3.64*	1.84	0.08
-7	10	4	3.61*	0.70	0.08
-6	10	4	2.29*	4.72	0.03
-5	10	4	3.62*	5.80	0.08
-4	10	4	4.49*	3.57	0.16
-3	10	4	3.50*	0.22	0.08
-2	10	4	8.12	8.70	2.36
-1	10	4	10.62	10.45	2.96
0	10	4	3.17*	2.35	0.10
1	10	4	7.87	8.12	2.46
2	10	4	6.60	7.53	2.27
3	10	4	5.08*	5.58	1.35
4	10	4	5.17*	4.46	0.19
5	10	4	3.22*	4.98	0.08
-6	10	5	3.77*	3.50	0.07
-5	10	5	3.86*	5.49	0.07
-4	10	5	3.66*	0.49	0.09
-3	10	5	3.61*	2.41	0.08
-2	10	5	3.86*	1.04	0.07
-1	10	5	2.74*	2.52	0.03
0	10	5	3.68*	1.73	0.07
1	10	5	3.50*	2.40	0.08
2	10	5	5.64*	6.33	1.09
1	11	0	13.00	12.24	6.41
2	11	0	2.35*	1.22	0.19
3	11	0	10.47	10.38	6.75
4	11	0	10.94	11.02	6.11
5	11	0	15.42	16.05	4.52
6	11	0	6.46	6.40	3.06
7	11	0	8.94	9.68	4.08
8	11	0	8.73	9.13	3.39
9	11	0	3.32*	1.27	0.09
-10	11	1	2.54*	3.25	0.05
-9	11	1	3.32*	0.13	0.09
-8	11	1	2.59*	7.12	0.06
-7	11	1	8.85	8.73	3.73
-6	11	1	16.49	16.34	3.93
-5	11	1	13.00	13.01	4.31
-4	11	1	17.63	17.55	4.31
-3	11	1	15.70	15.28	5.09
-2	11	1	16.85	16.86	4.82
-1	11	1	24.40	24.46	2.71
0	11	1	1.76*	4.32	0.07
1	11	1	10.12	10.00	6.33
2	11	1	6.97	7.05	5.21
3	11	1	12.14	12.46	5.55
4	11	1	5.05*	4.83	0.35
5	11	1	2.97*	5.57	0.12
6	11	1	4.40*	1.28	0.33
7	11	1	4.43*	0.60	0.30
8	11	1	3.34*	2.52	0.12
9	11	1	2.05*	2.40	0.04
-9	11	2	3.41*	1.60	0.09
-8	11	2	5.26*	5.04	0.28
-7	11	2	9.85	10.27	4.03
-6	11	2	3.25*	3.30	0.09
-5	11	2	4.43*	1.70	0.23
-4	11	2	1.05*	3.88	0.01
-3	11	2	19.65	19.27	3.66
-2	11	2	5.02*	5.49	0.47
-1	11	2	9.06	9.07	5.19
0	11	2	10.61	10.61	5.28
1	11	2	17.86	18.32	4.04
2	11	2	2.63*	0.98	0.14
3	11	2	2.89*	0.55	0.12
4	11	2	14.42	13.70	4.28
5	11	2	3.42*	0.90	0.19
6	11	2	8.65	9.78	3.78
7	11	2	3.20*	0.58	0.10
8	11	2	4.78*	4.73	0.20
-8	11	3	3.52*	3.33	0.09
-7	11	3	3.31*	0.04	0.09
-6	11	3	7.58	8.60	2.39
-5	11	3	10.80	10.43	3.67
-4	11	3	8.52	8.65	2.92
-3	11	3	3.97*	3.29	0.14
-2	11	3	3.35*	4.82	0.10
-1	11	3	1.10*	6.39	0.01
0	11	3	1.97*	2.38	0.26
1	11	3	10.09	10.12	3.35
2	11	3	6.26*	5.54	0.38
3	11	3	4.64*	4.41	1.38
4	11	3	2.96*	0.12	0.10
5	11	3	5.20*	5.45	0.26
6	11	3	5.77*	0.16	0.33
7	11	3	5.91*	3.06	0.33
8	11	3	5.08*	0.73	0.33
-8	11	4	3.39*	0.99	0.09
-7	11	4	2.41*	0.86	0.04
-6	11	4	3.43*	1.09	0.08
-5	11	4	4.68*	4.23	0.18
-4	11	4	7.28	7.90	1.88
-3	11	4	13.65	14.47	3.14
-2	11	4	16.21	16.50	3.25
-1	11	4	3.02*	4.90	0.07
0	11	4	3.27*	2.50	0.09
1	11	4	3.81*	4.38	0.15
2	11	4	9.73	9.37	3.25
3	11	4	4.26*	3.67	0.13
4	11	4	1.40*	1.93	0.01
5	11	4	3.37*	0.65	0.09
-6	11	5	5.06*	2.56	0.15
-5	11	5	1.43*	0.55	0.01
-4	11	5	4.20*	1.12	0.11
-3	11	5	3.57*	3.18	0.08
-2	11	5	1.95*	3.42	0.02
-1	11	5	6.35*	4.73	0.25
0	11	5	3.52*	1.45	0.08
1	11	5	4.93*	2.47	0.13
2	11	5	5.64*	3.70	0.19
0	12	0	50.37	49.76	0.75
1	12	0	9.30	8.91	7.10
2	12	0	1.85*	1.82	0.13
3	12	0	4.13*	1.78	0.42
4	12	0	1.03*	0.35	0.03
5	12	0	10.66	11.57	4.50
6	12	0	8.47	8.10	4.21
7	12	0	5.36	5.72	2.79
8	12	0	3.71*	1.07	1.37
9	12	0	5.61	4.88	1.84
-9	12	1	1.98*	1.21	0.04
-8	12	1	3.22*	3.22	0.11
-7	12	1	12.16	11.62	4.43
-6	12	1	13.45	13.63	4.19
-5	12	1	5.32	5.50	2.09
-4	12	1	1.03*	0.31	0.02
-3	12	1	9.31	9.55	5.47
-2	12	1	3.77*	0.18	0.35
-1	12	1	3.96	3.86	2.71
0	12	1	13.54	13.80	5.95
1	12	1	6.32	6.46	4.89
2	12	1	14.74	14.62	5.61
3	12	1	8.67	8.69	5.09
4	12	1	2.86*	1.40	0.15
5	12	1	15.73	15.47	4.08
6	12	1	8.52	7.98	3.78
7	12	1	3.44*	1.98	0.18
8	12	1	4.58*	1.72	0.25
9	12	1	3.31*	1.00	0.09
-8	12	2	4.89*	3.92	0.22
-8	12	2	4.36*	6.65	1.06
-7	12	2	6.18*	6.31	0.38
-6	12	2	3.39*	4.97	0.09
-5	12	2	3.25*	3.48	0.09
-4	12	2	3.06*	1.84	0.12
-3	12	2	4.89*	4.05	0.32
-2	12	2	2.75*	1.34	0.13
-1	12	2	3.32*	4.74	0.18
0	12	2	5.32	6.44	2.90
1	12	2	3.71*	1.04	0.22
2	12	2	4.87	3.66	2.24
3	12	2	2.95*	3.54	0.80
4	12	2	3.27*	6.28	0.09
5	12	2	7.37	7.52	3.19
6	12	2	4.87*	1.94	0.31
7	12	2	2.76*	2.72	0.09
8	12	2	6.02*	3.80	0.35
-9	12	3	3.42*	0.49	0.09
-8	12	3	4.89*	1.38	0.22
-7	12	3	4.38*	0.52	0.22
-6	12	3	6.83	7.16	2.59
-5	12	3	10.81	11.21	3.58
-4	12	3	13.56	14.06	3.32
-3	12	3	1.14*	6.17	0.01
-2	12	3	13.26	13.48	3.58
-1	12	3	3.35*	6.43	0.10
0	12	3	3.95*	3.04	1.10
1	12	3	3.05*	0.19	0.11
2	12	3	11.59	11.78	3.79
3	12	3	3.01*	0.62	0.13
4	12	3	5.13*	4.08	0.30
5	12	3	3.20*	0.15	0.10
6	12	3	3.20*	0.76	0.10
-8	12	4	6.37	6.59	1.47
-7	12	4	5.45*	7.81	0.19
-6	12	4	8.02	8.31	2.08
-5	12	4	3.38*	1.33	0.09
-4	12	4	6.67*	7.08	0.29
-3	12	4	11.47	12.03	3.22
-2	12	4	3.96*	2.87	0.12
-1	12	4	3.54*	0.35	0.10
0	12	4	2.19*	4.08	0.05
1	12	4	3.29*	0.12	0.09
2	12	4	1.32*	2.73	0.02
3	12	4	3.31*	3.33	0.09
4	12	4	3.39*	0.80	0.08
-5	12	5	5.98	5.47	1.15
-4	12	5	2.46*	5.82	0.03
-3	12	5	4.21*	8.00	0.07
-2	12	5	4.96*	5.84	0.89
-1	12	5	6.43*	0.73	0.28
0	12	5	3.79*	0.88	0.07
1	12	5	9.61	10.12	2.53
2	13	0	18.19	17.78	4.49
3	13	0	13.37	13.73	5.75
4	13	0	1.51*	0.48	0.44
5	13	0	20.74	20.37	3.47
6	13	0	7.73	7.94	3.87
7	13	0	5.35*	5.96	0.30
8	13	0	4.11*	4.21	1.51
9	13	0	3.17*	0.81	0.10
-9	13	1	3.31*	2.02	0.09
-8	13	1	3.32*	0.54	0.09
-7	13	1	1.89*	2.37	0.04
-6	13	1	6.26	6.10	2.90
-5	13	1	5.44*	1.96	0.35
-4	13	1	2.97*	1.48	0.11
-3	13	1	2.88*	1.06	0.12
-2	13	1	2.78*	3.96	0.13
-1	13	1	18.69	19.13	4.28
0	13	1	29.20	29.01	2.02
1	13	1	24.48	23.51	2.79
2	13	1	9.82	9.80	6.24
3	13	1	2.61*	2.36	0.15
4	13	1	5.26*	5.59	0.44
5	13	1	18.46	19.03	3.88
6	13	1	4.72	4.37	2.21
7	13	1	3.03*	0.42	0.11
8	13	1	3.23*	4.31	0.11
9	13	1	2.80*	1.85	0.07
-9	13	2	4.29*	3.10	0.17
-8	13	2	4.28*	0.97	0.21
-7	13	2	3.15*	0.08	0.10
-6	13	2	11.98	12.14	3.97
-5	13	2	9.98	9.67	3.60
-4	13	2	9.30	10.41	3.51
-3	13	2	19.01	19.00	3.66
-2	13	2	17.96	17.33	3.70
-1	13	2	10.54	10.32	4.63
0	13	2	8.80	8.87	4.23
1	13	2	4.73*	3.94	0.33
2	13	2	3.01*	0.85	0.11
3	13	2	1.14*	4.18	0.02
4	13	2	3.12*	1.42	0.10
5	13	2	2.91*	1.82	0.12
6	13	2	1.32*	3.09	0.02
7	13	2	3.13*	1.99	0.09
-8	13	3	7.24	7.04	1.97
-7	13	3	14.23	14.19	3.33
-6	13	3	10.04	10.86	3.51
-5	13	3	3.38*	2.60	0.09
-4	13	3	3.14*	1.28	0.10
-3	13	3	17.21	17.49	3.44
-2	13	3	12.44	12.44	3.52
-1	13	3	3.32*	2.63	0.09
0	13	3	6.52*	6.55	0.30
1	13	3	3.26*	4.35	0.09
2	13	3	2.96*	6.58	0.07
3	13	3	10.39	10.23	4.07
4	13	3	9.01	9.57	3.13
5	13	3	3.86*	4.33	0.96
6	13	3	3.20*	0.78	0.10
-7	13	4	6.05*	4.65	0.24
-6	13	4	6.16*	3.27	0.23
-5	13	4	3.28*	1.73	0.08
-4	13	4	3.47*	1.45	0.08
-3	13	4	3.26*	0.30	0.09
-2	13	4	4.42*	2.65	0.16
-1	13	4	1.80*	3.59	0.02
0	13	4	3.41*	3.11	0.10
1	13	4	4.54*	5.01	0.19
2	13	4	8.44	8.26	2.76
3	13	4	3.92*	0.82	0.14
4	13	4	2.87*	1.69	0.06
-5	13	5	5.66*	5.94	0.20
-4	13	5	3.71*	1.50	0.07
-3	13	5	2.01*	0.35	0.02
-2	13	5	4.01*	1.05	0.10
-1	13	5	6.36*	0.23	0.30
0	13	5	3.77*	2.15	0.07
1	13	5	4.13*	0.52	0.14
0	14	0	24.47	23.70	2.76
1	14	0	19.52	18.34	4.34
2	14	0	2.65*	1.11	0.20
3	14	0	2.84*	4.75	0.12
4	14	0	18.97	19.20	3.62
5	14	0	10.18	10.93	3.91
6	14	0	2.73*	0.31	0.13
7	14	0	2.78*	3.46	0.62
8	14	0	3.06*	0.89	0.11
9	14	0	3.11*	1.87	0.10
-9	14	1	3.28*	0.28	0.09
-8	14	1	2.35*	1.21	0.07
-7	14	1	5.89*	7.74	0.26
-6	14	1	2.86*	1.76	0.12
-5	14	1	12.44	11.80	4.26
-4	14	1	7.89	7.76	3.69
-3	14	1	4.91*	4.33	0.32
-2	14	1	13.09	12.84	5.18
-1	14	1	3.59*	3.83	0.31
0	14	1	11.71	10.93	5.59
1	14	1	4.99	4.78	2.98
2	14	1	2.73*	0.61	0.13
3	14	1	12.76	12.81	4.72
4	14	1	20.12	20.33	3.44
5	14	1	17.72	17.79	3.93
6	14	1	9.44	9.38	4.02
7	14	1	4.65*	3.07	0.20
8	14	1	6.52*	4.02	0.36
-8	14	2	3.30*	1.39	0.09
-8	14	2	3.11*	0.68	0.10
-7	14	2	3.22*	1.77	0.10
-6	14	2	4.81*	2.36	0.25
-5	14	2	3.14*	0.26	0.12
-4	14	2	5.83	5.56	2.17
-3	14	2	4.27*	0.49	0.20
-2	14	2	13.48	13.51	4.41
-1	14	2	3.20*	4.37	0.12
0	14	2	12.02	11.68	4.50
1	14	2	9.40	9.01	4.32
2	14	2	3.88*	4.55	0.14
3	14	2	2.96*	2.32	0.11
4	14	2	5.96*	4.95	0.41
5	14	2	3.84*	4.68	0.19
6	14	2	3.81*	1.35	0.23
7	14	2	3.74*	0.08	1.11
-8	14	3	3.49*	5.18	0.08
-7	14	3	3.57*	2.18	0.08
-6	14	3	2.26*	1.84	0.05
-5	14	3	3.33*	5.22	0.10
-4	14	3	5.03*	2.17	0.24
-3	14	3	10.41	10.61	3.26
-2	14	3	24.47	23.90	2.55
-1	14	3	18.88	19.01	3.36
0	14	3	10.63	10.78	3.60
1	14	3	3.08*	1.02	0.11
2	14	3	11.92	11.93	3.98
3	14	3	6.87	7.33	2.87
4	14	3	4.40*	2.86	0.23
5	14	3	5.18*	0.47	0.31
6	14	3	3.43*	3.65	0.08
-7	14	4	3.67*	1.64	0.07
-6	14	4	5.77*	2.08	0.21
-5	14	4	3.60*	3.78	0.10
-4	14	4	3.46*	0.93	0.08
-3	14	4	5.92	6.53	1.54
-2	14	4	3.40*	1.69	0.09
-1	14	4	4.31*	0.28	0.15
0	14	4	5.71*	4.69	0.29
1	14	4	9.39	9.31	3.00
2	14	4	6.55*	8.21	0.32
3	14	4	4.45*	6.03	0.14
4	14	4	3.22*	1.25	0.10
-4	14	5	3.26*	4.04	0.06
-3	14	5	1.40*	0.31	0.08
-2	14	5	3.71*	1.43	0.07
-1	14	5	7.22*	6.56	0.26
0	14	5	3.77*	5.42	0.07
1	15	0	8.38	8.00	5.85
2	15	0	2.08*	4.18	0.07
3	15	0	3.04*	3.58	0.15
4	15	0	8.83	8.77	4.55
5	15	0	28.10	28.08	2.12
6	15	0	10.04	10.21	4.90
7	15	0	2.60*	3.65	0.56
8	15	0	6.40*	6.62	0.35
-9	15	1	3.39*	1.66	0.09
-8	15	1	1.95*	0.52	0.05
-7	15	1	5.23*	3.57	0.32
-6	15	1	4.80*	2.32	0.31
-5	15	1	4.56*	5.96	0.23
-4	15	1	5.40*	4.76	0.42
-3	15	1	14.13	13.88	4.47
-2	15	1	2.80*	2.96	0.13
-1	15	1	2.70*	3.05	0.14
0	15	1	17.63	17.58	4.20
1	15	1	9.48	10.03	4.27
2	15	1	9.05	8.79	4.47
3	15	1	3.56*	3.39	1.20
4	15	1	15.36	15.72	4.15
5	15	1	5.48*	4.48	0.40
6	15	1	2.99*	1.14	0.11
7	15	1	3.86*	0.27	0.27
8	15	1	2.88*	3.56	0.10
-8	15	2	5.42*	1.19	0.32
-7	15	2	3.24*	1.56	0.10
-6	15	2	4.75*	5.96	0.25
-5	15	2	9.12	9.52	3.40
-4	15	2	1.17*	3.26	0.01
-3	15	2	10.80	11.10	3.83
-2	15	2	19.43	19.89	3.43
-1	15	2	12.16	12.35	4.02
0	15	2	14.84	14.84	4.13
1	15	2	2.95*	0.84	0.11
2	15	2	11.42	11.80	4.11
3	15	2	5.72*	3.23	0.41
4	15	2	4.74	3.34	2.11
5	15	2	3.07*	0.61	0.11
6	15	2	3.29*	3.76	0.09
7	15	2	3.41*	0.88	0.09
8	15	2	3.45*	1.56	0.08
-8	15	3	4.89*	6.26	1.15
-7	15	3	6.24*	5.72	0.29
-6	15	3	3.15*	4.76	0.10
-5	15	3	3.28*	5.56	0.09
-4	15	3	3.29*	4.34	0.09
-3	15	3	5.11*	7.42	0.23
-2	15	3	16.15	16.52	3.67
-1	15	3	8.80	9.37	3.05
0	15	3	8.58	8.10	3.62
1	15	3	3.08*	1.59	0.11
2	15	3	1.30*	3.09	0.01
3	15	3	2.36*	4.01	0.38
4	15	3	3.43*	0.57	0.08

h	k	l	Fo	Fc	weight
-7	15	4	3.52*	0.19	0.08
-6	15	4	4.26*	1.07	0.13
-5	15	4	5.35*	2.32	0.29
-4	15	4	3.55*	2.43	0.08
-3	15	4	3.26*	1.57	0.08
-2	15	4	3.50*	7.54	0.09
-1	15	4	3.31*	1.61	0.09
0	15	4	4.22*	1.01	0.21
1	15	4	3.47*	5.14	0.08
2	15	4	10.69	10.59	3.01
3	15	4	4.04*	0.30	0.14
-3	15	5	3.53*	1.37	0.08
-2	15	5	2.82*	0.34	0.06
-1	15	5	2.93*	4.27	0.06
0	16	0	7.85	7.52	4.66
1	16	0	2.94*	6.64	0.12
2	16	0	4.27*	5.27	1.89
3	16	0	4.00*	4.58	0.28
4	16	0	5.78*	7.35	0.28
5	16	0	9.83	10.23	4.32
6	16	0	3.02*	0.14	0.11
7	16	0	4.46*	3.56	0.20
8	16	0	3.08*	1.44	0.11
-8	16	1	3.98*	6.67	0.14
-7	16	1	4.86*	4.83	1.43
-6	16	1	3.59*	1.69	0.20
-5	16	1	4.83*	0.25	0.29
-4	16	1	2.43*	4.82	0.47
-3	16	1	10.09	10.04	4.24
-2	16	1	13.78	13.91	4.42
-1	16	1	10.13	10.14	4.64
0	16	1	2.83*	2.03	0.13
1	16	1	7.98	6.92	4.17
2	16	1	2.22*	2.27	0.07
3	16	1	7.54	7.93	3.31
4	16	1	5.95	4.87	2.98
5	16	1	3.84*	5.04	1.22
6	16	1	3.12*	3.24	0.10
7	16	1	3.41*	4.48	0.11
8	16	1	6.39*	6.01	0.31
-8	16	2	5.13*	0.45	0.24
-7	16	2	3.21*	3.63	0.10
-6	16	2	6.44	7.00	2.22
-5	16	2	7.36	6.81	3.37
-4	16	2	2.07*	4.87	0.04
-3	16	2	16.04	15.98	3.75
-2	16	2	11.43	11.48	4.00
-1	16	2	13.08	12.77	4.23
0	16	2	9.89	9.74	3.64
1	16	2	5.41*	6.52	0.30
2	16	2	4.26*	1.66	0.30
3	16	2	2.93*	2.07	0.12
4	16	2	3.05*	0.10	0.11
5	16	2	3.21*	0.60	0.10
6	16	2	5.22*	3.49	0.21
7	16	2	3.25*	0.02	0.09
-7	16	3	3.15*	3.74	0.06
-6	16	3	7.80	7.24	2.56
-5	16	3	11.83	11.90	3.47
-4	16	3	10.40	10.43	3.56
-3	16	3	12.34	12.71	3.80
-2	16	3	6.64*	9.26	0.29
-1	16	3	11.33	10.87	4.08
0	16	3	3.48*	8.05	0.08
1	16	3	3.33*	4.32	0.08
2	16	3	6.97	7.72	2.69
3	16	3	3.35*	3.03	0.09
4	16	3	2.87*	3.09	0.66
5	16	3	4.29*	4.79	0.20
-6	16	4	6.13*	0.97	0.31
-5	16	4	3.39*	2.09	0.09
-4	16	4	5.84*	3.04	0.24
-3	16	4	4.50*	4.06	0.16
-2	16	4	8.20	8.17	2.49
-1	16	4	1.35*	0.46	0.02
0	16	4	4.08*	2.32	0.15
1	16	4	3.27*	1.82	0.09
2	16	4	5.28*	3.10	0.20
3	16	4	3.28*	1.99	0.09
1	17	0	2.91*	3.93	0.12
2	17	0	8.93	8.69	4.57
3	17	0	5.49*	5.43	0.45
4	17	0	5.63	6.38	2.68
5	17	0	3.73*	2.50	0.18
6	17	0	3.19*	0.26	0.10
7	17	0	9.60	9.72	3.45
8	17	0	5.96*	2.37	0.38
-8	17	1	3.27*	4.22	0.09
-7	17	1	5.79	6.78	1.79
-6	17	1	2.96*	4.48	0.11
-5	17	1	3.04*	0.39	0.11
-4	17	1	10.05	10.34	4.45
-3	17	1	4.46*	5.25	0.22
-2	17	1	8.04	8.61	3.36
-1	17	1	4.43*	0.99	0.43
0	17	1	7.81	8.06	3.54
1	17	1	16.24	16.24	3.89
2	17	1	16.92	16.58	4.07
3	17	1	6.81	6.98	3.07
4	17	1	9.35	9.56	4.28
5	17	1	3.08*	3.13	0.11
6	17	1	1.90*	3.83	0.03
7	17	1	5.45	5.81	1.69
-8	17	2	4.09*	2.50	0.17
-7	17	2	4.37*	4.37	0.15
-6	17	2	7.70	6.96	3.11
-5	17	2	11.08	10.74	4.25
-4	17	2	3.48*	3.27	0.13
-3	17	2	8.64	8.88	3.70
-2	17	2	9.27	9.79	3.33
-1	17	2	3.02*	0.72	0.11
0	17	2	11.14	11.38	3.85
1	17	2	3.56*	0.85	0.15
2	17	2	3.21*	3.51	0.12
3	17	2	12.33	12.52	4.54
4	17	2	5.36*	6.65	0.34
5	17	2	10.43	10.88	3.25
6	17	2	1.42*	4.03	0.02
-7	17	3	2.48*	6.57	0.03
-6	17	3	3.91*	4.21	0.11
-5	17	3	4.44*	1.27	0.22
-4	17	3	3.21*	0.55	0.10
-3	17	3	3.13*	5.93	0.10
-2	17	3	6.44	6.09	2.56
-1	17	3	3.03*	0.54	0.11
0	17	3	6.41	6.36	2.41
1	17	3	12.53	12.87	4.00
2	17	3	3.23*	0.59	0.10
3	17	3	3.39*	2.90	0.09
4	17	3	2.43*	0.04	0.06
5	17	3	4.37*	1.28	0.22
-6	17	4	5.30*	1.77	0.18
-5	17	4	7.93	5.69	2.49
-4	17	4	8.77	9.02	2.48
-3	17	4	3.92*	5.04	0.08
-2	17	4	2.87*	3.77	0.44
-1	17	4	3.42*	2.23	0.09
0	17	4	6.36*	5.36	0.31
1	17	4	6.45*	1.93	0.37
2	17	4	3.23*	0.53	0.10
0	18	0	5.38*	5.86	0.34
1	18	0	7.87	7.97	3.61
2	18	0	3.25*	4.57	0.17
3	18	0	6.42	7.36	2.66
4	18	0	4.91*	4.56	1.81
5	18	0	4.77*	0.43	0.34
6	18	0	6.17	6.15	2.36
-7	18	1	2.43*	4.84	0.06
-6	18	1	2.62*	2.33	0.07
-5	18	1	4.17*	4.64	0.16
-4	18	1	3.18*	0.47	0.10
-3	18	1	3.07*	1.72	0.11
-2	18	1	11.81	11.77	4.12
-1	18	1	21.25	21.33	3.12
0	18	1	8.59	8.01	3.72
1	18	1	5.85*	6.78	0.41
2	18	1	14.60	14.54	4.39
3	18	1	10.83	11.06	4.42
4	18	1	3.02*	1.40	0.11
5	18	1	2.96*	1.47	0.11
6	18	1	4.18*	3.57	0.35
-7	18	2	3.04*	3.28	0.11
-6	18	2	3.89*	1.61	0.18
-5	18	2	3.53*	0.81	0.15
-4	18	2	4.46*	1.26	0.14
-3	18	2	3.11*	2.12	0.10
-2	18	2	3.36*	1.88	0.09
-1	18	2	2.91*	2.63	0.12
0	18	2	3.07*	0.96	0.11
1	18	2	4.84*	3.60	0.25
2	18	2	6.24*	8.16	0.38
3	18	2	18.79	18.54	3.50
4	18	2	19.92	20.18	3.43
5	18	2	17.59	17.91	3.90
6	18	2	2.22*	4.74	0.05
7	18	2	3.10*	2.95	0.10
-8	18	3	4.59*	4.36	0.17
-7	18	3	5.21*	3.59	0.25
-6	18	3	4.31*	3.60	1.01
-5	18	3	3.46*	3.33	0.08
-4	18	3	1.96*	0.45	0.26
-3	18	3	4.00*	1.23	0.15
-2	18	3	4.53*	0.90	0.22
-1	18	3	4.48*	0.29	0.24
0	18	3	1.29*	0.21	0.02
1	18	3	5.95	5.69	2.06
2	18	3	3.22*	5.60	0.09
3	18	3	3.25*	4.10	0.09
4	18	3	3.09*	1.23	0.07
-8	18	4	3.42*	1.58	0.09
-7	18	4	5.75	5.49	1.35
-6	18	4	2.02*	0.01	0.04
-5	18	4	2.00*	1.72	0.03
-4	18	4	3.71*	1.73	0.11
-3	18	4	3.44*	0.76	0.09
-2	18	4	3.31*	0.10	0.09
-1	18	4	2.87*	1.06	0.06
0	18	4	3.57*	4.31	0.08
1	19	0	2.02*	3.68	0.04
2	19	0	1.68*	1.23	0.04
3	19	0	12.13	11.88	4.77
4	19	0	4.70*	2.71	0.30
5	19	0	4.89*	2.08	0.33
6	19	0	4.92*	2.99	0.24
7	19	0	3.39*	0.31	0.09
-7	19	1	3.38*	0.40	0.09
-6	19	1	3.59*	4.50	0.12
-5	19	1	2.26*	0.05	0.07
-4	19	1	17.78	17.51	3.58
-3	19	1	2.99*	2.59	0.10
-2	19	1	5.21*	7.35	0.28
-1	19	1	3.02*	2.12	0.11
0	19	1	2.99*	3.92	0.11
1	19	1	5.46*	4.53	0.39
2	19	1	13.25	13.45	4.39
3	19	1	7.87	8.28	3.45
4	19	1	4.09*	5.43	0.25
5	19	1	4.66*	0.34	0.29
6	19	1	1.40*	0.91	0.02
-7	19	2	3.52*	1.48	0.11
-6	19	2	3.13*	2.50	0.10
-5	19	2	4.81*	3.82	0.22
-4	19	2	15.79	15.60	3.74
-3	19	2	15.09	15.03	4.17
-2	19	2	4.97*	5.34	0.25
-1	19	2	3.04*	0.06	0.11
0	19	2	12.79	13.14	4.37
1	19	2	9.08	10.13	3.64
2	19	2	4.24*	1.37	0.34
3	19	2	3.48*	1.02	0.14
4	19	2	4.30*	0.43	0.20
5	19	2	1.96*	1.70	0.26

h	k	l	Fo	Fc	weight
-6	19	3	3.80*	3.59	0.11
-5	19	3	3.34*	0.15	0.09
-4	19	3	4.72*	1.46	0.22
-3	19	3	2.99*	2.11	0.09
-2	19	3	3.24*	0.52	0.09
-1	19	3	3.40*	0.75	0.09
0	19	3	2.30*	0.13	0.06
1	19	3	3.42*	2.13	0.09
2	19	3	3.89*	0.33	0.14
3	19	3	3.26*	0.06	0.09
4	19	3	2.91*	2.18	0.08
-4	19	4	3.66*	0.00	0.07
-3	19	4	3.62*	2.75	0.08
-2	19	4	6.24*	0.56	0.37
-1	19	4	4.30*	1.46	0.14
0	19	4	5.59*	4.66	0.22
1	19	4	5.40	5.19	1.24
0	20	0	10.56	10.90	4.23
1	20	0	8.57	8.57	4.07
2	20	0	0.40*	0.81	0.02
3	20	0	2.80*	2.37	0.08
4	20	0	8.77	9.50	3.38
5	20	0	2.98*	1.39	0.11
6	20	0	3.24*	1.18	0.10
7	20	0	5.83*	3.07	0.33
-7	20	1	5.97*	0.77	0.31
-6	20	1	4.16*	0.24	0.27
-5	20	1	3.13*	0.46	0.10
-4	20	1	1.29*	5.39	0.02
-3	20	1	3.36*	4.48	0.09
-2	20	1	2.85*	3.94	0.84
-1	20	1	4.04*	3.71	0.21
0	20	1	2.92*	1.10	0.12
1	20	1	2.13*	1.69	0.06
2	20	1	5.30*	4.03	0.39
3	20	1	8.63	8.97	3.69
4	20	1	5.78*	5.71	0.46
5	20	1	3.36*	3.57	0.09
6	20	1	4.97*	3.83	0.24
-7	20	2	3.33*	2.23	0.09
-6	20	2	3.72*	1.99	0.88
-5	20	2	3.17*	1.87	0.10
-4	20	2	10.05	10.14	3.47
-3	20	2	3.03*	0.82	0.11
-2	20	2	3.62*	3.99	0.16
-1	20	2	4.92*	0.72	0.32
0	20	2	1.80*	1.93	0.04
1	20	2	6.23	6.28	2.73
2	20	2	5.41*	4.27	0.34
3	20	2	3.57*	2.69	0.15
4	20	2	3.09*	1.16	0.10
5	20	2	3.22*	1.68	0.10
-6	20	3	3.55*	3.07	0.08
-5	20	3	5.70*	5.26	0.21
-4	20	3	5.75*	2.96	0.28
-3	20	3	3.88*	1.14	0.14
-2	20	3	3.46*	4.14	0.08
-1	20	3	1.35*	0.28	0.02
0	20	3	1.93*	1.34	0.27
1	20	3	3.18*	2.20	0.10
2	20	3	3.14*	1.06	0.11
3	20	3	4.78*	4.06	0.22
-3	20	4	3.52*	2.51	0.08
-2	20	4	5.06*	1.66	0.19
-1	20	4	1.46*	7.40	0.01
0	21	0	9.91	9.49	4.34
1	21	0	3.98*	6.73	0.19
2	21	0	20.23	20.14	3.44
3	21	0	9.41	8.65	3.88
4	21	0	3.12*	1.72	0.10
5	21	0	4.94*	1.56	0.30
6	21	0	3.17*	0.14	0.17
-6	21	1	3.41*	3.21	0.09
-5	21	1	9.52	9.99	3.62
-4	21	1	1.83*	0.84	0.05
-3	21	1	1.79*	1.21	0.04
-2	21	1	4.17*	3.55	0.20
-1	21	1	3.17*	1.51	0.10
0	21	1	2.93*	3.54	0.12
1	21	1	4.07*	2.19	0.21
2	21	1	2.64*	4.15	0.08
3	21	1	2.96*	1.17	0.11
4	21	1	3.12*	0.65	0.10
5	21	1	3.46*	0.74	0.08
-6	21	2	3.54*	4.12	0.09
-5	21	2	3.38*	2.57	0.09
-4	21	2	3.29*	0.40	0.08
-3	21	2	4.61*	1.04	0.24
-2	21	2	3.19*	4.24	0.64
-1	21	2	1.65*	0.24	0.03
0	21	2	2.62*	1.01	0.09
1	21	2	5.82*	7.13	0.27
2	21	2	2.96*	1.34	0.11
3	21	2	1.89*	1.77	0.28
4	21	2	4.72*	2.81	0.24
-5	21	3	3.57*	3.80	0.08
-4	21	3	2.85*	3.70	0.06
-3	21	3	3.34*	0.15	0.09
-2	21	3	3.38*	2.30	0.09
-1	21	3	4.60*	0.38	0.21
0	21	3	5.21*	5.26	0.25
1	21	3	3.27*	3.87	0.09
2	21	3	2.03*	0.53	0.04
0	22	0	5.10*	2.81	0.25
1	22	0	4.24*	4.48	1.86
2	22	0	4.85*	2.14	0.33
3	22	0	5.32	6.07	1.71
4	22	0	3.01*	1.24	0.11
5	22	0	3.40*	1.22	0.09
6	22	0	4.84*	3.16	0.15
-6	22	1	2.51*	3.08	0.06
-5	22	1	5.43*	0.41	0.27
-4	22	1	3.17*	1.74	0.10
-3	22	1	6.32	6.94	2.11
-2	22	1	2.98*	0.05	0.11
-1	22	1	6.64*	4.45	0.31
0	22	1	2.24*	0.43	0.07
1	22	1	2.26*	4.53	0.04
2	22	1	3.24*	4.09	0.10
3	22	1	13.08	13.30	4.00
4	22	1	3.13*	3.68	0.10
5	22	1	3.40*	0.08	0.09
-5	22	2	3.20*	2.53	0.08
-4	22	2	3.94*	4.63	0.14
-3	22	2	2.98*	1.29	0.11
-2	22	2	4.67*	0.77	0.22
-1	22	2	3.18*	2.19	0.10
0	22	2	3.12*	4.08	0.10
1	22	2	3.10*	0.19	0.10
2	22	2	4.98*	3.76	0.36
3	22	2	2.83*	0.71	0.08
4	22	2	3.30*	0.30	0.09
-4	22	3	3.26*	3.11	0.10
-3	22	3	1.98*	1.31	0.26
-2	22	3	5.32*	2.27	0.31
-1	22	3	4.02*	2.34	0.12
0	22	3	3.48*	2.94	0.08
1	22	3	7.52	8.69	2.32
2	22	3	4.15*	7.06	0.11
1	23	0	3.14*	4.29	0.10
2	23	0	3.09*	3.51	0.11
3	23	0	6.78	6.74	2.64
4	23	0	3.25*	1.89	0.09
5	23	0	5.19*	3.63	0.27
-5	23	1	3.24*	1.22	0.10
-4	23	1	2.78*	5.16	0.06
-3	23	1	5.79*	1.44	0.33
-2	23	1	4.46*	4.65	0.22
-1	23	1	9.24*	3.30	0.10
0	23	1	3.77*	0.95	0.18
1	23	1	4.24*	3.55	0.22
2	23	1	9.75	9.08	3.82
3	23	1	6.21*	4.39	0.38
4	23	1	4.10*	3.16	1.17
-5	23	2	3.39*	3.92	0.09
-4	23	2	3.27*	1.15	0.09
-3	23	2	6.43*	7.32	0.28
-2	23	2	3.52*	1.08	0.08
-1	23	2	5.11	5.31	1.54
0	23	2	6.73	6.85	2.10
1	23	2	6.33	6.18	2.24
2	23	2	5.84*	4.56	0.31
3	23	2	3.13*	1.78	0.10
-3	23	3	6.57*	2.98	0.34
-2	23	3	3.46*	2.78	0.08
-1	23	3	5.04*	0.18	0.26
0	23	3	3.35*	1.09	0.09
0	24	0	3.81*	3.70	1.16
1	24	0	4.30*	4.62	0.19
2	24	0	3.06*	0.30	0.11
3	24	0	4.20*	1.02	0.17
4	24	0	2.03*	2.93	0.03
-4	24	1	6.72*	4.78	0.30
-3	24	1	3.71*	5.47	0.10
-2	24	1	3.13*	1.31	0.10
-1	24	1	3.33*	4.83	0.09
0	24	1	9.50	8.81	3.47
1	24	1	2.39*	0.37	0.06
2	24	1	3.42*	3.38	0.14
3	24	1	3.04*	0.29	0.11
4	24	1	3.44*	2.98	0.08
-4	24	2	3.12*	1.95	0.10
-3	24	2	2.03*	1.23	0.03
-2	24	2	1.09*	0.03	0.09
-1	24	2	3.21*	2.16	0.10
0	24	2	2.01*	3.10	0.03
1	24	2	2.86*	3.09	0.07
2	24	2	2.05*	5.45	0.03
3	25	0	2.96*	0.72	0.11
2	25	0	3.74*	5.75	0.11
3	25	0	3.52*	2.10	0.14
4	25	0	1.47*	1.70	0.02
-3	25	1	1.40*	3.26	0.12
-2	25	1	7.39	7.05	2.93
-1	25	1	1.99*	2.48	0.03
0	25	1	2.78*	3.18	0.13
1	25	1	5.30*	2.78	0.32
2	25	1	5.92*	5.86	0.25
3	25	1	3.58*	0.40	0.13
-2	25	2	3.12*	0.79	0.10
-1	25	2	4.11*	3.43	0.14
0	25	2	1.45*	3.53	0.02
1	25	2	5.49*	0.29	0.24
0	26	0	3.13*	1.72	0.10
1	26	0	3.80*	1.01	0.12
2	26	0	4.35*	2.85	0.24
-2	26	1	5.83*	2.38	0.42
-1	26	1	3.22*	0.41	0.10
0	26	1	4.80*	3.87	0.25
1	26	1	3.27*	0.70	0.09

1834 reflections

2,3,4α,4aβ,6,7,8aβ-heptamethyl-4aβ,5,8,8aβ-tetrahydro-1-naphthoquin-4β-ol

h	k	l	Fo	Fc	weight
-9	7	1	3.02*	3.21	0.88
-9	6	1	0.75*	0.41	0.07
-9	5	1	3.22*	2.70	1.17
-9	4	1	1.71*	1.54	0.34
-9	3	1	1.64*	1.52	0.37
-9	2	1	5.09	4.56	11.30
-9	1	1	2.51*	2.71	0.64
-9	0	2	5.44	5.51	10.33
-9	1	2	6.74	6.57	11.90
-9	2	2	1.66*	2.57	0.36
-9	3	2	7.01	7.16	11.04
-9	4	2	0.73*	0.71	0.06
-9	5	2	2.18*	1.83	3.44
-9	6	2	1.65*	1.09	0.37
-9	7	2	4.17	5.05	6.76
-9	8	3	2.42*	2.62	3.33
-9	7	3	1.63*	1.15	0.38
-9	6	3	1.47*	1.05	0.27
-9	5	3	7.98	7.94	11.46
-9	4	3	3.40*	3.99	1.09
-9	3	3	2.49*	2.51	0.83
-9	2	3	2.43*	2.29	4.41
-9	1	3	7.41	7.47	11.88
-9	0	4	4.52	4.13	9.24
-9	1	4	1.75*	2.52	0.36
-9	2	4	6.65	6.00	12.71
-9	3	4	5.97	5.36	13.54
-9	4	4	4.54	4.12	9.80
-9	5	4	2.82*	1.13	1.26
-9	6	4	2.33*	0.56	0.77
-9	7	4	3.15*	2.21	1.40
-9	8	4	1.76*	2.90	0.32
-9	8	5	1.70*	0.82	0.35
-9	7	5	1.65*	0.65	0.37
-9	6	5	5.84	5.77	10.64
-9	5	5	3.26*	1.43	1.32
-9	4	5	3.82	3.15	10.25
-9	3	5	1.67*	0.06	0.36
-9	2	5	3.12*	1.66	1.24
-9	1	5	1.53*	0.58	0.43
-9	0	6	9.11	8.85	11.53
-9	1	6	1.70*	1.98	0.34
-9	2	6	2.97*	3.21	1.26
-9	3	6	4.17	4.41	7.95
-9	4	6	1.19*	0.87	1.02
-9	5	6	1.80*	3.30	0.36
-9	6	6	1.96*	0.66	0.92
-9	7	6	1.74*	0.73	0.33
-9	7	7	1.07*	1.88	0.13
-9	6	7	5.97	4.60	10.93
-9	5	7	3.22*	2.68	1.48
-9	4	7	1.47*	0.48	0.29
-9	3	7	2.61*	2.43	4.35
-9	2	7	5.29	5.39	9.21
-9	1	7	2.61*	1.09	1.06
-9	0	8	1.68*	1.29	0.36
-9	1	8	2.84*	0.85	1.45
-8	2	8	1.69*	0.02	0.35
-8	3	8	2.55*	0.79	1.11
-8	4	8	2.97*	0.51	1.29
-8	5	8	3.81	2.90	8.52
-8	6	8	1.76*	1.38	0.32
-8	4	9	3.10*	2.15	0.93
-8	3	9	2.86	2.55	4.70
-8	2	9	2.23*	1.90	0.64
-8	1	9	1.75*	1.48	0.33
-9	0	10	1.73*	0.42	0.33
-9	1	10	2.50*	3.35	0.60
-8	4	12	2.82*	3.07	0.78
-8	3	12	2.59*	0.23	0.82
-8	2	12	2.24*	0.88	0.68
-8	1	12	2.58*	0.31	1.88
-8	0	12	3.50	3.17	7.47
-8	1	11	1.66*	0.86	0.36
-8	2	11	4.47	4.90	8.29
-8	3	11	2.42*	2.23	0.71
-8	4	11	7.07	6.71	11.12
-8	5	11	5.38	5.06	10.55
-8	6	11	1.73*	0.66	0.33
-8	7	11	1.07*	1.20	0.15
-8	8	10	2.90*	2.53	0.60
-8	7	10	10.41	10.23	9.61
-8	6	10	5.11	4.33	9.65
-8	5	10	3.16*	3.22	1.45
-8	4	10	3.13*	2.80	1.07
-8	3	10	4.49	4.42	8.41
-8	2	10	1.67*	3.45	0.36
-8	1	10	1.42*	1.43	0.33
-8	0	10	1.75*	3.92	0.33
-8	1	9	2.78*	3.42	1.21
-8	2	9	4.42	4.46	8.17
-8	3	9	0.70*	1.23	0.09
-8	4	9	4.80	5.32	9.57
-8	5	9	11.67	11.45	9.60
-8	6	9	3.26	3.17	5.95
-8	7	9	5.24	4.80	11.76
-8	8	9	0.73*	0.80	0.07
-8	9	9	5.32	5.11	8.59
-8	10	8	3.07*	2.63	1.25
-8	9	8	5.20	5.08	10.53
-8	8	8	4.43	3.92	8.79
-8	7	8	10.95	10.80	10.22
-8	6	8	1.56*	0.29	0.41
-8	5	8	8.06	7.37	12.93
-8	4	8	3.92	4.21	8.59
-8	3	8	6.50	6.05	13.75
-8	2	8	3.61	4.27	7.44
-8	1	8	1.52*	4.04	0.26
-8	0	8	7.58	7.09	13.37
-8	1	7	2.33*	3.17	0.82
-8	2	7	2.61*	2.43	1.15
-8	3	7	5.16	5.40	12.11
-8	4	7	2.81*	2.18	1.32
-8	5	7	5.09	4.82	12.02
-8	6	7	3.62	3.20	7.84
-8	7	7	1.89*	1.70	0.69
-8	8	7	1.60*	2.76	0.38
-8	9	7	9 19	8.97	11.01
-8	10	7	5.87	5.45	9.55
-8	11	7	3.24	3.59	5.68
-8	11	6	2.10*	3.30	0.42
-8	10	6	2.31*	2.54	0.65
-8	9	6	2.27*	0.22	0.86
-8	8	6	1.72*	2.29	0.34
-8	7	6	6.94	6.99	11.67
-8	6	6	1.91*	0.51	3.65
-8	5	6	3.09	4.03	6.71
-8	4	6	1.72*	1.90	0.34
-8	3	6	1.54*	0.14	0.42
-8	2	6	7.88	7.55	13.31
-8	1	6	5.97	6.13	13.31
-8	0	6	6.31	6.00	12.28
-8	1	5	3.23	3.77	8.03
-8	2	5	7.67	7.78	12.90
-8	3	5	3.67	3.70	8.06
-8	4	5	8.28	8.23	13.04
-8	5	5	5.77	5.51	12.86
-8	6	5	6.34	6.17	14.16
-8	7	5	1.06*	0.82	1.02
-8	8	5	2.53*	0.29	1.41
-8	9	5	5.92	6.10	10.81
-8	10	5	6.86	6.82	12.29
-8	11	5	3.38*	2.19	1.10
-8	12	5	1.68*	0.77	0.36
-8	12	4	6.98	6.82	10.41
-8	11	4	1.64*	0.26	0.37
-8	10	4	3.25	2.89	6.16
-8	9	4	1.53*	0.61	0.43
-8	8	4	2.80*	0.39	1.67
-8	7	4	3.79	3.34	9.49
-8	6	4	2.59	2.48	5.89
-8	5	4	1.43*	1.16	2.20
-8	4	4	5.60	5.61	12.22
-8	3	4	8.34	8.11	12.34
-8	2	4	8.37	8.47	13.31
-8	1	4	4.27	3.80	13.12
-8	0	4	0.93*	2.35	0.14
-8	1	3	1.64*	3.20	0.37
-8	2	3	5.69	5.70	13.82
-8	3	3	4.39	4.24	11.66
-8	4	3	10.01	9.86	12.32
-8	5	3	1.65*	2.00	0.45
-8	6	3	0.96*	1.30	0.17
-8	7	3	2.39*	1.62	0.86
-8	8	3	2.29*	2.46	3.55
-8	9	3	3.47	3.32	6.75
-8	10	3	1.02*	1.06	0.14
-8	11	3	1.66*	0.07	0.36
-8	12	3	1.58*	1.33	0.40
-8	12	2	2.61*	1.20	0.86
-8	11	2	4.77	4.50	8.90
-8	10	2	4.12	3.51	8.53
-8	9	2	2.37*	1.96	1.10
-8	8	2	1.55*	0.39	0.42
-8	7	2	1.70*	0.46	0.48
-8	6	2	1.68*	2.00	0.36
-8	5	2	4.56	4.49	9.93
-8	4	2	3.35*	2.88	1.35
-8	3	2	6.13	6.52	13.74
-8	2	2	3.23	3.67	7.48
-8	1	2	4.42	4.44	12.15
-8	0	2	7.69	8.05	14.28
-8	1	1	4.05	3.46	10.07
-8	2	1	11.52	11.98	9.54
-8	3	1	12.30	11.84	9.61
-8	4	1	1.91*	3.11	0.45
-8	5	1	8.30	8.63	12.86
-8	6	1	2.39*	0.80	1.09
-8	7	1	0.70*	1.60	0.07
-8	8	1	1.60*	1.05	0.39
-8	9	1	1.67*	0.44	0.36
-8	10	1	1.79*	1.18	0.46
-8	11	1	4.69	4.35	8.84
-7	14	1	3.09	1.89	5.39
-7	13	1	4.15	3.88	8.12
-7	12	1	1.05*	0.53	0.91
-7	11	1	2.59*	1.95	1.16
-7	10	1	2.96*	0.58	1.75
-7	9	1	2.72	2.48	5.71
-7	8	1	2.85*	3.22	1.67
-7	7	1	7.03	6.67	13.64
-7	6	1	16.50	16.82	5.09
-7	5	1	2.17*	2.19	0.82
-7	4	1	11.12	11.18	11.66
-7	3	1	8.61	8.00	14.35
-7	2	1	4.20	4.56	12.11
-7	1	1	11.02	11.10	11.12
-7	0	2	2.25*	2.78	1.29
-7	1	2	6.69	7.10	17.42
-7	2	2	14.69	15.16	6.04
-7	3	2	1.05*	1.01	0.29
-7	4	2	16.10	16.65	5.50
-7	5	2	6.99	6.43	14.55
-7	6	2	2.44*	3.27	1.58
-7	7	2	2.12*	0.41	1.49
-7	8	2	4.28	4.19	12.81
-7	9	2	1.51*	0.64	0.44
-7	10	2	0.67*	1.47	0.09
-7	11	2	4.99	4.79	12.76
-7	12	2	1.05*	1.51	0.91
-7	13	2	5.08	4.79	9.93
-7	14	2	2.86*	2.64	1.15
-7	15	2	3.23	3.34	5.27
-7	15	3	1.68*	2.58	0.26
-7	14	3	6.09	6.29	10.36
-7	13	3	3.64	3.56	6.67
-7	12	3	6.16	5.36	12.80
-7	11	3	4.37	4.35	10.40
-7	10	3	3.21	3.27	8.70
-7	9	3	3.29	3.18	8.47
-7	8	3	2.21*	1.59	5.95
-7	7	3	4.99	5.37	13.70

h	k	l	Fo	Fc	weight
-7	6	3	9.74	9.63	12 39
-7	5	3	3 53	3 52	10.89
-7	4	3	15.97	15 92	5 71
-7	3	3	8.65	8 67	14.58
-7	2	3	4.72	4.43	14.67
-7	1	3	6.51	6.88	17.49
-7	0	4	1.99*	0.86	1.55
-7	1	4	4.46	4.44	15.57
-7	2	4	10.51	10.25	12.70
-7	3	4	6.01	6 40	14.98
-7	4	4	13.89	13.53	7.33
-7	5	4	15.41	15.28	5 76
-7	6	4	5.32	5.21	13.70
-7	7	4	1.46*	1.43	0.47
-7	8	4	3.00	2.48	8.33
-7	9	4	7.67	7.73	15.07
-7	10	4	1.65*	1.54	0.41
-7	11	4	1.51*	1.14	0.44
-7	12	4	6.30	6.04	13.24
-7	13	4	2.16*	1.08	0.78
-7	14	4	2.95*.	2.09	1.02
-7	15	4	1.67*	1.33	0.36
-7	14	5	3.78	3.62	6.70
-7	13	5	1.25*	0.12	0.26
-7	12	5	2.12*	1.85	0.76
-7	11	5	1.60*	0.16	0.39
-7	10	5	1.53*	0.55	0.43
-7	9	5	4.07	3.67	13.46
-7	8	5	2.16*	0.67	1.06
-7	7	5	5.34	5.61	13.90
-7	6	5	11.96	12.87	9.11
-7	5	5	16.86	16.64	5.01
-7	4	5	7.75	8.18	15.66
-7	3	5	7.86	8.00	15.70
-7	2	5	13.58	13.18	7.44
-7	1	5	2.86	2.59	9.13
-7	0	6	11.11	11.10	11.66
-7	1	6	2.21*	0.86	1.49
-7	2	6	1.06*	1.07	0.28
-7	3	6.	1.45*	1.52	0.47
-7	4	6	14.60	15.37	6.65
-7	5	6	1.49*	0.34	0.45
-7	6	6	1.04*	0.58	1.27
-7	7	6	7.60	7.70	15.18
-7	8	6	1.14*	1.29	0.24
-7	9	6	1.50*	0.92	0.36
-7	10	6	4.12	3 43	10.53
-7	11	6	2.52*	0.01	1.71
-7	12	6	2.10*	1.51	4.02
-7	13	6	3.09*	2.73	1.15
-7	14	6	3.49*	4.19	1.23
-7	14	7	2.82*	2.08	0.82
-7	13	7	1.80*	1.28	0.31
-7	12	7	5.51	5.47	11.91
-7	11	7	2.34*	0.73	0.80
-7	10	7	3.46	3.29	7.87
-7	9	7	5.59	5.69	12.62
-7	8	7	6.36	6.49	12.30
-7	7	7	4.04	4.82	10.01
-7	6	7	1.51*	2.24	0.44
-7	5	7	1.49*	0.67	0.45
-7	4	7	5.12	4.55	15.51
-7	3	7	4.42	4.15	13.89
-7	2	7	7.02	7.09	16.59
-7	1	7	3.47	3.10	12.54
-7	0	8	2.00*	2.26	0.71
-7	1	8	10.41	10.53	11.23
-7	2	8	0.90*	0.24	0.20
-7	3	8	2.22*	1.58	1.47
-7	4	8	1.49*	1.83	0.45
-7	5	8	3 18	2.51	10.08
-7	6	8	3.43	3.48	8.53
-7	7	8	2.91*	3.57	1.35
-7	8	8	1.57*	0.01	0.41
-7	9	8	1.55*	0.35	0.41
-7	10	8	1.57*	3.69	0.32
-7	11	8	1.60*	3.12	0.34
-7	12	8	1.46*	0.91	0.31
-7	13	8	2.24*	2.24	0.54
-7	12	9	1.64*	1.57	0.37
-7	11	9	2.53*	0.97	1.05
-7	10	9	1.24*	2.63	0.21
-7	9	9	1.64*	0.21	0.37
-7	8	9	5.57	4.70	11.84
-7	7	9	1.93*	1.30	0.52
-7	6	9	1.62*	3.17	0.38
-7	5	9	1.55*	0.76	0.41
-7	4	9	1.50*	1.26	0.44
-7	3	9	5.38	4.91	15.70
-7	2	9	1.51*	0.20	0.44
-7	1	9	9.52	9.40	13.28
-7	0	10	4.01	4.17	8.39
-7	1	10	11.43	10.98	10.57
-7	2	10	1.66*	1.51	0.36
-7	3	10	8.82	8.67	12.28
-7	4	10	4.98	5.24	10.69
-7	5	10	2.46*	1.89	5.43
-7	6	10	5.31	6.11	10.23
-7	7	10	4.73	4.84	9.00
-7	8	10	1.68*	0.38	0.36
-7	9	10	4.21	4.01	8.08
-7	10	10	4.48	4.11	9.67
-7	11	10	3.16*	0.56	1.40
-7	10	11	1.75*	1.64	2.01
-7	9	11	4.72	4.80	10.19
-7	8	11	6.12	6.15	11.96
-7	7	11	4.72	4.50	11.31
-7	6	11	1.58*	2.67	0.33
-7	5	11	5.92	6.13	12.30
-7	4	11	2.31*	1.94	0.83
-7	3	11	2.18*	4.90	0.36
-7	2	11	6.02	6.30	11.84
-7	1	11	11.80	11.58	9.67
-7	0	12	0.41*	1.49	0.11
-7	1	12	8.97	8.84	12.61
-7	2	12	1.51*	0.06	0.44
-7	3	12	8.35	8.44	11 48
-7	4	12	8.23	7.72	12.51
-7	5	12	1.02*	1.22	0.12
-7	6	12	6.34	5.40	10.92
-7	7	12	1.80*	2.10	0.31
-7	8	12	1.65*	0.03	0.37
-7	6	13	2.62*	3.15	3.93
-7	5	13	2.68*	4.20	0.65
-7	4	13	8.95	8.55	10.49
-7	3	13	3.59*	3.88	1.14
-7	2	13	1.55*	2.00	1.63
-7	1	13	7.59	7.45	11.05
-7	0	14	2.13*	2.13	0.50
-7	1	14	1.73*	0.25	0.33
-7	2	14	5.26	5.37	9.44
-6	1	15	1.78*	1.67	0.32
-6	2	15	5.32	4.70	9.62
-6	7	14	0.75*	1.21	0.10
-6	6	14	7.61	6.82	10.86
-6	5	14	3.30*	2.41	1.36
-6	4	14	1.80*	1.17	0.38
-6	3	14	2 42*	0 08	0.85
-6	2	14	3.57	4.07	6.18
-6	1	14	2.90*	4.34	0.76
-6	0	14	1.76*	0.18	0.32
-6	1	13	4.82	4.91	10.92
-6	2	13	2.04*	3.04	2.62
-6	3	13	7.03	6.91	12.24
-6	4	13	1.58*	1.59	0.55
-6	5	13	1.61*	0.55	0.39
-6	6	13	2.97*	3.16	1.01
-6	7	13	1.26*	0.23	0.22
-6	8	13	7.80	7.50	11.17
-6	9	13	1.79*	2.22	0.31
-6	11	12	1.84*	2.44	0.29
-6	10	12	1.69*	1.00	0.35
-6	9	12	1.76*	0.36	0.32
-6	8	12	2.02*	2.99	0.48
-6	7	12	1.58*	0.31	0.40
-6	6	12	6.33	5.96	12.42
-6	5	12	2.50*	2.69	5.02
-6	4	12	1.64*	2.42	0.37
-6	3	12	2.63*	2.01	1.46
-6	2	12	1.64*	1.17	0.37
-6	1	12	5.18	5.21	12.58
-6	0	12	8.16	8.19	13.34
-6	1	11	2.43*	0.17	1.50
-6	2	11	0.92*	0.24	0.25
-6	3	11	1.48*	0.62	0.46
-6	4	11	2.83	2.85	6.76
-6	5	11	2.90*	3.14	1.61
-6	6	11	1.51*	0.21	0.36
-6	7	11	0.68*	0.45	0.09
-6	8	11	2.08*	0.06	0.59
-6	9	11	1.58*	0.61	0.40
-6	10	11	2.48*	3.19	0.95
-6	11	11	2.19*	0.39	0.88
-6	12	11	5.26	5.30	9.16
-6	13	10	5.42	5.39	9.81
-6	12	10	1.78*	0.05	0.53
-6	11	10	1.42*	0.57	0.33
-6	10	10	2.09*	2.86	0.65
-6	9	10	12.05	12.28	8.60
-6	8	10	2.16*	1.98	4.09
-6	7	10	1.15*	0.92	0.25
-6	6	10	1.53*	1.04	0.43
-6	5	10	3.00	3.44	8.67
-6	4	10	2.71*	3.39	1.29
-6	3	10	1.48*	0.91	0.46
-6	2	10	1.89*	2.03	4.82
-6	1	10	1.43*	0.70	0.49
-6	0	10	4.75	4.68	15.12
-6	1	9	5.85	6.03	17.17
-6	2	9	8.89	8.63	14.83
-6	3	9	1.23*	2.19	0.33
-6	4	9	2.48*	3.13	1.52
-6	5	9	1.46*	0.11	0.47
-6	6	9	0.90*	1.15	0.20
-6	7	9	12.11	12.53	8.96
-6	8	9	1.73*	1.23	0.62
-6	9	9	4.68	4.72	10.47
-6	10	9	0.96*	1.09	0.18
-6	11	9	6.74	7.07	13.11
-6	12	9	1.52*	0.71	0.43
-6	13	9	2.81*	2.52	0.94
-6	14	9	3.18	3.38	5.35
-6	15	8	4.61	4.23	8.99
-6	14	8	1.71*	1.08	0.34
-6	13	8	2.36*	1.42	0.95
-6	12	8	2.09*	3.30	0.69
-6	11	8	5.51	5.58	11.47
-6	10	8	5.43	5.36	12.09
-6	9	8	8.07	8.35	14.06
-6	8	8	3.51	3.49	9.61
-6	7	8	2.18*	3.18	0.72
-6	6	8	1.48*	0.82	0.46
-6	5	8	9.00	9.11	14.77
-6	4	8	1.35*	1.63	0.50
-6	3	8	2.80*	3.15	1.74
-6	2	8	12.50	12.39	8.52
-6	1	8	13.53	13.59	7 37
-6	0	8	9.83	9.73	13.51
-6	1	7	18.83	19.09	4.42
-6	2	7	3.81	3.61	11.82
-6	3	7	9.41	8.61	14.58
-6	4	7	4.63	4.56	16.23
-6	5	7	5.58	5.62	17.72
-6	6	7	1.47*	1.13	0.46
-6	7	7	3.83	4.49	11.71
-6	8	7	8.80	9.32	14.22
-6	9	7	12.47	12.78	8.39
-6	10	7	1.42*	0.21	0.49
-6	11	7	1.76*	0.43	0.73
-6	12	7	2.05*	3.20	0.51
-6	13	7	7.73	7.63	13.36
-6	14	7	3.29*	3.48	1.42

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight 3
-6	15	7	0.74*	1.12	0.12	-6	6	3	14.22	14.26	6.77	-5	6	1	6.93	6.32	20.75	-5	15	4	2.64*	2.36	1.02
-6	16	7	2.13*	1.68	0.50	-6	7	3	4.28	3.98	14.12	-5	5	1	8.89	9.31	16.47	-5	16	4	1.52*	1.72	0.43
-6	16	6	3.25*	4.26	0 70	-6	8	3	6.47	6.71	17.90	-5	4	1	6.81	6.21	24.29	-5	17	4	1.57*	1.18	0.41
-6	15	6	5.79	5.86	9.23	-6	9	3	5.16	5.30	16.02	-5	3	1	13 77	14.96	7.31	-5	18	4	5.26	4.61	9.86
-6	14	6	3.39	3.10	7.31	-6	10	3	9.27	9.27	13.84	-5	2	1	2.57	2.42	14.74	-5	18	5	2.37*	1.98	0.65
-6	13	6	2.49*	1.63	1.03	-6	11	3	2.65*	2.71	1.21	-5	1	1	1.55*	2.52	1.84	-5	17	5	2.97	2.42	5.86
-6	12	6	2.52*	2.66	5.42	-6	12	3	2.47*	2.15	1.08	-5	0	2	32.75	33.76	1.96	-5	16	5	2.45*	0.22	1.12
-6	11	6	6.19	6.45	13.41	-6	13	3	2.87*	2.72	1.33	-5	1	2	20.88	21.42	3.95	-5	15	5	2.51	1.78	6.10
-6	10	6	8.30	8.17	13.79	-6	14	3	1.20*	0.45	0.33	-5	2	2	4.09	3.01	25.35	-5	14	5	2.58*	1.08	1.75
-6	9	6	1.52*	1.41	0.43	-6	15	3	1.49*	1.32	0.45	-5	3	2	5.17	5.09	25.26	-5	13	5	1.30*	1.89	0.37
-6	8	6	6.43	6.17	16.23	-6	16	3	1.79*	0.56	0.31	-5	4	2	1.95*	1.62	2.64	-5	12	5	1.26*	0.32	0.45
-6	7	6	1.44*	0.52	0.48	-6	17	3	0.75*	3.16	0.06	-5	5	2	5.34	5.60	23.23	-5	11	5	2.03*	2.36	0.91
-6	6	6	15.17	16.36	6.13	-6	17	2	3.15	3.42	5.45	-5	6	2	3.65	3.78	19.57	-5	10	5	2.13*	2.58	5.15
-6	5	6	10.23	10.68	12.77	-6	16	2	5.08	4.53	10.35	-5	7	2	4.61	4.52	17.87	-5	9	5	6.07	5.63	18.55
-6	4	6	8.77	8.53	16.87	-6	15	2	1.63*	0.40	0.38	-5	8	2	21.14	20.74	3.50	-5	8	5	9.93	10.68	13.29
-6	3	6	8.28	8.76	16.76	-6	14	2	2.08*	1.00	0.73	-5	9	2	1.38*	1.18	0.52	-5	7	5	13.05	12.97	8.37
-6	2	6	19.17	19.59	4.35	-6	13	2	3.55	3.15	9.15	-5	10	2	3.64	3.35	12.00	-5	6	5	9.28	9.02	15.72
-6	1	6	19.04	20.09	4.46	-6	12	2	3.78	3.38	10.20	-5	11	2	12.83	13.03	9.53	-5	5	5	22.35	22.56	3.37
-6	0	6	7.72	7.88	16.81	-6	11	2	5.29	5.07	13.69	-5	12	2	3.10	3.14	9.12	-5	4	5	1.27*	0.79	0.62
-6	1	5	16.23	17.15	5.49	-6	10	2	2.80*	3.06	1.14.	-5	13	2	2.97	2.93	7.36	-5	3	5	14.52	14.84	6.98
-6	2	5	5.25	5.76	15.60	-6	9	2	7.32	7.43	16.19	-5	14	2	2.54*	3.24	0.75	-5	2	5	5.48	5.54	25.08
-6	3	5	21.36	21.61	3.42	-6	8	2	1.99*	0.66	1.18	-5	15	2	1.14*	0.08	1.36	-5	1	5	19.83	20.02	4.27
-6	4	5	7.58	7.41	16.37	-6	7	2	17.60	17.55	4.82	-5	16	2	2.48*	2.33	4.93	-5	0	6	21.91	21.65	3.56
-6	5	5	6.19	6.25	17.67	-6	6	2	16.32	15.02	5.47	-5	17	2	1.57*	0.26	0.40	-5	1	6	14.12	13.77	6.92
-6	6	5	3.57	4.23	11.40	-6	5	2	8.70	8.36	15.41	-5	18	2	4.71	4.21	9.70	-5	2	6	9.89	9.80	14.00
-6	7	5	18.80	19.43	4.39	-6	4	2	3.03	2.28	11.89	-5	18	3	2.10*	0.22	0.71	-5	3	6	20.67	20.37	3.83
-6	8	5	13.88	13.98	6.95	-6	3	2	14.19	13.97	7.19	-5	17	3	1.61*	1.32	0.38	-5	4	6	5.01	4.80	19.71
-6	9	5	3.72	2.78	13.30	-6	2	2	5.12	5.07	19.85	-5	16	3	1.58*	0.96	0.40	-5	5	6	1.34*	1.18	3.18
-6	10	5	7.24	7.43	15.31	-6	1	2	11.99	12.27	10.01	-5	15	3	2.62*	2.41	1.37	-5	6	6	1.27*	0.37	0.62
-6	11	5	3.60	3.27	9.86	-6	0	2	13.25	13.03	8.77	-5	14	3	5.05	4.57	14.07	-5	7	6	3.22	3.04	12.71
-6	12	5	5.07	4.67	13.64	-6	1	1	10.51	10.18	13.82	-5	13	3	3.19*	3.90	1.44	-5	8	6	1.37*	1.53	0.53
-6	13	5	8.26	7.21	12.24	-6	2	1	8.95	8.60	17.56	-5	12	3	1.48*	2.89	0.45	-5	9	6	5.72	5.88	16.13
-6	14	5	3.88	3.85	8.60	-6	3	1	10.06	10.86	13.67	-5	11	3	1.36*	0.72	0.54	-5	10	6	8.04	7.26	15.67
-6	15	5	3.75	3.96	7 14	-6	4	1	11.15	11.00	11.43	-5	10	3	11.15	11.18	11.38	-5	11	6	1.86*	0.78	0.82
-6	16	5	2.22*	0.31	0.80	-6	5	1	22 60	23.15	3.24	-5	9	3	14.18	13.96	7.58	-5	12	6	1.55*	0.65	0.41
-6	17	4	2.82*	1.28	1.41	-6	6	1	0.82*	0.64	0.17	-5	8	3	9.41	9.26	13.96	-5	13	6	1.40*	1.06	0.51
-6	16	4	3.03*	0.81	1.47	-6	7	1	2.21*	1.05	1.42	-5	7	3	15.81	16.05	5.98	-5	14	6	1.55*	1.00	0.41
-6	15	4	3.82	3.55	7.83	-6	8	1	3.14	3.07	9.79	-5	6	3	6.87	6.92	22.25	-5	15	6	2.51*	2.04	0.86
-6	14	4	3.05	2.84	6.06	-6	9	1	1.38*	0.59	0.58	-5	5	3	1.24*	0.33	0.65	-5	16	6	3.12*	3.55	0.91
-6	13	4	2.63*	2.87	1.20	-6	10	1	2 18*	0.21	1.31	-5	4	3	4.78	4.88	23.93	-5	17	6	1.69*	0.75	0.35
-6	12	4	4.66	5.66	10.78	-6	11	1	5.89	5.96	14.76	-5	3	3	1.11*	1.25	0.82	-5	17	7	1.83*	2.32	0.39
-6	11	4	4.68	4.14	12 17	-6	12	1	4.82	4.44	12.98	-5	2	3	17.80	16.60	5.06	-5	16	7	4.30	3.88	8.31
-6	10	4	1.43*	1.32	0.49	-6	13	1	2.17*	3.11	3.42	-5	1	3	5.23	5.24	24.04	-5	15	7	1.68*	0.89	0.35
-6	9	4	1.94*	0.15	0.97	-6	14	1	1.71*	1.59	0.35	-5	0	4	14.67	15.18	6.98	-5	14	7	1.46*	0.58	0.47
-6	8	4	1.80*	2.14	0.93	-6	15	1	4.28	3.84	8.51	-5	1	4	1.21*	2.41	0.69	-5	13	7	1.57*	3.27	0 41
-6	7	4	1.67*	0.22	0.74	-6	16	1	1.75*	0.21	0.33	-5	2	4	8.66	9.21	18.77	-5	12	7	7.24	6.83	14.32
-6	6	4	3.83	3.37	12.84	-5	18	1	4.80	4.60	7.89	-5	3	4	17.22	16.63	5.55	-5	11	7	1.10*	0.01	0.30
-6	5	4	16.48	17.20	5.35	-5	17	1	1.61*	0.31	0.42	-5	4	4	7.55	7.18	20.68	-5	10	7	2.97	4.41	7.46
-6	4	4	18.07	19.08	4.73	-5	16	1	5.34	4.58	12.12	-5	5	4	8.98	8.43	15.73	-5	9	7	5.78	6.65	16.62
-6	3	4	17.90	17.96	4.98	-5	15	1	3.56	3.29	8.49	-5	6	4	9.01	8.82	17.57	-5	8	7	4.05	2.79	14.88
-6	2	4	13.76	14.07	7.96	-5	14	1	1.54*	1.14	0.42	-5	7	4	2.93	2.35	12.83	-5	7	7	4.11	3.86	15.00
-6	1	4	13.92	14.18	7.19	-5	13	1	2.71*	3 11	1.35	-5	8	4	1.46*	2.75	0.47	-5	6	7	1.96*	1.78	1.01
-6	0	4	3.76	3.54	16.70	-5	12	1	1.45*	1.70	0 47	-5	9	4	4.02	3 88	15.94	-5	5	7	16.00	15.19	5.63
-6	1	3	4.59	5.29	16.39	-5	11	1	2.89*	3.93	1.40	-5	10	4	10.72	11.09	12.24	-5	4	7	8.42	8.77	16.93
-6	2	3	7.77	7.82	17.96	-5	10	1	14.67	15.09	6.17	-5	11	4	8.20	8.89	15.32	-5	3	7	11.15	11.00	10.53
-6	3	3	16.17	15.81	5.67	-5	9	1	9.23	9.13	14.16	-5	12	4	4.80	4.53	15.09	-5	2	7	25.31	25.28	2.83
-6	4	3	13.74	13.63	7.93	-5	8	1	16.42	15.92	5.50	-5	13	4	1.28*	2.25	0.34	-5	1	7	12.87	13.67	8.53
-6	5	3	13.10	13.21	8.69	-5	7	1	9.17	8.77	15.84	-5	14	4	1.40*	0.65	0.51	-5	0	8	50.23	51.50	0.88

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight 4
-5	1	8	8.16	7.82	14.43	-5	4	11	3.43	3.37	11.60	-4	8	14	5.01	5.61	8.88	-4	9	10	1.10*	0.71	0.34
-5	2	8	17.53	17 35	5.00	-5	3	11	8.63	8 59	14.04	-4	7	14	1.59*	0.43	0.40	-4	8	10	2.56*	3.72	1.06
-5	3	8	16.73	16.62	5 49	-5	2	11	10.20	10.67	12.50	-4	6	14	1.87*	0.28	0.64	-4	7	10	7.38	7.78	16.06
-5	4	8	2.03*	0.54	1 45	-5	1	11	5.10	5.13	15.11	-4	5	14	2.22*	0.11	0.71	-4	6	10	9.16	9.23	14.24
-5	5	8	0.57*	1.39	0.10	-5	0	12	14.09	13.98	7.28	-4	4	14	5.28	5.90	11.62	-4	5	10	4.14	3.90	13.40
-5	6	8	2.54*	3.51	1.55	-5	1	12	4.26	3.65	12.91	-4	3	14	1 60*	0.81	0.39	-4	4	10	8 19	8.39	15.67
-5	7	8	11.58	11.97	10.63	-5	2	12	4.95	4.53	13.03	-4	2	14	2.83*	2.46	1.11	-4	3	10	10.53	10.44	11 81
-5	8	8	6.14	6.87	16.99	-5	3	12	10.51	9.96	11.55	-4	1	14	2.65*	1.63	1.18	-4	2	10	12.04	12.03	10.04
-5	9	8	2.23*	1.96	1.37	-5	4	12	5.88	5.67	14.96	-4	0	14	2.05*	2.35	0.58	-4	1	10	7.17	7.35	16.70
-5	10	8	1.39*	1.73	0.52	-5	5	12	1.75*	0.70	0.57	-4	1	13	2.72	2.71	7.25	-4	0	10	14.45	15.10	6.74
-5	11	8	6.52	6.87	14.04	-5	6	12	5.21	5.20	12.94	-4	2	13	8.26	8.27	13.21	-4	1	9	6.59	7.22	19.00
-5	12	8	7.35	7.20	13.78	-5	7	12	2.67	2.76	5.23	-4	3	13	5.23	5.16	14.50	-4	2	9	4.38	4.61	18.66
-5	13	8	1.80*	1.28	0.57	-5	8	12	1.09*	1.47	1.09	-4	4	13	3.55	3.77	8.63	-4	3	9	2.72	1.75	12.88
-5	14	8	2.32*	2.27	0.77	-5	9	12	0.70*	1.00	0.09	-4	5	13	2.81	3.01	6.74	-4	4	9	1.11*	0.88	0.58
-5	15	8	1.90*	0.99	0.52	-5	10	12	0.92*	0.53	0.79	-4	6	13	9.20	9.35	12.51	-4	5	9	8.68	9.55	16.44
-5	16	8	5.28	4.88	9.01	-5	11	12	1.72*	1.87	0.34	-4	7	13	2.75*	2.97	0.86	-4	6	9	8.39	9.13	16.37
-5	16	9	4.62	4.30	7.34	-5	12	12	1.94*	1.42	2.88	-4	8	13	3.56	3.55	8.62	-4	7	9	6.78	7.37	17.28
-5	15	9	3.11*	1 85	1.35	-5	11	13	4.40	4.31	8.58	-4	9	13	2.56*	1.75	0.83	-4	8	9	3.66	4.33	12.11
-5	14	9	1.60*	0.68	0.39	-5	10	13	1.85*	1.33	0.46	-4	10	13	5.33	4.85	11.83	-4	9	9	1.50*	0.63	0.62
-5	13	9	1.56*	2.03	0.36	-5	9	13	5.61	5.13	12.26	-4	11	13	4.76	4.04	9.67	-4	10	9	2.17*	1.99	1.17
-5	12	9	2.89*	1.02	1.80	-5	8	13	2.14*	1.07	0.79	-4	12	13	1.66*	0.28	0.36	-4	11	9	1.92*	2.27	1.15
-5	11	9	1.63*	1.17	0.49	-5	7	13	0.70*	1.15	0.09	-4	14	12	1.69*	2.72	0.32	-4	12	9	3.07	2.86	8.40
-5	10	9	1.53*	1.53	0.43	-5	6	13	2.70*	0.92	1.92	-4	13	12	1.81*	0.75	0.38	-4	13	9	4.12	3.87	9.16
-5	9	9	1.53*	0.88	0.43	-5	5	13	2.92*	0.19	1.44	-4	12	12	2.50*	2.82	0.71	-4	14	9	2.48*	2.29	4.30
-5	8	9	5.30	6.58	17.03	-5	4	13	1.49*	1.75	0.45	-4	11	12	1.73*	2.58	0.34	-4	15	9	2.94	3.06	5.25
-5	7	9	4.22	4.25	15.19	-5	3	13	5.50	5.62	11.57	-4	10	12	1.55*	0.79	0.42	-4	16	9	1.27*	0.53	0.29
-5	6	9	1.59*	2.41	0.66	-5	2	13	8.21	8.79	11.57	-4	9	12	1.65*	1.79	0.37	-4	17	9	4.98	4.90	7.74
-5	5	9	10.76	11.16	11.22	-5	1	13	2.61*	1.38	1.04	-4	8	12	5.26	5.01	14.17	-4	17	8	1.70*	0.15	0.35
-5	4	9	4.37	4.07	16.67	-5	0	14	7.51	6.84	12.34	-4	7	12	1.75*	1.63	0.69	-4	16	8	8.97	8.18	10.51
-5	3	9	9.22	9.19	14.60	-5	1	14	1.55*	1.69	0.42	-4	6	12	6.67	6.86	14.02	-4	15	8	2.51*	2.87	0.75
-5	2	9	18.63	19.16	4 54	-5	2	14	1.59*	0.76	0.40	-4	5	12	7.69	7.77	14.01	-4	14	8	4.35	4.56	10.13
-5	1	9	5.71	5.48	17.17	-5	3	14	1.87*	0.64	0.70	-4	4	12	4.01	3.99	11.00	-4	13	8	8.62	8.67	12.75
-5	0	10	22.72	23.42	3.12	-5	4	14	1.42*	2.78	0.24	-4	3	12	5.26	5.28	13.86	-4	12	8	4.45	4.17	12.16
-5	1	10	7.31	7.69	15.92	-5	5	14	2.58*	3.29	0.81	-4	2	12	12.57	13.01	8.34	-4	11	8	7.05	7.29	15.81
-5	2	10	9.29	9.46	14.43	-5	6	14	2.61*	1.00	1.06	-4	1	12	9.92	10.37	12.57	-4	10	8	1.37*	0.78	0.54
-5	3	10	4.82	4.74	14.44	-5	7	14	6.64	6.22	12.64	-4	0	12	2.25*	1.07	1.07	-4	9	8	9.44	10.27	13.54
-5	4	10	1.44*	0.81	0.48	-5	8	14	5.60	4.98	9.73	-4	1	11	2.79*	4.09	1.13	-4	8	8	6.42	6.44	18.47
-5	5	10	6.51	6.99	15.66	-5	9	14	2.81*	0.84	1.21	-4	2	11	8.43	8.21	15.43	-4	7	8	4.44	4.90	19.24
-5	6	10	0.62*	1.34	0.11	-5	6	15	2.49*	0.46	0.92	-4	3	11	6.78	6.85	15.63	-4	6	8	3.97	3.47	17.19
-5	7	10	1.79*	1.40	0.75	-5	5	15	1.73*	2.67	0.34	-4	4	11	5.96	6.01	17.13	-4	5	8	1.34*	0.56	0.56
-5	8	10	0.95*	0.57	1.11	-5	4	15	1.74*	1.66	0.33	-4	5	11	11.80	11.62	10.02	-4	4	8	1.14*	1.75	0.77
-5	9	10	5.08	4.93	14.93	-5	3	15	3.29*	3.87	0.86	-4	6	11	1.39*	0.76	0.53	-4	3	8	11.32	10.51	10.65
-5	10	10	2.76*	0.26	1.92	-5	2	15	2.91	3.82	4.73	-4	7	11	1.51*	0.35	0.44	-4	2	8	7.22	7.42	20.50
-5	11	10	2.27*	0.33	1.20	-5	1	15	3.01*	2.53	1.22	-4	8	11	5.90	6.58	16.35	-4	1	8	2.37*	2.18	2.05
-5	12	10	1.50*	0.74	0.44	-4	3	16	2.50*	0.31	0.71	-4	9	11	1.31*	0.62	0.36	-4	0	8	20.72	21.05	3.78
-5	13	10	4.26	3.47	9.00	-4	2	16	1.70*	1.68	0.35	-4	10	11	7.02	6.60	14.79	-4	1	7	10.00	9.13	13.93
-5	14	10	5.22	5.11	10.12	-4	1	16	1.98*	0.77	0.54	-4	11	11	1.37*	2.01	0.36	-4	2	7	20.92	20.66	3.93
-5	15	10	2.49*	2.14	0.67	-4	0	16	2.24*	1.16	0.92	-4	12	11	1.56*	0.56	0.42	-4	3	7	5.66	5.90	24.45
-5	14	11	1.80*	1.39	0.31	-4	1	15	1.90*	1.47	0.63	-4	13	11	5.72	5.26	11.39	-4	4	7	1.87	2.33	8.52
-5	13	11	1.80*	2.74	0.45	-4	2	15	1.02*	0.47	0.15	-4	14	11	1.47*	0.57	0.26	-4	5	7	15.98	16.91	6.12
-5	12	11	2.27*	1.20	0.75	-4	3	15	2.60*	1.40	1.15	-4	15	11	1.72*	0.73	0.34	-4	6	7	1.59*	0.41	1.34
-5	11	11	5.34	5.05	12.34	-4	4	15	2.62*	2.05	0.83	-4	16	10	0.75*	1.59	0.08	-4	7	7	2.37*	1.55	1.86
-5	10	11	1.69*	0.52	0.35	-4	5	15	1.60*	2.12	0.39	-4	15	10	6.38	6.14	10.47	-4	8	7	5.48	5.80	20.32
-5	9	11	3.99	3.82	9.52	-4	6	15	5.25	5.27	9.41	-4	14	10	3.41*	3.27	1.12	-4	9	7	4.20	4.69	15.47
-5	8	11	3.37	3.16	8.52	-4	7	15	1.46*	1.55	1.44	-4	13	10	1.96*	3.11	0.48	-4	10	7	3.66	2.99	15.21
-5	7	11	1.37*	2.01	0.54	-4	8	15	1.68*	2.28	0.35	-4	12	10	6.08	5.75	12.99	-4	11	7	2.77*	3.25	1.79
-5	6	11	6.26	6.20	14.72	-4	10	14	4.83	4.10	8.31	-4	11	10	2.53	2.91	5.88	-4	12	7	4.43	4.61	13.93
-5	5	11	3.35	3.23	9.84	-4	9	14	5.53	5.39	10.33	-4	10	10	2.82*	2.54	1.81	-4	13	7	4.25	4.33	12.26

h	k	l	Fo	Fc	weight
-4	14	7	5.60	5.67	13.00
-4	15	7	6.78	6.58	13.34
-4	16	7	2.89*	2 25	1 12
-4	17	7	2.04*	2.09	0.46
-4	18	7	5.51	5.19	8.86
-4	18	6	1.62*	0.70	0.38
-4	17	6	3.29	2.21	7.26
-4	16	6	1.20*	3.32	0.22
-4	15	6	2.59*	2.84	1.17
-4	14	6	3.72	3.29	10.63
-4	13	6	12.43	11.77	9.28
-4	12	6	4.37	5.05	12.58
-4	11	6	3.54	3.87	12.37
-4	10	6	5.44	7.00	18.02
-4	9	6	1.36*	0.61	3 77
-4	8	6	2.77	2.80	10 53
-4	7	6	7.28	7.78	19.98
-4	6	6	9.37	10.08	15.55
-4	5	6	20.62	20 44	4.02
-4	4	6	21.62	20.77	3.83
-4	3	6	2.87	2.80	20.11
-4	2	6	5.16	4.89	25.39
-4	1	6	4.59	3.82	27.09
-4	0	6	34.97	36.01	1.77
-4	1	5	11.46	11 44	10.73
-4	2	5	20.03	18.67	4.43
-4	3	5	5.96	4.92	26.88
-4	4	5	2.15	2.50	15.53
-4	5	5	0.97*	0.96	0.53
-4	6	5	2.67	3.17	16.64
-4	7	5	26.83	26.63	2.69
-4	8	5	11.44	11.93	10.51
-4	9	5	6.00	6.25	18.30
-4	10	5	0.56*	1.82	0.10
-4	11	5	4.76	4.61	15.23
-4	12	5	6.80	7.35	16.67
-4	13	5	6.89	6.66	16.46
-4	14	5	0.64*	1.16	0.09
-4	15	5	4.36	3.59	10.59
-4	16	5	1.80*	1.07	0.61
-4	17	5	1.57*	0.62	0.52
-4	18	5	4.02	3.99	8.59
-4	19	5	3.08*	2.19	1.10
-4	19	4	0.74*	1.13	0.11
-4	18	4	1.34*	1.64	1.35
-4	17	4	1.70*	0.11	0.58
-4	16	4	1.57*	0.26	0.40
-4	15	4	5.14	5.13	13.20
-4	14	4	4.08	3.93	12 50
-4	13	4	3.32	3.61	10.44
-4	12	4	4.44	4.72	13.44
-4	11	4	5.70	6.05	15.76
-4	10	4	6.21	6.91	18.06
-4	9	4	11.63	11.65	10.08
-4	8	4	3.95	3.84	19.36
-4	7	4	12.47	11.98	9.92
-4	6	4	1.09*	0.09	0.82
-4	5	4	2.01*	0.53	3.23
-4	4	4	4.20	4.49	29.41
-4	3	4	2.78	2.04	22.02
-4	2	4	20.14	18.46	4.47
-4	1	4	1.77*	2.27	2.03
-4	0	4	1.59*	0.71	2.85
-4	1	3	0.97*	0.67	0.64
-4	2	3	11.56	11.62	11.57
-4	3	3	1.11*	0.24	0.81
-4	4	3	17.84	16.81	5.30
-4	5	3	7.35	7.31	24.25
-4	6	3	2.05	1.66	13.62
-4	7	3	1.26*	2.09	4.33
-4	8	3	7.72	7.87	19.75
-4	9	3	11.53	11.78	10.72
-4	10	3	1.36*	1.64	0.54
-4	11	3	17.40	17.71	5.05
-4	12	3	22.78	22.61	3.07
-4	13	3	2.57*	2.42	1.67
-4	14	3	7.50	7.53	16.24
-4	15	3	1.52*	1.80	0.43
-4	16	3	2.41*	2.96	1.10
-4	17	3	1.57*	2.50	0.41
-4	18	3	2.26*	2.53	0.65
-4	19	3	3.13*	2.91	1.12
-4	19	2	1.75*	0.03	0.33
-4	18	2	1.59*	0.19	0.41
-4	17	2	1.19*	1.64	0.24
-4	16	2	2.91*	3.06	1.43
-4	15	2	1.45*	0.54	0.47
-4	14	2	1.76*	2.37	0.73
-4	13	2	2.89	2.94	9.24
-4	12	2	4.87	4.50	16.93
-4	11	2	8.38	8.52	14.49
-4	10	2	28.72	28.74	2.28
-4	9	2	33.67	33.54	1.81
-4	8	2	4.06	3.75	21.09
-4	7	2	11.19	11.25	11.24
-4	6	2	11.18	11.95	11.11
-4	5	2	6.08	5.76	28.37
-4	4	2	4.44	3.92	33.02
-4	3	2	17.59	16.09	5.37
-4	2	2	18.61	17.80	5.14
-4	1	2	8.46	7.43	19.79
-4	0	2	17.89	18.02	5.43
-4	1	1	9.38	8.14	15.56
-4	2	1	18.64	18.45	5.14
-4	3	1	1.05*	2.44	0.91
-4	4	1	6.13	5.44	28.12
-4	5	1	28.14	26.15	2.59
-4	6	1	1.75*	0.98	10.30
-4	7	1	7.28	7.82	21.98
-4	8	1	23.86	24.41	3.18
-4	9	1	6.85	6.44	18.99
-4	10	1	13.09	13.55	7.95
-4	11	1	19.15	19.36	4.28
-4	12	1	1.29*	0.47	0.60
-4	13	1	1.44*	0.33	0.48
-4	14	1	6.10	6.00	15.44
-4	15	1	1.40*	0.11	0.51
-4	16	1	4.68	5.07	10.16
-4	17	1	1.61*	0.10	0.39
-4	18	1	2.02*	0.71	0.72
-4	19	1	3.58	3.03	7.77
-3	20	1	3.13*	0.99	1.25
-3	19	1	1.91*	1.45	3.16
-3	18	1	2.85*	0.34	1.29
-3	17	1	1.61*	1.23	3.06
-3	16	1	8.11	7.88	13.28
-3	15	1	7.54	8.05	15.64
-3	14	1	3.02	3.58	9.12
-3	13	1	0.89*	1.00	0.34
-3	12	1	14.93	14.16	6.68
-3	11	1	13.11	13.47	8.60
-3	10	1	12.81	12.07	8.91
-3	9	1	15.77	15.13	6.33
-3	8	1	4.47	4.69	28.22
-3	7	1	0.90*	0.13	0.66
-3	6	1	19.76	18.16	4.57
-3	5	1	9.71	9.61	15.20
-3	4	1	15.53	13.32	6.58
-3	3	1	12.02	12.13	10.55
-3	2	1	6.47	6.07	29.98
-3	1	1	1.52*	3.25	2.76
-3	0	2	37.38	38.14	1.65
-3	1	2	50.53	48.08	0.93
-3	2	2	22.41	19.87	4.06
-3	3	2	13.14	13.92	9.46
-3	4	2	3.08	3.46	28.05
-3	5	2	1.81*	1.96	2.60
-3	6	2	29.87	28.21	2.39
-3	7	2	18.66	18.16	4.93
-3	8	2	13.83	13.04	7.79
-3	9	2	8.13	9.16	17.00
-3	10	2	20.34	19.46	3.99
-3	11	2	7.84	7.45	17.84
-3	12	2	14.57	14.74	6.76
-3	13	2	1.15*	0.13	0.36
-3	14	2	5.32	5.33	14.89
-3	15	2	1.45*	0.54	0.47
-3	16	2	2.41*	1.23	1.34
-3	17	2	1.63*	1.32	0.40
-3	18	2	1.54*	0.86	0.54
-3	19	2	1.47*	0.04	0.47
-3	20	2	1.66*	1.34	0.36
-3	20	3	1.63*	0.99	0.38
-3	19	3	1.62*	0.78	0.38
-3	18	3	1.54*	0.74	0.42
-3	17	3	1.64*	1.23	0.63
-3	16	3	3.02	3.19	8.54
-3	15	3	1.47*	0.02	0.46
-3	14	3	3.32	4.07	10.96
-3	13	3	9.24	9.28	14.49
-3	12	3	1.32*	1.40	0.57
-3	11	3	4.80	4.80	20.72
-3	10	3	1.33*	2.12	0.56
-3	9	3	6.13	6.00	25.93
-3	8	3	2.40	1.86	17.33
-3	7	3	18.46	18.47	4.90
-3	6	3	15.26	14.58	7.35
-3	5	3	41.16	40.42	1.34
-3	4	3	60.30	56.41	0.66
-3	3	3	20.72	21.43	4.48
-3	2	3	7.26	7.23	25.66
-3	1	3	13.11	12.32	9.69
-3	0	4	8.56	9.29	18.52
-3	1	4	31.77	32.26	2.21
-3	2	4	19.87	19.25	4.66
-3	3	4	30.80	29.86	2.31
-3	4	4	41.56	40.76	1.33
-3	5	4	11.23	10.19	12.03
-3	6	4	34.10	33.30	1.87
-3	7	4	11.49	11.12	10.45
-3	8	4	1.99*	0.60	2.97
-3	9	4	15.54	15.47	6.41
-3	10	4	6.65	6.74	21.72
-3	11	4	5.14	4.87	19.79
-3	12	4	7.56	7.41	18.01
-3	13	4	1.42*	0.45	0.50
-3	14	4	6.50	6.68	16.02
-3	15	4	2.25	1.02	7.57
-3	16	4	4.02	4.25	9.09
-3	17	4	1.55*	0.17	0.42
-3	18	4	1.56*	2.92	0.30
-3	19	4	2.28*	2.56	0.75
-3	20	4	2.89*	0.60	1.60
-3	20	5	2.92*	0.47	1.49
-3	19	5	2.06*	1.93	0.53
-3	18	5	3.24*	4.39	1.25
-3	17	5	3.37	3.39	8.08
-3	16	5	3.26	2.64	7.44
-3	15	5	1.91*	0.84	0.78
-3	14	5	1.41*	1.45	0.50
-3	13	5	7.24	7.49	17.54
-3	12	5	8.48	8.68	15.82
-3	11	5	1.28*	1.87	0.61
-3	10	5	2.39*	1.31	2.11
-3	9	5	4.84	5.34	24.95
-3	8	5	1.86*	2.72	1.38
-3	7	5	3.77	3.65	24.72
-3	6	5	3.84	2.76	25.10
-3	5	5	12.07	12.47	10.46
-3	4	5	33.86	30.72	1.92
-3	3	5	14.15	13.24	8.06
-3	2	5	35.85	35.33	1.76
-3	1	5	26.36	26.16	3.02
-3	0	6	14.46	13.61	7.78
-3	1	6	1.60*	1.89	11.24
-3	2	6	15.40	14.38	7.26
-3	3	6	8.28	8.10	18.35
-3	4	6	1.11*	0.37	0.81
-3	5	6	28.35	26.63	2.55
-3	6	6	7.02	6.57	24.63
-3	7	6	6.29	5.81	24.67
-3	8	6	11.90	11.31	10.59

h	k	l	Fo	Fc	weight
-3	9	6	9.75	9.95	13.94
-3	10	6	1.76*	1.87	5.19
-3	11	6	9.02	10.04	15.38
-3	12	6	6.59	6 73	17.75
-3	13	6	2.91*	2.50	1.74
-3	14	6	7.79	7.79	15.07
-3	15	6	2.76*	3.62	1.31
-3	16	6	1.64*	1.93	0.37
-3	17	6	2.78*	1.76	1.22
-3	18	6	2.27*	0 25	1.00
-3	19	6	1.28*	0.07	0.25
-3	19	7	1.34*	1 27	1.15
-3	18	7	1.63*	0.07	0.45
-3	17	7	3.51	3.23	7.00
-3	16	7	4.18	3.92	11.09
-3	15	7	2.57*	3.04	1.19
-3	14	7	9.50	9.65	12.10
-3	13	7	4.98	4.88	13 70
-3	12	7	1.38*	0.12	0.53
-3	11	7	9.16	8.98	14.56
-3	10	7	1.79*	0.58	1.03
-3	9	7	7.29	7.24	18.06
-3	8	7	10.84	10.76	12.41
-3	7	7	9.49	9.47	14.47
-3	6	7	4.09	3.96	22.66
-3	5	7	7.57	8.13	20.92
-3	4	7	3.67	4.16	24.64
-3	3	7	12.76	12.91	8.63
-3	2	7	1.48*	0.79	2.18
-3	1	7	4.83	5.12	28.43
-3	0	8	3.78	3.57	24.90
-3	1	8	1.39*	0.39	1.32
-3	2	8	9.41	8.81	14.73
-3	3	8	7.51	7.35	22.29
-3	4	8	9.49	9.48	16.13
-3	5	8	6.77	7.24	22.01
-3	6	8	1.21*	1.53	0.69
-3	7	8	5.33	5.12	20.22
-3	8	8	8.44	8.28	16.79
-3	9	8	15.67	15.08	6.24
-3	10	8	2.42*	2.31	1.53
-3	11	8	2.76*	2.94	1.72
-3	12	8	1.33*	0.83	0.57
-3	13	8	6.01	5.85	16.10
-3	14	8	7.62	7.37	13.38
-3	15	8	1.57*	1.17	0.40
-3	16	8	3.78	3.89	8.29
-3	17	8	3.95	3.91	7.57
-3	18	8	0.68*	1.49	0.31
-3	17	9	3.13*	3.49	1.33
-3	16	9	2.69*	2.82	0.61
-3	15	9	4.73	4.70	10.76
-3	14	9	2.11*	2.32	4.49
-3	13	9	1.32*	0.88	0.29
-3	12	9	2.40*	0.97	1.44
-3	11	9	5.31	5.42	15.48
-3	10	9	4.90	4.61	15.49
-3	9	9	7.89	7.95	16.46
-3	8	9	2.94	2.94	11.05
-3	7	9	12.22	11.95	8.74
-3	6	9	2.28	1.96	9.50
-3	5	9	5.81	5.83	18.15
-3	4	9	1.42*	0.10	0.88
-3	3	9	6.63	6.99	21.95
-3	2	9	3.85	4.08	19.38
-3	1	9	13.81	13.60	7.87
-3	0	10	1.38*	1.81	0.53
-3	1	10	1.37*	1.45	0.53
-3	2	10	8.19	8.30	17.58
-3	3	10	12.31	12.57	9.40
-3	4	10	1.36*	0.80	0.54
-3	5	10	14.06	14.60	6.76
-3	6	10	1.37*	0.29	0.53
-3	7	10	12.68	12.48	7.64
-3	8	10	1.40*	0.24	0.51
-3	9	10	7.39	7.43	16.32
-3	10	10	1.55*	0.01	0.90
-3	11	10	2.05*	2.55	0.93
-3	12	10	7.12	7.32	13.30
-3	13	10	0.96*	0.67	0.15
-3	14	10	2.10*	2.19	3.34
-3	15	10	2.27*	1.23	1.00
-3	16	10	3.61*	3.80	1.00
-3	15	11	1.83*	1.01	0.30
-3	14	11	1.68*	0.04	0.35
-3	13	11	2.40*	2.12	4.03
-3	12	11	1.94*	0.02	0.68
-3	11	11	5.34	5.24	12.83
-3	10	11	4.85	4.20	14.57
-3	9	11	4.12	4.49	11.42
-3	8	11	3.48	3.22	10.18
-3	7	11	10.80	10.88	11.05
-3	6	11	9.67	9.73	12.92
-3	5	11	1.47*	0.76	0.46
-3	4	11	6.52	6.90	16.26
-3	3	11	5.86	5.99	16.68
-3	2	11	14.37	14.73	6.90
-3	1	11	10.68	10.87	12.20
-3	0	12	11.03	10.81	10.29
-3	1	12	4.69	4.71	14.11
-3	2	12	1.47*	0.48	0.46
-3	3	12	1.38*	0.81	0.53
-3	4	12	17.55	17.70	4.49
-3	5	12	2.27*	2.56	1.05
-3	6	12	2.39*	1.87	1.46
-3	7	12	6.45	6.74	13.95
-3	8	12	1.74*	0.73	0.61
-3	9	12	7.41	7.15	12.83
-3	10	12	1.54*	1.39	0.42
-3	11	12	1.21*	0.17	0.24
-3	12	12	1.23*	0.95	0.23
-3	13	12	2.52*	1.03	0.82
-3	14	12	4.65	4.85	8.28
-3	13	13	1.72*	1.68	0.34
-3	12	13	9.35	8.69	10.32
-3	11	13	1.48*	0.53	0.45
-3	10	13	2.83*	2 87	1.09
-3	9	13	1.63*	0 90	0.38
-3	8	13	3.67	3.36	10.21
-3	7	13	4.51	4.75	10.32
-3	6	13	6.06	6.31	14.41
-3	5	13	8.18	7.79	12.89
-3	4	13	1.57*	0.50	0 41
-3	3	13	2.05*	1.11	0.93
-3	2	13	5.27	5.52	14.63
-3	1	13	7.24	7.08	14.21
-3	0	14	1.91*	2.31	0.66
-3	1	14	4.33	4.12	10.81
-3	2	14	4.10	3.88	10.43
-3	3	14	2.41*	3.10	4.25
-3	4	14	8.57	8.06	12.09
-3	5	14	1.63*	0.46	0.38
-3	6	14	2.88*	0.68	1.52
-3	7	14	3.41	3.96	6.97
-3	8	14	2.48*	0.25	1.17
-3	9	14	1.51*	0.07	0.44
-3	10	14	5.49	5.73	10.01
-3	11	14	2.26*	1.82	0.53
-3	8	15	1.81*	1.72	0.30
-3	7	15	3.39*	2 58	1.20
-3	6	15	2.31*	1.86	0.78
-3	5	15	2.05*	1.76	0.61
-3	4	15	5.75	5.93	9.95
-3	3	15	1.57*	0.32	0.40
-3	2	15	1.57*	1.72	0.41
-3	1	15	1.58*	0.14	0.40
-3	0	16	3.29	3.03	5.91
-3	1	16	3.23*	0.25	1.38
-3	2	16	1.74*	2.71	0.33
-3	3	16	1.66*	1.06	0.36
-3	4	16	1.52*	0.97	0.43
-2	4	16	3.27*	3.06	1.07
-2	3	16	1.73*	1.16	0.33
-2	2	16	1.69*	1.60	0.35
-2	1	16	3.23*	2.78	0.95
-2	0	16	5.37	5.25	9.59
-2	1	15	1.63*	1.12	0.38
-2	2	15	5.61	5.66	11.09
-2	3	15	6.55	6.26	11.18
-2	4	15	4.27	5.07	7.26
-2	5	15	1.56*	0.39	0.41
-2	6	15	1.79*	1.62	0.41
-2	7	15	6.36	6.21	9.33
-2	8	15	6.28	6.24	10.26
-2	11	14	1.76*	1.94	0.32
-2	10	14	7.76	7.58	10.07
-2	9	14	3.01	2.93	5.27
-2	8	14	2.48*	2.12	1.02
-2	7	14	2.12*	1.06	1.13
-2	6	14	8.13	7.83	11.78
-2	5	14	7.00	6.48	12.17
-2	4	14	5.96	5.73	11.69
-2	3	14	4.73	4.52	10.92
-2	2	14	7.97	7.66	12.76
-2	1	14	2.52*	3.19	0.78
-2	0	14	2.23*	1.37	1.34
-2	1	13	2.86*	2.90	1.82
-2	2	13	2.77	2.29	7.88
-2	3	13	2.81*	2.78	1.38
-2	4	13	11.16	11.57	10.12
-2	5	13	4.49	4.87	11.23
-2	6	13	3.37	3.61	7.75
-2	7	13	2.13*	2.59	3.93
-2	8	13	1.18*	0.82*	0.27
-2	9	13	1.64*	3.26	0.37
-2	10	13	3.43	2.96	7.76
-2	11	13	1.25*	0.72	0.17
-2	12	13	1.92*	2.11	2.61
-2	13	13	1.89*	4.43	0.28
-2	14	12	2.22*	0.93	0.74
-2	13	12	2.61*	0.68	1.06
-2	12	12	3.47	2.61	9.12
-2	11	12	1.83*	0.84	0.78
-2	10	12	1.36*	2.44	0.25
-2	9	12	2.88	2.55	7.12
-2	8	12	7.60	7.23	13.71
-2	7	12	1.29*	0.46	0.32
-2	6	12	1.42*	2.09	0.37
-2	5	12	5.52	5.34	14.53
-2	4	12	0.87*	0.36	0.26
-2	3	12	0.94*	1.41	1.10
-2	2	12	7.08	7.05	16.83
-2	1	12	2.35*	1.84	1.22
-2	0	12	2.42	3.39	6.52
-2	1	11	8.30	8.31	16.40
-2	2	11	2.89	2.81	9.65
-2	3	11	2.27*	2.24	6.86
-2	4	11	1.85*	1.80	0.91
-2	5	11	2.72*	1.39	1.78
-2	6	11	2.46	2.31	8.14
-2	7	11	12.25	12.19	9.11
-2	8	11	1.53*	0.69	0.59
-2	9	11	3.48	3.78	10.16
-2	10	11	4.49	4.87	12.80
-2	11	11	5.89	5.31	13.45
-2	12	11	4.58	4.24	11.26
-2	13	11	1.61*	2.08	0.38
-2	14	11	2.02*	1.86	0.50
-2	15	11	1.60*	0.89	0.39
-2	16	11	3.01*	1.93	0.93
-2	17	10	1.99*	2.08	0.44
-2	16	10	2.19*	2.18	0.51
-2	15	10	1.59*	1.08	0.47
-2	14	10	1.85*	1.01	0.33
-2	13	10	5.01	4.52	11.19
-2	12	10	2.84*	0.85	1.81
-2	11	10	1.52*	2.18	0.43
-2	10	10	5.86	6.14	16.57
-2	9	10	8.67	8.86	16.09
-2	8	10	2.53*	0.28	1.93
-2	7	10	7.71	7.42	16.93
-2	6	10	1.62*	2.75	3.24

h	k	l	Fo	Fc	weight
-2	5	10	8.02	7.74	15.69
-2	4	10	23.17	23.52	3.06
-2	3	10	0.59*	1.04	0.64
-2	2	10	6.78	6.77	19.11
-2	1	10	1.20*	0.51	0.70
-2	0	10	5.42	5.47	19.21
-2	1	9	2.33*	1.19	2.54
-2	2	9	3.62	3.15	20.12
-2	3	9	1.93*	0.71	1.85
-2	4	9	2.52	2.90	11.36
-2	5	9	14.10	14.92	7.51
-2	6	9	6.65	6.91	19.37
-2	7	9	13.36	13.70	7.25
-2	8	9	9.03	8.75	15.13
-2	9	9	1.30*	0.75	0.60
-2	10	9	6.14	6.27	16.48
-2	11	9	2.59	2.30	7.44
-2	12	9	4.07	4.48	11.33
-2	13	9	1.54*	1.46	0.42
-2	14	9	1.90*	2.53	0.71
-2	15	9	1.57*	0.04	0.41
-2	16	9	3.93	3.25	10.26
-2	17	9	2.31*	0.40	0.96
-2	18	9	1.30*	1.74	0.24
-2	18	8	0.74*	0.29	0.09
-2	17	8	2.94*	2.21	1.57
-2	16	8	1.56*	0.74	0.41
-2	15	8	0.67*	0.75	0.08
-2	14	8	2.52*	1.50	1.39
-2	13	8	3.11	2.83	11.74
-2	12	8	4.40	3.86	14.09
-2	11	8	4.51	4.94	14.86
-2	10	8	2.23*	2.04	1.30
-2	9	8	9.43	10.06	13.60
-2	8	8	1.88*	2.56	1.20
-2	7	8	1.18*	1.43	0.51
-2	6	8	9.74	10.05	14.79
-2	5	8	10.99	10.32	12.05
-2	4	8	1.17*	0.73	0.73
-2	3	8	1.82*	2.89	9.03
-2	2	8	5.45	5.09	25.69
-2	1	8	27.24	27.65	2.70
-2	0	8	36.31	37.01	1.66
-2	1	7	10.08	10.05	12.96
-2	2	7	13.86	13.71	7.99
-2	3	7	20.41	19.97	4.30
-2	4	7	12.22	10.94	9.79
-2	5	7	3.38	3.61	22.30
-2	6	7	6.58	6.06	24.09
-2	7	7	5.96	6.15	24.03
-2	8	7	2.36	2.70	10.74
-2	9	7	6.41	6.22	19.14
-2	10	7	10.51	10.17	13.11
-2	11	7	9.95	9.88	13.39
-2	12	7	2.51*	2.57	1.51
-2	13	7	1.06*	1.65	0.23
-2	14	7	1.41*	0.46	0.43
-2	15	7	7.08	7.26	14.71
-2	16	7	1.54*	1.07	0.42
-2	17	7	3.65	3.37	8.20
-2	18	7	2.03*	1.56	0.70
-2	19	7	0.74*	0.84	0.08
-2	20	6	1.89*	1.09	0.44
-2	19	6	3.57	3.46	6.50
-2	18	6	1.63*	0.65	0.38
-2	17	6	3.21	2.57	7.66
-2	16	6	2.72*	2.17	1.34
-2	15	6	1.49*	1.59	0.45
-2	14	6	3.48	3.32	11.35
-2	13	6	9.89	10.22	13.32
-2	12	6	20.40	20.50	3.86
-2	11	6	18.31	18.65	4.48
-2	10	6	9.17	9.61	16.05
-2	9	6	7.41	7.55	20.67
-2	8	6	3.46	3.39	20.31
-2	7	6	4.46	3.60	26.28
-2	6	6	29.07	27.59	2.46
-2	5	6	3.13	3.20	24.51
-2	4	6	24.65	24.61	3.30
-2	3	6	15.47	14.82	6.53
-2	2	6	1.04*	1.15	0.93
-2	1	6	6.10	6.30	30.72
-2	0	6	0.92*	0.65	0.80
-2	1	5	5.46	4.97	33.68
-2	2	5	31.54	29.85	2.24
-2	3	5	1.06*	0.52	0.88
-2	4	5	52.11	50.44	0.87
-2	5	5	0.73*	3.59	0.39
-2	6	5	1.52*	1.17	1.59
-2	7	5	5.45	5.49	29.27
-2	8	5	4.59	5.04	27.46
-2	9	5	1.14*	0.28	0.77
-2	10	5	10.48	10.68	12.66
-2	11	5	4.24	3.97	17.36
-2	12	5	4.69	4.51	16.31
-2	13	5	4.46	4.11	14.18
-2	14	5	12.43	12.29	8.58
-2	15	5	4.78	4.54	16.11
-2	16	5	1.47*	1.60	0.46
-2	17	5	6.38	6.12	12.54
-2	18	5	1.05*	1.06	0.91
-2	19	5	5.50	5.30	10.53
-2	20	5	2.57*	1.63	0.94
-2	20	4	2.20*	0.55	0.66
-2	19	4	4.03	4.09	8.29
-2	18	4	3.49	3.57	7.07
-2	17	4	1.50*	0.97	0.44
-2	16	4	7.20	7.18	13.28
-2	15	4	2.38*	1.67	1.91
-2	14	4	1.49*	1.91	3.28
-2	13	4	2.34	2.08	7.23
-2	12	4	16.39	17.38	5.54
-2	11	4	12.91	12.99	8.85
-2	10	4	10.28	10.69	12.75
-2	9	4	2.15*	2.01	2.88
-2	8	4	0.80*	0.67	0.45
-2	7	4	4.15	3.89	29.09
-2	6	4	40.58	37.27	1.39
-2	5	4	6.82	7.73	24.98
-2	4	4	59.87	57.22	0.67
-2	3	4	48.87	48.32	1.00
-2	2	4	1.00*	1.17	1.01
-2	1	4	8.73	9.15	17.98
-2	0	4	3.84	3.94	36.86
-2	1	3	9.09	10.27	16.95
-2	2	3	79.27	79.77	0.33
-2	3	3	5.38	5.59	29.81
-2	4	3	64.87	65.40	0.58
-2	5	3	14.78	13.93	7.09
-2	6	3	56.00	53.57	0.76
-2	7	3	15.53	15.71	6.43
-2	8	3	14.62	14.20	7.63
-2	9	3	6.70	7.12	25.01
-2	10	3	2.30*	2.45	2.03
-2	11	3	7.60	7.61	20.48
-2	12	3	12.32	12.34	10.03
-2	13	3	11.13	11.16	11.16
-2	14	3	10.65	11.11	11.85
-2	15	3	5.48	5.20	17.00
-2	16	3	1.55*	0.75	0.42
-2	17	3	2.07*	1.43	1.20
-2	18	3	2.71*	3.37	1.43
-2	19	3	1.60*	0.82	0.39
-2	20	3	1.78*	2.18	0.32
-2	21	3	2.72*	1.40	1.23
-2	21	2	2.37*	1.05	0.85
-2	20	2	2.05*	0.82	0.61
-2	19	2	1.85*	0.30	0.54
-2	18	2	3.02*	3.36	1.26
-2	17	2	1.51*	1.38	0.44
-2	16	2	7.21	6.45	15.90
-2	15	2	4.23	4.79	13.08
-2	14	2	1.47*	0.91	3.18
-2	13	2	4.00	3.71	14.87
-2	12	2	5.17	5.07	20.87
-2	11	2	4.18	4.29	22.93
-2	10	2	1.20*	1.64	0.69
-2	9	2	20.36	20.77	4.22
-2	8	2	9.86	9.58	14.62
-2	7	2	1.05*	0.28	0.91
-2	6	2	29.67	26.88	2.48
-2	5	2	53.61	51.34	0.83
-2	4	2	66.90	66.29	0.54
-2	3	2	8.65	8.67	17.67
-2	2	2	79.94	78.25	0.33
-2	1	2	18.34	18.51	5.87
-2	0	2	14.04	14.16	8.70
-2	1	1	34.55	33.84	1.96
-2	2	1	27.53	29.07	2.93
-2	3	1	3.99	4.62	36.75
-2	4	1	16.71	16.00	6.53
-2	5	1	12.48	12.10	10.36
-2	6	1	36.20	34.53	1.74
-2	7	1	5.70	5.41	31.49
-2	8	1	6.31	5.62	27.92
-2	9	1	8.50	9.39	18.95
-2	10	1	8.55	8.57	18.90
-2	11	1	1.13*	2.47	0.44
-2	12	1	1.06*	0.51	0.69
-2	13	1	2.14*	2.00	1.41
-2	14	1	16.89	17.67	5.07
-2	15	1	6.68	6.78	15.11
-2	16	1	1.08*	2.47	0.24
-2	17	1	1.50*	0.73	0.44
-2	18	1	2.43*	1.76	1.32
-2	19	1	2.21*	0.23	1.06
-2	20	1	1.63*	0.54	0.38
-2	21	1	1.06*	0.89	0.14
-1	21	1	2.56*	2.68	0.64
-1	20	1	1.64*	0.85	0.37
-1	19	1	1.54*	2.14	0.25
-1	18	1	1.51*	1.40	0.44
-1	17	1	1.49*	0.29	0.45
-1	16	1	4.97	5.05	15.96
-1	15	1	3.52	4.20	12.40
-1	14	1	6.94	6.86	16.37
-1	13	1	0.76*	0.17	0.20
-1	12	1	2.12*	2.40	1.54
-1	11	1	13.88	13.27	7.16
-1	10	1	6.95	6.91	25.17
-1	9	1	2.93	2.61	21.74
-1	8	1	11.08	12.09	12.14
-1	7	1	3.12	3.41	29.89
-1	6	1	14.21	14.46	7.84
-1	5	1	0.93*	1.64	4.16
-1	4	1	4.28	4.82	37.35
-1	3	1	44.14	43.35	1.24
-1	2	1	70.64	71.28	0.44
-1	1	1	65.76	65.23	0.51
-1	0	2	79.62	79.83	0.35
-1	1	2	16.99	16.93	6.97
-1	2	2	33.53	32.47	2.09
-1	3	2	79.55	79.22	0.34
-1	4	2	9.35	9.03	16.12
-1	5	2	41.27	40.06	1.38
-1	6	2	35.44	35.58	1.82
-1	7	2	14.69	14.36	7.22
-1	8	2	11.95	11.95	11.06
-1	9	2	16.43	17.15	5.80
-1	10	2	1.75*	1.39	1.49
-1	11	2	6.88	7.36	21.36
-1	12	2	10.78	10.80	12.53
-1	13	2	12.17	12.47	8.85
-1	14	2	10.87	10.92	10.71
-1	15	2	5.69	5.50	16.12
-1	16	2	0.62*	1.07	0.08
-1	17	2	2.31*	3.07	0.92
-1	18	2	1.49*	0.74	0.45
-1	19	2	2.76*	4.23	0.95
-1	20	2	1.57*	1.15	0.40
-1	21	2	2.57*	0.36	0.94
-1	21	3	1.84*	2.57	0.30

h	k	l	Fo	Fc	weight
-1	20	3	1.55*	0.56	0.41
-1	19	3	0.98*	1.41	0.17
-1	18	3	3.68	3.58	9.41
-1	17	3	7.92	7.70	13.54
-1	16	3	2.56*	0.80	2.22
-1	15	3	7.14	7.05	17.62
-1	14	3	1.45*	0.94	0.48
-1	13	3	4.99	5.07	15.93
-1	12	3	17.10	16.93	5.28
-1	11	3	1.33*	1.28	0.57
-1	10	3	24.19	25.04	3.24
-1	9	3	7.72	7.17	22.62
-1	8	3	10.57	10.82	13.27
-1	7	3	24.21	23.00	3.49
-1	6	3	16.43	15.75	6.47
-1	5	3	12.32	12.77	10.72
-1	4	3	34.76	34.99	1.92
-1	3	3	1.80*	0.99	3.57
-1	2	3	34.20	34.12	1.89
-1	1	3	25.04	24.54	3.56
-1	0	4	86.50	87.05	0.29
-1	1	4	10.92	11.49	12.93
-1	2	4	7.70	7.72	23.78
-1	3	4	30.68	29.64	2.39
-1	4	4	1.76*	1.37	3.52
-1	5	4	5.51	5.24	35.17
-1	6	4	14.76	15.21	7.01
-1	7	4	6.81	5.32	27.67
-1	8	4	1.98	1.40	15.06
-1	9	4	0.94*	0.83	0.57
-1	10	4	14.39	14.10	7.13
-1	11	4	8.91	9.48	15.87
-1	12	4	6.62	6.87	17.72
-1	13	4	18.33	18.70	4.68
-1	14	4	2.43	2.31	6.65
-1	15	4	1.47*	2.01	0.46
-1	16	4	7.18	7.06	14.42
-1	17	4	1.60*	0.25	0.39
-1	18	4	1.52*	0.28	0.43
-1	19	4	2.99*	2.36	1.68
-1	20	4	2.63*	2.72	0.98
-1	21	4	3.20*	1.77	1.46
-1	20	5	1.86*	2.42	2.50
-1	19	5	2.78*	2.97	4.57
-1	18	5	4.17	3.75	10.91
-1	17	5	2.66*	3.76	0.84
-1	16	5	6.42	6.17	14.82
-1	15	5	7.77	7.96	14.49
-1	14	5	2.73*	1.79	1.76
-1	13	5	10.76	11.03	10.87
-1	12	5	23.99	24.53	2.99
-1	11	5	27.32	27.85	2.46
-1	10	5	20.37	20.96	3.90
-1	9	5	11.81	11.93	10.40
-1	8	5	4.62	4.72	29.21
-1	7	5	1.42*	1.12	1.36
-1	6	5	1.81	2.74	12.25
-1	5	5	2.26	2.73	19.08
-1	4	5	9.62	9.83	15.23
-1	3	5	1.58*	0.93	2.24
-1	2	5	33.30	31.62	2.06
-1	1	5	2.98	3.08	32.52
-1	0	6	25.84	26.40	3.15
-1	1	6	16.98	16.61	6.02
-1	2	6	30.71	30.17	2.31
-1	3	6	12.02	12.78	9.84
-1	4	6	13.14	13.44	8.92
-1	5	6	2.81	3.34	23.42
-1	6	6	6.85	7.25	25.96
-1	7	6	1.18*	1.23	0.72
-1	8	6	20.03	20.14	4.27
-1	9	6	27.86	28.30	2.52
-1	10	6	24.72	25.56	2.97
-1	11	6	8.56	8.13	14.76
-1	12	6	5.10	4.91	14.39
-1	13	6	8.82	8.98	14.73
-1	14	6	1.34*	0.01	0.56
-1	15	6	0.63*	1.51	0.09
-1	16	6	4.74	4.45	12.32
-1	17	6	5.07	4.50	14.46
-1	18	6	1.65*	0.83	0.37
-1	19	6	1.92*	1.96	2.43
-1	20	6	2.80*	1.85	0.99
-1	19	7	1.68*	1.08	0.35
-1	18	7	3.69	4.26	6.97
-1	17	7	2.32*	2.69	3.92
-1	16	7	3.15*	2.84	1.51
-1	15	7	3.25*	3.26	1.38
-1	14	7	0.89*	0.82	0.19
-1	13	7	1.49*	0.47	0.45
-1	12	7	2.56*	4.25	0.84
-1	11	7	19.47	19.37	4.23
-1	10	7	7.62	6.98	16.57
-1	9	7	1.91*	0.05	1.34
-1	8	7	1.27*	1.83	0.62
-1	7	7	5.75	6.30	23.33
-1	6	7	19.16	18.16	4.50
-1	5	7	17.24	17.56	5.14
-1	4	7	11.16	10.80	11.87
-1	3	7	3.80	4.04	29.17
-1	2	7	5.06	5.04	31.13
-1	1	7	6.39	6.18	27.33
-1	0	8	19.15	18.63	4.53
-1	1	8	21.81	22.41	3.78
-1	2	8	12.55	12.77	9.68
-1	3	8	11.53	11.16	11.08
-1	4	8	20.75	20.31	4.00
-1	5	8	12.98	12.30	8.88
-1	6	8	6.07	5.85	21.47
-1	7	8	16.24	16.69	5.68
-1	8	8	34.72	34.81	1.70
-1	9	8	14.44	14.45	6.55
-1	10	8	6.42	6.47	15.79
-1	11	8	11.79	11.87	10.06
-1	12	8	6.17	5.84	17.31
-1	13	8	1.99*	1.44	0.76
-1	14	8	1.71*	1.38	0.67
-1	15	8	4.09	3.67	11.44
-1	16	8	2.18*	2.50	3.65
-1	17	8	1.66*	1.03	0.36
-1	18	8	1.65*	1.54	0.37
-1	18	9	2.13*	1.42	0.48
-1	17	9	1.73*	1.20	0.33
-1	16	9	2.46*	0.34	0.97
-1	15	9	4.91	4.28	10.96
-1	14	9	1.59*	0.73	0.39
-1	13	9	2.43*	2.75	0.95
-1	12	9	1.55*	0.57	0.42
-1	11	9	2.13*	1.72	1.14
-1	10	9	2.61*	3.65	1.35
-1	9	9	15.92	16.05	5.64
-1	8	9	12.05	12.01	9.50
-1	7	9	10.86	11.45	11.24
-1	6	9	28.52	28.86	2.32
-1	5	9	5.52	5.36	21.07
-1	4	9	9.38	9.87	14.13
-1	3	9	7.70	8.43	19.96
-1	2	9	15.35	15.73	6.45
-1	1	9	9.14	9.68	16.02
-1	0	10	1.62*	1.93	4.54
-1	1	10	1.33*	1.50	0.60
-1	2	10	1.63*	2.19	0.87
-1	3	10	13.31	13.55	7.60
-1	4	10	6.14	6.37	18.16
-1	5	10	7.67	8.13	16.16
-1	6	10	11.42	12.15	9.63
-1	7	10	7.59	8.00	16.57
-1	8	10	11.18	11.06	9.69
-1	9	10	1.53*	0.56	0.43
-1	10	10	9.89	9.78	13.44
-1	11	10	2.31*	0.04	1.36
-1	12	10	2.08*	0.04	1.19
-1	13	10	1.61*	1.93	0.39
-1	14	10	1.58*	1.52	0.40
-1	15	10	1.42*	0.15	0.49
-1	16	10	1.79*	1.85	0.49
-1	17	10	1.06*	1.69	0.12
-1	16	11	1.66*	0.70	0.36
-1	15	11	1.71*	0.93	0.34
-1	14	11	2.03*	0.87	0.55
-1	13	11	1.53*	0.15	0.43
-1	12	11	0.97*	0.49	0.14
-1	11	11	3.18	3.14	7.72
-1	10	11	7.56	7.38	14.48
-1	9	11	1.52*	1.11	0.43
-1	8	11	13.70	13.16	7.46
-1	7	11	11.54	11.18	9.33
-1	6	11	11.43	11.64	10.44
-1	5	11	6.94	7.08	17.58
-1	4	11	3.57	4.29	12.40
-1	3	11	2.60*	3.37	1.62
-1	2	11	2.81	3.52	9.53
-1	1	11	7.43	7.69	17.99
-1	0	12	4.91	5.03	16.34
-1	1	12	4.66	4.70	15.56
-1	2	12	13.47	13.85	7.34
-1	3	12	2.61*	3.27	1.45
-1	4	12	6.76	7.09	15.63
-1	5	12	2.59*	1.44	1.48
-1	6	12	4.40	4.16	11.87
-1	7	12	1.43*	0.50	0.49
-1	8	12	3.78	3.69	10.26
-1	9	12	3.61	3.99	8.80
-1	10	12	5.98	5.56	12.71
-1	11	12	1.68*	2.02	0.36
-1	12	12	1.42*	3.27	0.21
-1	13	12	1.81*	1.69	0.31
-1	14	12	1.29*	0.10	1.34
-1	13	13	1.75*	2.46	0.33
-1	12	13	1.61*	0.00	0.39
-1	11	13	4.54	4.96	8.44
-1	10	13	0.71*	1.20	0.08
-1	9	13	5.26	5.40	10.89
-1	8	13	1.77*	2.84	0.32
-1	7	13	4.55	4.50	10.03
-1	6	13	1.64*	1.37	0.55
-1	5	13	3.29	3.66	7.97
-1	4	13	8.00	8.48	13.01
-1	3	13	1.30*	1.17	0.37
-1	2	13	8.66	8.74	13.58
-1	1	13	1.52*	0.93	0.43
-1	0	14	3.98	9.12	12.17
-1	1	14	1.57*	0.71	0.40
-1	2	14	6.06	6.43	10.95
-1	3	14	2.71*	3.30	4.59
-1	4	14	1.05*	0.55	0.90
-1	5	14	1.39*	0.14	0.31
-1	6	14	1.64*	1.82	0.37
-1	7	14	5.77	5.94	11.39
-1	8	14	1.71*	2.12	0.34
-1	9	14	5.85	5.90	10.23
-1	10	14	3.55	2.60	6.79
-1	11	14	6.49	6.24	9.82
-1	8	15	4.48	4.79	7.38
-1	7	15	0.74*	1.71	0.08
-1	6	15	4.20	3.38	7.91
-1	5	15	2.30*	3.26	2.96
-1	4	15	1.09*	1.93	0.84
-1	3	15	1.92*	1.82	3.05
-1	2	15	3.52	2.99	7.53
-1	1	15	1.59*	0.28	0.39
-1	0	16	1.83*	1.72	0.47
0	0	16	0.43*	0.15	0.14
-1	1	16	1.68*	0.81	0.39
-1	2	16	1.78*	1.39	0.32
-1	3	16	1.78*	1.39	0.32
0	1	15	1.26*	0.59	0.23
0	2	15	2.18*	0.30	0.76
0	3	15	2.64*	1.43	1.04
0	4	15	1.59*	1.94	1.68
0	5	15	5.14	5.26	8.65
0	6	15	3.26*	3.52	0.98
0	10	14	3.82	4.01	6.76

h	k	l	Fo	Fc	weight
0	9	14	0.74*	0.97	0.08
0	8	14	4.10	3.07	7.99
0	7	14	5.96	5.51	11.11
0	6	14	2.47*	4.63	0.76
0	5	14	2.45*	1.49	0.78
0	4	14	2.80*	1.51	1.13
0	3	14	3.60	3.35	7.24
0	2	14	7.48	7.47	12.61
0	1	14	1.97*	2.14	3.13
0	0	14	6.87	6.37	12.39
0	1	13	1.60*	2.84	0.39
0	2	13	7.33	7.40	12.94
0	3	13	6.38	6.60	14.21
0	4	13	6.92	6.71	12.85
0	5	13	6.22	6.53	13.24
0	6	13	1.60*	1.69	0.39
0	7	13	2.25*	2.10	3.44
0	8	13	8.84	8.32	11.44
0	9	13	4.36	3.92	9.00
0	10	13	2.17*	1.62	0.83
0	11	13	5.29	5.17	9.16
0	12	13	3.67	3.26	6.37
0	14	12	0.75*	1.37	0.07
0	13	12	5.83	5.12	11.06
0	12	12	2.48*	2.68	3.41
0	11	12	1.66*	1.32	0.36
0	10	12	2.49*	2.22	0.92
0	9	12	3.66	3.59	9.23
0	8	12	1.58*	1.06	0.40
0	7	12	7.53	7.40	14.38
0	6	12	5.51	5.59	13.08
0	5	12	7.16	7.82	13.20
0	4	12	4.77	4.58	12.77
0	3	12	1.41*	0.47	0.51
0	2	12	0.62*	0.66	0.09
0	1	12	2.78*	2.14	1.49
0	0	12	19.84	20.08	3.74
0	1	11	7.14	7.45	15.46
0	2	11	16.35	16.33	5.58
0	3	11	8.29	9.46	14.47
0	4	11	3.22	2.61	10.47
0	5	11	13.16	13.82	7.55
0	6	11	7.15	7.44	13.97
0	7	11	6.29	6.23	14.23
0	8	11	8.79	8.88	13.12
0	9	11	6.84	7.41	12.99
0	10	11	1.15*	0.53	0.26
0	11	11	4.39	4.61	8.71
0	12	11	1.61*	1.56	0.38
0	13	11	2.00*	1.11	0.73
0	14	11	1.03*	0.21	0.95
0	15	11	3.34	2.91	4.92
0	16	10	1.65*	0.04	1.95
0	15	10	2.88*	4.24	0.84
0	14	10	1.64*	0.76	0.37
0	13	10	3.13*	2.82	1.41
0	12	10	1.55*	0.95	0.41
0	11	10	4.67	5.15	13.44
0	10	10	2.19*	2.42	1.02
0	9	10	1.07*	0.22	0.25
0	8	10	18.86	18.27	4.32
0	7	10	18.89	19.46	4.19
0	6	10	4.69	4.82	14.65
0	5	10	6.09	6.32	18.49
0	4	10	1.34*	1.25	0.56
0	3	10	3.87	3.82	13.64
0	2	10	7.61	7.87	17.40
0	1	10	7.89	7.87	18.45
0	0	10	8.64	8.29	15.09
0	1	9	2.07*	2.59	2.06
0	2	9	9.10	9.19	15.80
0	3	9	5.90	5.14	22.07
0	4	9	16.61	17.26	5.62
0	5	9	7.44	6.80	18.43
0	6	9	2.65*	2.46	1.79
0	7	9	1.59*	1.06	0.67
0	8	9	1.10*	1.56	1.74
0	9	9	14.13	14.90	7.40
0	10	9	8.91	8.96	13.79
0	11	9	2.83	2.74	7.46
0	12	9	2.39*	2.75	6.06
0	13	9	1.14*	0.27	0.27
0	14	9	6.45	6.53	12.28
0	15	9	1.97*	1.71	0.62
0	16	9	3.04	3.18	5.47
0	17	9	5.30	4.70	9.48
0	18	8	3.69	3.40	7.36
0	17	8	4.01	3.14	7.53
0	16	8	4.16	3.91	10.03
0	15	8	4.93	4.78	10.77
0	14	8	1.13*	1.11	0.28
0	13	8	3.75	3.56	10.21
0	12	8	2.13*	1.01	1.08
0	11	8	3.50	3.73	11.82
0	10	8	11.29	11.66	9.91
0	9	8	10.80	10.81	10.64
0	8	8	14.66	15.03	6.70
0	7	8	3.77	3.97	16.73
0	6	8	6.11	6.43	20.46
0	5	8	16.02	16.55	6.04
0	4	8	13.68	13.29	8.08
0	3	8	5.19	4.96	25.43
0	2	8	9.46	9.22	14.87
0	1	8	14.19	14.16	7.57
0	0	8	2.78	3.92	15.57
0	1	7	5.64	5.95	28.63
0	2	7	13.55	13.24	8.01
0	3	7	4.76	4.34	27.36
0	4	7	8.61	10.09	15.82
0	5	7	2.72	2.31	15.17
0	6	7	3.74	3.89	19.16
0	7	7	29.55	30.11	2.26
0	8	7	2.39*	0.93	2.55
0	9	7	6.47	6.18	17.48
0	10	7	17.09	17.21	5.10
0	11	7	0.99*	0.74	0.29
0	12	7	0.59*	1.14	0.09
0	13	7	4.58	4.56	14.32
0	14	7	5.23	5.02	15.27
0	15	7	2.12*	1.74	4.39
0	16	7	6.44	6.47	12.64
0	17	7	2.96*	2.94	0.99
0	18	7	2.39*	1.37	0.82
0	19	7	2.88*	1.25	1.21
0	20	6	1.58*	0.11	0.40
0	19	6	2.78	2.25	5.04
0	18	6	7.39	7.17	10.97
0	17	6	4.18	3.60	10.34
0	16	6	0.66*	0.64	0.07
0	15	6	3.16	2.96	8.91
0	14	6	7.18	7.22	15.85
0	13	6	7.95	8.20	15.53
0	12	6	4.82	4.50	15.76
0	11	6	1.74*	2.20	0.94
0	10	6	2.38*	0.23	2.62
0	9	6	7.02	6.89	20.18
0	8	6	9.87	9.52	14.33
0	7	6	10.27	10.84	12.62
0	6	6	4.06	4.04	27.96
0	5	6	8.85	9.08	18.48
0	4	6	35.80	34.32	1.74
0	3	6	25.18	25.65	3.19
0	2	6	3.60	3.50	27.39
0	1	6	17.61	15.88	5.50
0	0	6	27.61	27.37	2.77
0	1	5	26.40	25.48	3.09
0	2	5	31.43	28.73	2.25
0	3	5	3.84	4.56	34.36
0	4	5	12.30	13.40	9.48
0	5	5	21.80	21.26	4.12
0	6	5	13.35	14.06	8.87
0	7	5	11.74	12.15	10.15
0	8	5	6.23	5.81	25.83
0	9	5	17.35	17.09	5.59
0	10	5	4.56	5.00	19.89
0	11	5	3.69	3.23	17.96
0	12	5	5.78	5.79	18.39
0	13	5	6.91	6.81	17.50
0	14	5	2.16*	2.01	1.11
0	15	5	8.03	8.13	14.54
0	16	5	4.59	4.43	12.12
0	17	5	2.21*	2.27	0.80
0	18	5	1.55*	0.86	0.38
0	19	5	1.66*	0.85	0.36
0	20	5	6.45	5.59	9.72
0	21	4	1.85*	2.11	0.29
0	20	4	1.26*	0.32	0.22
0	19	4	1.99*	1.99	0.47
0	18	4	5.86	5.12	12.97
0	17	4	7.20	7.23	11.75
0	16	4	1.55*	0.86	0.58
0	15	4	13.84	13.70	7.42
0	14	4	1.94*	1.65	0.87
0	13	4	5.24	5.81	16.66
0	12	4	1.33*	1.27	0.56
0	11	4	13.45	13.74	7.91
0	10	4	16.12	15.78	6.22
0	9	4	10.58	10.60	12.48
0	8	4	7.49	7.55	21.96
0	7	4	4.06	4.10	26.04
0	6	4	7.16	6.37	24.42
0	5	4	19.11	19.68	5.06
0	4	4	33.04	33.47	2.06
0	3	4	40.66	42.42	1.42
0	2	4	27.86	27.90	2.85
0	1	4	16.80	17.63	6.62
0	0	4	20.82	21.28	4.70
0	1	3	61.95	62.23	0.52
0	2	3	60.04	62.63	0.53
0	3	3	23.93	24.20	3.75
0	4	3	37.71	37.25	1.64
0	5	3	24.55	24.60	3.53
0	6	3	22.72	22.63	3.99
0	7	3	12.11	12.51	9.84
0	8	3	22.27	21.49	3.87
0	9	3	3.61	4.30	26.25
0	10	3	7.90	7.71	21.07
0	11	3	7.00	7.25	21.43
0	12	3	1.29*	0.62	0.60
0	13	3	1.35*	2.31	0.55
0	14	3	8.47	8.41	14.49
0	15	3	2.07*	0.17	0.99
0	16	3	5.72	5.68	13.23
0	17	3	12.14	11.87	7.98
0	18	3	10.08	9.67	10.21
0	19	3	5.61	5.93	10.13
0	20	3	4.41	3.99	8.08
0	21	3	3.34*	2.60	1.26
0	21	2	1.81*	0.78	0.48
0	20	2	2.79	3.21	4.76
0	19	2	0.98*	0.89	0.14
0	18	2	2.97	3.20	6.33
0	17	2	1.11*	2.53	0.22
0	16	2	11.50	11.65	10.23
0	15	2	1.96*	2.60	0.58
0	14	2	7.92	8.10	16.72
0	13	2	2.59*	2.49	1.74
0	12	2	1.23*	0.25	0.66
0	11	2	11.32	11.46	10.47
0	10	2	4.78	4.72	27.14
0	9	2	2.61	2.77	20.80
0	8	2	11.90	11.52	10.48
0	7	2	9.36	10.18	16.84
0	6	2	8.02	7.88	22.09
0	5	2	13.84	13.87	8.71
0	4	2	14.75	16.26	7.92
0	3	2	21.17	21.18	4.77
0	2	2	59.17	59.51	0.59
0	1	2	26.56	27.16	3.24
0	0	2	103.11	105.23	0.22
0	1	1	1.40*	1.73	13.13
0	2	1	135.85	139.02	0.13

h	k	l	Fo	Fc	weight
0	3	1	62.19	62.90	0.54
0	4	1	17.72	18.05	6.34
0	5	1	19.51	18.64	5.36
0	6	1	6.91	6.78	26.72
0	7	1	21.92	21.42	4.19
0	8	1	12.39	14.20	9.78
0	9	1	3.75	2.57	27.69
0	10	1	14.85	14.34	7.23
0	11	1	3.15	2.85	20.76
0	12	1	8.64	8.70	18.47
0	13	1	1.31*	2.07	0.58
0	14	1	2.68	2.75	10.31
0	15	1	1.42*	0.33	0.49
0	16	1	2.11*	3.85	0.64
0	17	1	1.49*	1.42	0.45
0	18	1	2.83	3.31	6.00
0	19	1	1.59*	0.32	0.39
0	20	1	1.23*	0.44	0.20
0	21	1	3.21*	2.11	1.49
0	20	0	2.13*	0.93	0.59
0	18	0	4.04	4.32	9.83
0	16	0	3.22	3.12	10.70
0	14	0	4.42	4.28	15.14
0	12	0	2.09*	1.94	1.70
0	10	0	15.48	14.62	6.68
0	8	0	30.73	30.93	2.32
0	6	0	17.09	18.55	6.32
0	4	0	5.33	4.99	32.62
0	2	0	25.15	25.86	3.61
1	0	0	8.06	7.95	19.35
1	1	0	73.67	75.00	0.42
1	2	0	66.28	67.20	0.49
1	3	0	1.31*	1.17	1.63
1	4	0	27.71	29.69	2.94
1	5	0	8.50	9.03	17.36
1	6	0	5.70	5.52	34.96
1	7	0	5.47	4.75	31.63
1	8	0	48.09	48.51	1.01
1	9	0	16.16	14.85	5.69
1	10	0	9.28	9.26	16.43
1	11	0	8.46	7.84	18.30
1	12	0	13.20	13.05	8.06
1	13	0	2.19*	2.99	7.50
1	14	0	5.20	5.71	15.30
1	15	0	1.31*	1.84	0.59
1	16	0	9.52	9.75	13.36
1	17	0	1.91*	3.84	0.52
1	18	0	1.55*	0.12	0.41
1	19	0	1.38*	0.34	0.33
1	20	0	2.57*	0.95	1.37
1	21	0	2.45*	0.21	0.95
1	21	1	1.72*	0.06	0.34
1	20	1	3.29	3.24	6.12
1	19	1	4.84	4.35	11.78
1	18	1	1.60*	3.06	0.39
1	17	1	5.57	6.29	12.33
1	16	1	6.11	5.53	14.41
1	15	1	8.95	8.56	14.12
1	14	1	7.85	7.86	15.72
1	13	1	7.69	7.70	18.23
1	12	1	11.91	11.44	9.77
1	11	1	1.24*	0.18	0.65
1	10	1	7.25	6.88	22.49
1	9	1	10.15	10.21	13.39
1	8	1	23.52	21.94	3.56
1	7	1	23.54	22.56	3.60
1	6	1	35.90	34.90	1.77
1	5	1	50.23	50.29	0.95
1	4	1	18.64	18.87	5.58
1	3	1	10.20	10.73	13.91
1	2	1	22.74	22.71	4.19
1	1	1	34.39	33.49	1.99
1	0	2	75.83	76.91	0.37
1	1	2	39.97	39.53	1.49
1	2	2	31.28	30.80	2.35
1	3	2	23.37	23.20	3.95
1	4	2	75.68	77.58	0.36
1	5	2	21.22	20.09	4.40
1	6	2	53.65	54.26	0.83
1	7	2	7.02	7.66	24.25
1	8	2	11.76	11.65	10.79
1	9	2	17.09	16.88	5.43
1	10	2	3.41	3.28	22.18
1	11	2	1.00*	1.17	0.46
1	12	2	4.18	4.52	17.05
1	13	2	0.78*	1.98	0.20
1	14	2	12.91	13.43	8.21
1	15	2	18.43	18.90	4.18
1	16	2	1.24*	1.80	0.33
1	17	2	3.10*	3.70	1.54
1	18	2	3.89	4.21	8.31
1	19	2	6.10	5.71	10.87
1	20	2	1.70*	0.67	0.35
1	21	2	3.03	2.71	5.53
1	21	3	1.30*	1.67	0.20
1	20	3	5.41	5.03	9.61
1	19	3	3.14*	1.73	1.50
1	18	3	5.07	5.27	10.58
1	17	3	4.30	4.42	10.22
1	16	3	3.21	3.58	8.08
1	15	3	2.18*	1.65	5.60
1	14	3	1.84*	0.96	0.84
1	13	3	11.73	12.11	9.64
1	12	3	10.12	10.50	13.37
1	11	3	1.19*	1.06	0.71
1	10	3	2.56	3.02	13.52
1	9	3	13.06	12.86	8.10
1	8	3	15.72	14.80	6.91
1	7	3	51.98	49.29	0.86
1	6	3	62.55	61.09	0.61
1	5	3	14.97	14.67	7.04
1	4	3	3.91	3.46	31.97
1	3	3	22.04	22.52	4.24
1	2	3	25.18	24.14	3.44
1	1	3	2.65	2.90	26.81
1	0	4	29.68	30.29	2.54
1	1	4	19.95	20.10	4.91
1	2	4	60.67	60.43	0.66
1	3	4	29.94	28.86	2.45
1	4	4	31.85	30.91	2.15
1	5	4	44.32	41.92	1.19
1	6	4	15.94	16.76	5.78
1	7	4	17.64	17.61	5.10
1	8	4	1.17*	1.97	0.72
1	9	4	1.37*	1.49	0.77
1	10	4	4.71	4.29	23.75
1	11	4	2.11*	1.05	1.50
1	12	4	1.25*	0.72	0.64
1	13	4	1.72*	2.60	0.70
1	14	4	2.85*	3.46	1.67
1	15	4	1.49*	1.55	0.45
1	16	4	3.95	4.44	10.71
1	17	4	1.88*	0.83	0.61
1	18	4	2.42*	2.84	3.84
1	19	4	1.01*	2.24	0.12
1	20	4	3.21*	1.84	1.31
1	20	5	2.90*	1.97	1.12
1	19	5	2.71*	2.20	0.94
1	18	5	1.60*	0.13	0.39
1	17	5	4.01	3.85	8.76
1	16	5	4.38	4.51	12.92
1	15	5	1.57*	1.42	0.41
1	14	5	2.17*	1.80	5.93
1	13	5	4.71	5.03	14.08
1	12	5	1.39*	1.20	0.52
1	11	5	5.33	5.52	18.59
1	10	5	10.27	10.31	13.36
1	9	5	5.58	5.43	21.05
1	8	5	11.17	11.50	10.72
1	7	5	9.07	8.28	17.54
1	6	5	18.87	18.59	4.75
1	5	5	30.27	30.60	2.33
1	4	5	44.21	42.85	1.18
1	3	5	40.23	38.97	1.41
1	2	5	39.51	39.01	1.45
1	1	5	32.03	30.10	2.15
1	0	6	45.33	44.76	1.12
1	1	6	1.07*	0.85	0.88
1	2	6	5.24	4.85	29.51
1	3	6	22.15	22.54	3.83
1	4	6	16.35	17.74	4.99
1	5	6	9.57	8.92	15.01
1	6	6	2.40*	4.08	2.63
1	7	6	15.13	15.53	6.70
1	8	6	12.13	12.41	9.67
1	9	6	15.74	16.24	5.90
1	10	6	20.43	20.91	3.64
1	11	6	1.78*	2.03	0.82
1	12	6	4.96	4.14	15.21
1	13	6	10.55	10.36	11.94
1	14	6	4.70	4.94	13.55
1	15	6	1.45*	1.95	0.44
1	16	6	3.61	3.30	9.40
1	17	6	4.51	3.90	12.11
1	18	6	1.75*	1.11	0.51
1	19	6	1.48*	0.11	0.29
1	19	7	3.14	2.61	5.62
1	18	7	3.02*	0.76	1.03
1	17	7	2.13*	0.34	0.86
1	16	7	2.01*	2.60	2.90
1	15	7	1.56*	0.77	0.41
1	14	7	2.24*	2.53	0.88
1	13	7	1.88*	2.29	4.28
1	12	7	7.28	7.67	16.61
1	11	7	11.16	11.61	11.14
1	10	7	0.57*	0.33	0.10
1	9	7	6.93	7.40	16.48
1	8	7	7.44	7.44	17.44
1	7	7	2.09*	1.71	1.46
1	6	7	3.99	4.32	17.56
1	5	7	26.71	26.50	2.74
1	4	7	1.21*	1.37	0.68
1	3	7	12.58	11.93	9.18
1	2	7	1.64*	1.98	1.32
1	1	7	8.03	7.61	19.78
1	0	8	5.41	4.74	21.74
1	1	8	12.96	12.68	8.46
1	2	8	10.18	10.15	13.25
1	3	8	7.87	7.75	20.01
1	4	8	1.36*	0.65	0.54
1	5	8	17.91	18.44	5.18
1	6	8	15.92	16.27	5.61
1	7	8	8.13	7.55	15.75
1	8	8	16.90	17.04	4.94
1	9	8	5.77	6.23	14.27
1	10	8	7.04	7.35	16.79
1	11	8	0.61*	2.96	0.07
1	12	8	1.46*	0.82	0.47
1	13	8	3.29	3.26	8.42
1	14	8	1.61*	0.85	0.39
1	15	8	1.60*	0.23	0.39
1	16	8	0.71*	0.89	0.08
1	17	8	5.03	3.94	10.16
1	18	8	1.84*	1.55	0.33
1	17	9	2.79	0.44	5.87
1	16	9	1.46*	3.07	0.25
1	15	9	3.02	2.10	5.92
1	14	9	2.49*	0.60	1.25
1	13	9	4.44	4.44	11.66
1	12	9	2.27*	0.79	1.07
1	11	9	1.54*	0.14	0.42
1	10	9	5.45	5.79	14.30
1	9	9	3.15*	2.89	1.47
1	8	9	15.66	15.27	5.72
1	7	9	9.89	10.52	13.01
1	6	9	7.33	7.29	16.11
1	5	9	7.93	8.27	16.31
1	4	9	1.38*	1.43	0.53
1	3	9	11.23	11.44	11.46
1	2	9	2.54*	2.45	2.12
1	1	9	2.15*	1.63	2.44
1	0	10	23.02	23.56	3.08

h	k	l	Fo	Fc	weight
1	1	10	8.81	9 05	14.72
1	2	10	5.12	5.40	16.14
1	3	10	6.17	7.20	15.69
1	4	10	11.03	11.71	11.81
1	5	10	4.37	4.41	13.24
1	6	10	18.91	17.91	4.39
1	7	10	4.60	3.84	14.44
1	8	10	1.00*	2.45	0.99
1	9	10	6.22	6.51	14.97
1	10	10	2.52*	3.64	1.02
1	11	10	2.87*	1.93	1.14
1	12	10	1.64*	0.55	0.37
1	13	10	2.61*	0.81	1.52
1	14	10	2.37*	0.72	0.88
1	15	10	1.27*	2.24	0.19
1	16	10	2.26*	1 17	0.63
1	14	11	2.67*	2.34	0.76
1	13	11	2.80*	2.30	0.86
1	12	11	4.83	4.57	9.16
1	11	11	1.64*	2.19	0.37
1	10	11	4.57	5.11	10 67
1	9	11	1.76*	0.03	0.73
1	8	11	6.69	6.86	12.88
1	7	11	2.87*	1.89	1.70
1	6	11	5.61	5.46	16.21
1	5	11	4.77	4.37	13 39
1	4	11	1.75*	0.64	0.95
1	3	11	7.25	7.70	16.88
1	2	11	11.38	12.00	10.54
1	1	11	3.47	3.75	10.84
1	0	12	3.29	3.42	9.18
1	1	12	4.84	4.34	15.29
1	2	12	1.57*	1.18	0.56
1	3	12	3.66	3.86	10.63
1	4	12	5.53	5.90	13 63
1	5	12	2.71*	3.00	1.21
1	6	12	2.58*	2.46	0.97
1	7	12	5.71	5.04	13.87
1	8	12	2.17*	0.86	1.31
1	9	12	2.87*	3.09	1.03
1	10	12	1.42*	0.15	0.22
1	11	12	4.27	3.79	7.71
1	12	12	1.91*	2.26	0.28
1	13	12	6.22	5.75	9.87
1	11	13	3.10*	1.32	0 93
1	10	13	1.28*	2.83	0.15
1	9	13	3.33*	2.95	1.08
1	8	13	3.82	4.15	7.64
1	7	13	4.57	4.35	10.79
1	6	13	2.21*	2 11	0.75
1	5	13	3.00	2.97	6.35
1	4	13	1.65*	2.00	0.37
1	3	13	3.54	3.07	9.02
1	2	13	3.00	3.44	6.96
1	1	13	3.78	3.55	10.48
1	0	14	1.55*	0.55	0.42
1	1	14	2.91	2.80	5.43
1	2	14	1.65*	1.25	0.37
1	3	14	3.12*	1.48	1.39
1	4	14	1.69*	0.24	0.35
1	5	14	2.29*	0.54	0.91
1	6	14	0.95*	1.96	0.58
1	7	14	4.12	4.01	7.28
1	8	14	2.70*	2.00	0.93
1	4	15	5.84	4.98	11.18
1	3	15	2.70*	2.11	0.74
1	2	15	1.81*	3.57	0.31
1	1	15	2.36*	2.83	0.63
2	5	14	4.37	4.03	6.47
2	4	14	3.07*	3.08	1.11
2	3	14	2.34*	2.63	0.57
2	2	14	1.47*	1.80	0.26
2	1	14	2.21*	2.63	0.44
2	0	14	2.75*	1.94	1.10
2	1	13	3.96	4.00	8.35
2	2	13	2.95	3.29	5.19
2	3	13	0.71*	0.62	0.06
2	4	13	1.65*	0.04	0.37
2	5	13	1.63*	1.22	2.16
2	6	13	1.56*	0.57	0.41
2	7	13	1.62*	1.02	0.38
2	8	13	1.05*	0.22	0.17
2	9	13	1.50*	0.40	0.34
2	11	12	1.49*	1.22	0.25
2	10	12	1.03*	0.37	0.14
2	9	12	1.69*	2.53	1.89
2	8	12	1.62*	1.96	0.38
2	7	12	1.72*	2.42	0.34
2	6	12	2.54*	2.56	4.86
2	5	12	1.71*	1.63	0.34
2	4	12	0.96*	1.25	0.17
2	3	12	5.26	4.94	12.52
2	2	12	4.47	4.28	12.64
2	1	12	1.53*	1.59	0.43
2	0	12	4.65	4.45	10.07
2	1	11	7.60	7 40	13.97
2	2	11	1.49*	0.76	0.45
2	3	11	4.88	5.31	12.50
2	4	11	1.37*	0.22	0.53
2	5	11	4.93	3.70	14.24
2	6	11	5.18	5.39	12.84
2	7	11	2.00*	1.49	0.75
2	8	11	1.57*	0.78	0.41
2	9	11	2.29*	0.56	1.18
2	10	11	3.90	2.91	8.33
2	11	11	0.72*	0.83	0.07
2	12	11	2.19*	2.05	0.63
2	13	11	1 29*	1.47	0.17
2	15	10	1.73*	0 25	0.33
2	14	10	3.14	3 07	4 80
2	13	10	1.90*	0.13	0.49
2	12	10	5.42	5.42	10.92
2	11	10	3.26	3.27	7.56
2	10	10	4.81	5.28	10.72
2	9	10	1.62*	3.41	0.45
2	8	10	11.21	11.29	10.59
2	7	10	1.52*	1.29	0.43
2	6	10	3.79	5.06	10.12
2	5	10	1.24*	2.90	0.31
2	4	10	7.78	7.70	14.92
2	3	10	1.41*	0.07	0.51
2	2	10	1.36*	0.83	0.54
2	1	10	1.59*	1.45	0.66
2	0	10	1.89*	0.21	1.09
2	1	9	12.76	13.23	8.83
2	2	9	14.79	14.91	6.43
2	3	9	1.47*	0.90	0.46
2	4	9	11.87	12.56	9.27
2	5	9	6.70	6.32	15.36
2	6	9	5.81	6.24	15.47
2	7	9	8.05	7.90	14.36
2	8	9	1.44*	1.74	0.48
2	9	9	1.89*	0.16	1.02
2	10	9	2.33*	0.93	1.34
2	11	9	1.50*	0.99	0.44
2	12	9	1.52*	0.25	0.43
2	13	9	1.56*	0.28	0.41
2	14	9	2.84*	1.67	1.76
2	15	9	1.62*	2.46	0.38
2	16	9	2.65*	2.11	4.72
2	17	8	3.34*	3.53	1.03
2	16	8	1.45*	0.13	0.34
2	15	8	2.55*	1.31	1.19
2	14	8	1.61*	1.89	0.39
2	13	8	1.77*	1.21	0.50
2	12	8	2.59	2.64	6.82
2	11	8	1.90*	3.30	0.67
2	10	8	4.56	5.83	11.46
2	9	8	2.02*	2.30	4.70
2	8	8	6.15	6.05	18.18
2	7	8	1.41*	0.68	0.48
2	6	8	15.62	16.09	5.52
2	5	8	19.56	19.79	4.24
2	4	8	6.84	7.00	15.69
2	3	8	24.38	24 77	2.91
2	2	8	19.67	19.66	3.96
2	1	8	5.47	5.88	17.73
2	0	8	8.59	8.54	16.55
2	1	7	4.13	4.68	22.74
2	2	7	10.92	11.45	11.65
2	3	7	1.21*	0.18	0.68
2	4	7	23.26	23.65	3.23
2	5	7	4.61	4.80	16.64
2	6	7	4.98	4.24	15.28
2	7	7	16.05	16.27	5.23
2	8	7	1.38*	0.49	0.52
2	9	7	1.42*	2.14	0.49
2	10	7	3.14	3.37	9.09
2	11	7	6.37	6.90	15.33
2	12	7	2.08*	2.88	0.72
2	13	7	5.93	6.07	14.29
2	14	7	1.42*	0.50	0.50
2	15	7	2.52*	2.37	4.97
2	16	7	1.54*	1.56	0.42
2	17	7	1.26*	0.51	0.24
2	18	7	1.73*	0.22	0.33
2	19	6	3.54*	4.31	0.83
2	18	6	1.72*	0.08	0.34
2	17	6	1.71*	2.25	0.34
2	16	6	1.66*	0.57	0.36
2	15	6	2.75*	2.25	1.93
2	14	6	4.06	5.19	9.17
2	13	6	5.73	5.14	14.55
2	12	6	5.12	4.63	16.52
2	11	6	5.18	6.47	12.57
2	10	6	7.63	8.90	14.93
2	9	6	1.38*	0.48	0.52
2	8	6	12.11	11.87	9.36
2	7	6	2.34*	0.42	2.72
2	6	6	3.14	3.60	14.56
2	5	6	1.99*	0.36	1.75
2	4	6	16.54	15.74	6.06
2	3	6	7.87	7.31	21.21
2	2	6	17.98	18.39	4.91
2	1	6	1.15*	1.16	0.75
2	0	6	10.98	11.32	11.75
2	1	5	16.76	18.45	5.65
2	2	5	1.17*	1.77	0.74
2	3	5	34.08	33.99	1.88
2	4	5	12.08	11.33	10.35
2	5	5	6.48	6.38	23.65
2	6	5	16.19	15.00	6.25
2	7	5	2.58	2.79	13.37
2	8	5	3.29	2.99	17.09
2	9	5	11.66	12.21	9.48
2	10	5	10.48	11.13	10.81
2	11	5	15.46	14.72	5.85
2	12	5	18.39	19.29	4.29
2	13	5	4.01	3.38	12.20
2	14	5	0.63*	2.57	0.06
2	15	5	7.20	6.87	13.49
2	16	5	3.63	3.31	9.24
2	17	5	1.61*	1.39	0.39
2	18	5	0.72*	1.20	0.07
2	19	5	3.14	2.42	5.72
2	20	4	3.19*	3.98	0.89
2	19	4	2.82*	1.65	1.47
2	18	4	0.70*	0.63	0.07
2	17	4	1.58*	0.19	0.40
2	16	4	2.37*	0.78	1.14
2	15	4	4.27	4.89	11.46
2	14	4	5.79	6.52	14.37
2	13	4	11.05	10.60	10.46
2	12	4	2.48*	3.58	1.28
2	11	4	2.68	3.29	8.60
2	10	4	1.06*	0.58	0.31
2	9	4	9.85	10.04	13.61
2	8	4	13.76	14.90	7.03
2	7	4	5.08	5.05	25.35
2	6	4	2.43*	2.20	2.49
2	5	4	18.48	16.84	5.10
2	4	4	42.32	39.47	1.26

h	k	l	Fo	Fc	weight
2	3	4	34.57	31.89	1.85
2	2	4	7.85	6.81	19 51
2	1	4	2.75	3.11	20.65
2	0	4	8.56	7.87	19.58
2	1	3	29.52	27 64	2.53
2	2	3	3.19	1.39	25.98
2	3	3	2.72	2.76	20.29
2	4	3	35.72	33.15	1.77
2	5	3	24.65	22.86	3.28
2	6	3	9.77	9.32	14.46
2	7	3	9.28	9.07	16.04
2	8	3	0.95*	0.14	0.56
2	9	3	3.24	3.79	17 24
2	10	3	9.19	9.58	15 28
2	11	3	4.47	4.24	18.33
2	12	3	2.72*	2 70	1.77
2	13	3	1.91*	1.98	1.08
2	14	3	4.78	4.08	14.41
2	15	3	2.24*	0.70	1.35
2	16	3	2.04*	2.01	0.75
2	17	3	2.50*	2.27	0 99
2	18	3	4.29	3.81	9 84
2	19	3	2.68*	2.00	0.75
2	20	3	2.96*	2.35	1.29
2	20	2	3.44*	4.50	0.94
2	19	2	2.24*	1.61	0.50
2	18	2	2.47*	1.90	0.85
2	17	2	3.78	3.61	9.42
2	16	2	8.49	8.18	12.92
2	15	2	5.86	5.41	15.15
2	14	2	9.60	10.43	12.99
2	13	2	11.36	12.21	9.40
2	12	2	2.55*	1 33	1.93
2	11	2	1.27*	0.48	0.62
2	10	2	1.00*	0.02	0.53
2	9	2	0.42*	0.08	0.50
2	8	2	6.10	6.08	26.82
2	7	2	41.45	41.09	1.31
2	6	2	1.02*	2.48	0.60
2	5	2	13.49	13.08	8.66
2	4	2	28.10	26.70	2.73
2	3	2	1.07*	1.29	0.88
2	2	2	10.01	9.97	14.18
2	1	2	0.49*	0.32	0.25
2	0	2	16.57	15.69	6.47
2	1	1	24.42	25.32	3.59
2	2	1	4.46	4.75	32.12
2	3	1	32.87	34 06	2.10
2	4	1	59.36	59.34	0.68
2	5	1	20.26	21.04	4.72
2	6	1	24.00	23.15	3.52
2	7	1	21.07	19.74	4.20
2	8	1	3.02	3.25	21.98
2	9	1	1.13*	0.76	0.78
2	10	1	22.30	22.34	3.47
2	11	1	9.46	9.58	14.01
2	12	1	12.88	12.59	8.89
2	13	1	8.85	8.67	15.35
2	14	1	5.46	5.42	13.97
2	15	1	10.25	10.65	12.06
2	16	1	5.62	6.13	14.57
2	17	1	1.49*	1.10	0.45
2	18	1	1.50*	0.75	0.45
2	19	1	1.53*	0.34	0.43
2	20	1	3.17*	3.05	1.21
2	21	1	3.97	3.85	7.27
2	21	0	1.50*	0.56	0.34
2	20	0	1.53*	0.24	0.43
2	19	0	4.39	4.51	9.06
2	18	0	4.64	4.21	9.94
2	17	0	5.34	5.69	12.44
2	16	0	13.70	13.42	6.97
2	15	0	2.17*	1.19	0.92
2	14	0	15.61	16.08	5.65
2	13	0	2.71*	3.86	1.41
2	12	0	14.61	15.37	6.75
2	11	0	11.46	12.12	10.61
2	10	0	2.21*	2.64	2.08
2	9	0	11.03	11.37	12.31
2	8	0	6.64	7.27	25.26
2	7	0	16.06	15.59	6.10
2	6	0	9.04	8.09	17.35
2	5	0	0.83*	0.45	0.57
2	4	0	6.08	6.22	30.89
2	3	0	26.22	25.76	3.16
2	2	0	3.91	3.42	23.93
2	1	0	14.30	13.75	7.89
2	0	0	75.22	71.74	0.37
3	0	0	5.93	5.86	23.19
3	1	0	3.19	2.89	19.20
3	2	0	2.39	1.98	14.58
3	3	0	18.13	18.97	5.52
3	4	0	38.53	39.21	1.53
3	5	0	17.35	18.81	5.56
3	6	0	4.81	4.49	26.81
3	7	0	12.66	12.60	9.29
3	8	0	14.29	14.45	7.05
3	9	0	8.51	7.90	16.58
3	10	0	19.06	19.65	4.74
3	11	0	5.21	5.71	17.12
3	12	0	3.18	3.32	10.82
3	13	0	14.51	14.90	6.40
3	14	0	5.46	5.89	15.38
3	15	0	3.98	4.31	11.13
3	16	0	4.58	4.68	10.78
3	17	0	0.95*	2.14	0.17
3	18	0	1.60*	1.39	0.39
3	18	0	0.72*	1.06	0.11
3	20	0	1.78*	2.77	0.32
3	20	1	1.62*	1.71	0.38
3	19	1	1.58*	0.14	0.40
3	18	1	1.39*	0.68	0.37
3	17	1	1.90*	2.08	0.59
3	16	1	9.15	9.27	11.50
3	15	1	6.08	6.70	13.52
3	14	1	5.31	4.67	16.90
3	13	1	5.71	6.16	16.46
3	12	1	8 78	8.98	14.23
3	11	1	3.27	4.20	10.28
3	10	1	12.52	12 48	8.86
3	9	1	13.68	13.74	7.56
3	8	1	1.88*	0.24	6.94
3	7	1	2.92	3.89	15.38
3	6	1	5.60	5.48	25.67
3	5	1	8.61	9.06	17.88
3	4	1	8.63	6.98	16.96
3	3	1	8.86	8.54	15.93
3	2	1	32.07	30.31	2.13
3	1	1	11.20	11.56	10.58
3	0	2	21.14	21.58	4.30
3	1	2	24.72	24.30	3.33
3	2	2	21.97	20.50	4.03
3	3	2	8.63	9.09	16.95
3	4	2	24.58	24.96	3.26
3	5	2	24.55	24.07	3.18
3	6	2	4.35	3.60	22.04
3	7	2	23.99	24.71	3.20
3	8	2	9.85	10.36	13.66
3	9	2	8.23	7.43	18.09
3	10	2	14.99	15.07	6.49
3	11	2	3.54	3.54	11.96
3	12	2	7.02	7.29	16.54
3	13	2	1.45*	1.71	0.44
3	14	2	1.96*	1.15	5.16
3	15	2	2.84*	0.39	1.84
3	16	2	3.72	3.10	9.63
3	17	2	5.63	5.93	12.31
3	18	2	4.68	4.62	10.07
3	19	2	2.91*	1.11	1.10
3	20	2	2.13*	4.01	0.41
3	19	3	1.50*	1.88	1.30
3	18	3	4.20	3.70	7.00
3	17	3	0.98*	0.69	0.18
3	16	3	1.03*	1.00	0.95
3	15	3	1.71*	2.54	0.47
3	14	3	3.32	3.87	8.06
3	13	3	1.05*	2.72	0.22
3	12	3	6.18	6.35	17.66
3	11	3	11.62	12.18	9.92
3	10	3	4.66	4.79	15.64
3	9	3	14.95	14.90	6.86
3	8	3	9.95	10.22	14.31
3	7	3	14.36	15.06	7.50
3	6	3	31.84	31.65	2.05
3	5	3	14.94	14.65	6.88
3	4	3	7.01	6 81	23.82
3	3	3	1.77*	0.31	1.64
3	2	3	3.63	3.16	23.00
3	1	3	1.29*	0.06	1.27
3	0	4	8.57	9.23	17.03
3	1	4	6.85	6.31	23.06
3	2	4	2.21*	1.87	2.39
3	3	4	10.67	10.98	12.63
3	4	4	13.30	12.47	7.63
3	5	4	11.47	11.13	10.15
3	6	4	1.28*	0.98	0.61
3	7	4	2.56*	1.34	2.23
3	8	4	1.29*	1.76	0.52
3	9	4	7.04	7.04	16.80
3	10	4	9.49	9.01	13.89
3	11	4	3.87	4.03	11.72
3	12	4	1.04*	2.00	0.27
3	13	4	5.65	4.41	14.35
3	14	4	9.12	9.66	13.31
3	15	4	7.21	7.14	12.39
3	16	4	1.56*	0.36	0.41
3	17	4	1.72*	3.22	0.34
3	18	4	5.48	5.10	10.37
3	19	4	4.19	3.43	6.57
3	18	5	3.05*	1.84	1.36
3	17	5	1.43*	1.42	0.27
3	16	5	3.42	3.60	6.79
3	15	5	1.65*	2.37	0.43
3	14	5	2.70*	0.84	1.52
3	13	5	2.62*	5.29	0.69
3	12	5	3.32	2.70	9.69
3	11	5	1.52*	3.17	0.43
3	10	5	5.48	6.33	14.46
3	9	5	4.20	4.41	13.52
3	8	5	4.50	3.85	15.62
3	7	5	1.28*	0.85	0.61
3	6	5	6.46	6.79	20.41
3	5	5	2.10*	2.29	1.50
3	4	5	25.33	25.11	2.84
3	3	5	3.44	2.57	16.22
3	2	5	5.02	5.28	19.88
3	1	5	8.09	8.16	19.71
3	0	6	15.00	16.09	6.23
3	1	6	16.37	16.17	5.74
3	2	6	21.28	21.88	3.78
3	3	6	12.67	13.08	9.18
3	4	6	1.42*	1.56	0.49
3	5	6	12.19	12.23	8.51
3	6	6	9.20	9.25	14.32
3	7	6	1.48*	0.14	0.76
3	8	6	5.29	5.32	16.62
3	9	6	3.98	4.30	13.34
3	10	6	8.20	8.59	14.48
3	11	6	2.55*	2.29	1.38
3	12	6	5.97	6.48	13.41
3	13	6	1.45*	0.40	0.48
3	14	6	2.23*	1.90	1.34
3	15	6	1.57*	1.21	0.41
3	16	6	1.74*	0.56	0.60
3	17	6	1.47*	0.59	0.26
3	18	6	3.54*	3.36	0.96
3	17	7	1.70*	0.16	0.34
3	16	7	2.92*	1.23	1.24
3	15	7	3.10*	0.79	1.60
3	14	7	2.85*	3.30	0.79
3	13	7	1.59*	0.72	0.40
3	12	7	1.61*	1.86	0.53

h	k	l	Fo	Fc	weight
3	11	7	2.31*	0.75	0.97
3	10	7	1.53*	1.91	0.53
3	9	7	5.26	6.12	13.67
3	8	7	5.27	5.41	16.43
3	7	7	3.41	3.41	11.72
3	6	7	8.91	9.28	14.19
3	5	7	1.85*	1.00	1.06
3	4	7	18.82	19.15	4.45
3	3	7	30.45	29.71	2.05
3	2	7	17.35	17.06	4.85
3	1	7	7.34	7.30	16.30
3	0	8	16.48	16.18	5.87
3	1	8	15.54	15.51	6.08
3	2	8	12.44	12.11	8.89
3	3	8	7.84	8.12	15.34
3	4	8	9.67	9.33	13.61
3	5	8	3.67	4.24	11.73
3	6	8	2.68*	4.20	1.46
3	7	8	1.36*	0.01	0.54
3	8	8	1.11*	0.83	1.66
3	9	8	4.56	5.14	12.64
3	10	8	1.50*	0.70	0.44
3	11	8	3.04*	0.66	1.57
3	12	8	2.15*	1.95	1.11
3	13	8	1.59*	2.39	0.40
3	14	8	2.47*	1.62	0.85
3	15	8	1.70*	1.21	0.35
3	16	8	2.30*	0.43	3.72
3	15	9	1.69*	1.29	0.36
3	14	9	3.58	3.24	6.32
3	13	9	1.02*	0.63	0.18
3	12	9	1.72*	0.29	0.34
3	11	9	4.10	4.96	8.44
3	10	9	1.71*	1.57	0.34
3	9	9	0.66*	3.24	0.06
3	8	9	1.51*	1.40	0.44
3	7	9	2.39*	0.49	1.67
3	6	9	1.26*	1.27	0.35
3	5	9	1.24*	1.02	1.62
3	4	9	1.48*	2.25	0.46
3	3	9	3.11	3.46	9.52
3	2	9	1.41*	0.63	0.50
3	1	9	3.77	3.60	12.91
3	0	10	5.15	5.06	15.48
3	1	10	0.97*	1.42	1.01
3	2	10	1.42*	2.22	0.34
3	3	10	7.40	6.55	14.90
3	4	10	1.43*	0.21	0.49
3	5	10	5.00	4.89	12.84
3	6	10	0.85*	1.29	0.79
3	7	10	2.59*	3.15	0.81
3	8	10	1.92*	2.35	0.50
3	9	10	1.54*	1.08	0.46
3	10	10	2.72*	3.00	0.91
3	11	10	4.14	3.13	8.35
3	12	10	6.39	6.58	8.29
3	13	10	8.24	7.77	9.46
3	11	11	6.15	6.71	8.16

h	k	l	Fo	Fc	weight
3	10	11	2.42*	1.85	0.56
3	9	11	1.75*	1.36	0.33
3	8	11	2.65*	4.26	0.55
3	7	11	2.32*	2.66	0.74
3	6	11	0.98*	3.78	0.12
3	5	11	1.67*	0.48	0.53
3	4	11	2.02*	1.18	0.83
3	3	11	2.60*	2.15	1.73
3	2	11	1.52*	1.08	0.43
3	1	11	8.93	8.53	12.40
3	0	12	4.25	3.70	8.81
3	1	12	5.14	4.68	11.02
3	2	12	4.54	3.29	10 00
3	3	12	2.90*	1.94	1.40
3	4	12	1.74*	1.37	0.60
3	5	12	1.66*	0.34	0.36
3	6	12	2.39*	0.33	1.07
3	7	12	2.31*	2.92	0.51
3	8	12	1.83*	2.51	0.30
3	9	12	1.76*	1.55	0.32
3	10	13	2.26*	2.57	2.44
3	9	13	1.29*	2.80	0.16
3	8	13	2.05*	1.42	3.04
3	7	13	2.95*	3.32	1.08
3	2	13	5.79	5.36	10.36
3	1	13	1.04*	1.22	0.15
4	5	12	2.60*	0.34	0.92
4	4	12	2.23*	2.85	0.54
4	3	12	3.05	3.58	4.22
4	2	12	1.85*	0.96	0.29
4	1	12	11.53	9.97	8.95
4	0	12	6.49	6.45	10.40
4	1	11	1.00*	1.35	0.14
4	2	11	7.54	7.48	11.36
4	3	11	3.47*	2.75	1.12
4	4	11	1.43*	2.83	0.20
4	5	11	1.63*	0.26	0.37
4	6	11	3.70	2.35	8.33
4	7	11	1.64*	1.00	0.29
4	8	11	1.79*	2.13	0.31
4	9	11	2.50*	1.13	0.75
4	11	10	0.75*	0.10	0.07
4	10	10	7.64	6.22	9.94
4	9	10	1.62*	2.91	0.28
4	8	10	1.89*	0.40	0.55
4	7	10	2.91*	2.61	0.88
4	6	10	4.09	3.72	8.12
4	5	10	1.65*	0.31	0.37
4	4	10	3.85	3.83	9.34
4	3	10	2.54*	1.74	1.14
4	2	10	3.83	3.67	8.45
4	1	10	1.68*	2.32	0.35
4	0	10	4.77	4.55	10.83
4	1	9	1.44*	1.11	0.44
4	2	9	3.57	3.78	9.62
4	3	9	3.18*	3.73	1.06
4	4	9	3.13	3.27	6.30
4	5	9	2.72*	2.68	1.34

h	k	l	Fo	Fc	weight
4	6	9	5.77	5.41	12.35
4	7	9	1.01*	0.42	0.99
4	8	9	6.34	5.69	12.45
4	9	9	5.17	5.32	9.25
4	10	9	3.41	2.99	6.14
4	11	9	1.91*	2.43	0.45
4	12	9	1.95*	0.55	0.46
4	13	9	2.26*	1.40	0.71
4	14	8	1.69*	0.30	0.35
4	13	8	1.62*	0.09	0.38
4	12	8	1.89*	0.35	0.44
4	11	8	1.87*	1.91	2.44
4	10	8	4.44	3.49	8.20
4	9	8	1.54*	1.40	0.42
4	8	8	2.14*	1.99	4.12
4	7	8	2.25*	3.66	0.88
4	6	8	1.69*	0.43	0.69
4	5	8	1.67*	1.25	0.57
4	4	8	2.42*	2.84	1.10
4	3	8	4.15	4.42	11.63
4	2	8	1.95*	0.13	0.92
4	1	8	3.06	2.87	9.02
4	0	8	3.24	3.20	10.31
4	1	7	1.55*	1.78	0.42
4	2	7	12.38	12.47	8.50
4	3	7	1.41*	0.75	0.50
4	4	7	0.93*	1.39	1.16
4	5	7	7.33	7.78	14.57
4	6	7	1.45*	0.57	0.48
4	7	7	3.61	5.05	7.79
4	8	7	1.90*	0.78	1.17
4	9	7	1.83*	1.82	0.58
4	10	7	2.47*	0.86	1.56
4	11	7	0.55*	1.95	0.25
4	12	7	1.54*	2.66	0.25
4	13	7	2.65*	0.72	1.11
4	14	7	3.24*	2.68	1.34
4	15	7	2.57*	1.26	0.83
4	16	6	1.96*	0.75	0.46
4	15	6	2.50*	1.46	0.88
4	14	6	4.54	4.09	10.28
4	13	6	4.55	4.67	10.00
4	12	6	1.59*	1.84	0.39
4	11	6	2.44*	2.32	4.90
4	10	6	2.02*	2.25	0.85
4	9	6	1.44*	0.13	0.48
4	8	6	10.99	10.90	10.07
4	7	6	1.48*	0 66	0.46
4	6	6	1 49*	2.38	0.45
4	5	6	8 05	8.06	15.54
4	4	6	7.12	6.95	14.56
4	3	6	4.79	4.48	15.13
4	2	6	1.47*	1.67	0.47
4	1	6	16.41	16.12	5.06
4	0	6	43.71	44.95	1.11
4	1	5	16.61	16.02	5.38
4	2	5	24.51	24.40	2.92
4	3	5	12.85	13.85	8.67

h	k	l	Fo	Fc	weight 13
4	4	5	9.67	8.98	12.60
4	5	5	3.57	3.91	10.92
4	6	5	6.37	5.78	15.47
4	7	5	1.79*	1.59	4.27
4	8	5	4.17	5.22	10.90
4	9	5	1.70*	1.30	0.61
4	10	5	1.95*	2.21	0.97
4	11	5	8.12	8.76	13.71
4	12	5	5.29	4.66	12.57
4	13	5	2.83*	1.15	1.18
4	14	5	1.73*	1.67	2.55
4	15	5	1.61*	1.44	0.39
4	16	5	1.92*	0.33	0.48
4	17	5	4.53	4.37	7.74
4	18	4	1.71*	1.52	0.34
4	17	4	1.73*	0.69	0.33
4	16	4	1.63*	2.09	0.38
4	15	4	2.39*	0.48	0.86
4	14	4	1.02*	0.09	0.96
4	13	4	1.30*	1.74	0.27.
4	12	4	3,98	4.22	10.57
4	11	4	5.00	4.36	12.92
4	10	4	5.81	6.02	15 57
4	9	4	9.74	10.10	13.04
4	8	4	3.20	4.37	9.29
4	7	4	2.83*	2.50	1.70
4	6	4	7.84	8.67	15.36
4	5	4	2.13*	2.81	1.36
4	4	4	4.55	4.28	17.34
4	3	4	1.38*	0.14	0.52
4	2	4	22.96	22.32	3.27
4	1	4	1.90*	1.58	1.07
4	0	4	16.29	15.74	5.56
4	1	3	14.07	13.60	7.33
4	2	3	16.77	17.72	5.60
4	3	3	9.72	9.84	12.64
4	4	3	9.60	8.67	14.35
4	5	3	4.74	4.87	17.51
4	6	3	1.41*	2.02	0.50
4	7	3	1.38*	0.95	0.53
4	8	3	12.47	12.93	8.63
4	9	3	10.87	11.02	10.74
4	10	3	7.18	7.92	15.43
4	11	3	9.92	9.52	12.82
4	12	3	1.95*	1.20	0.91
4	13	3	1.55*	0.27	0.41
4	14	3	6.53	6.43	13.66
4	15	3	2.34*	2.43	0.81
4	16	3	1.87*	1.38	0.62
4	17	3	5.53	5.39	8.38
4	18	3	0.68*	0.84	0.27
4	19	2	2.38*	2.17	0.50
4	18	2	1.68*	0.87	0.35
4	17	2	2.45*	1.34	1.30
4	16	2	1.82*	1.42	0.43
4	15	2	4.16	4.48	8.56
4	14	2	2.66*	2.89	1.06
4	13	2	1.41*	0.86	0.50

h	k	l	Fo	Fc	weight
4	12	2	1.49*	1.70	0.45
4	11	2	3.06	4.01	7.38
4	10	2	8.92	9.54	13.36
4	9	2	18.52	19.83	4.49
4	8	2	18.40	18.95	4.63
4	7	2	8.64	8.76	15.58
4	6	2	10.37	8.80	13.09
4	5	2	6.88	6.41	18.69
4	4	2	2.33*	2.96	1.50
4	3	2	16.02	14.82	6.01
4	2	2	1.05*	0.01	0.36
4	1	2	18.16	17.35	4.71
4	0	2	33.74	31.68	1.88
4	1	1	27.48	25.49	2.69
4	2	1	17.33	15.95	5.12
4	3	1	1.85*	0.00	6.49
4	4	1	10.35	9.71	12.34
4	5	1	21.56	22.00	3.76
4	6	1	13.76	13.79	7.71
4	7	1	12.88	13 16	8.67
4	8	1	9.97	10.31	11.63
4	9	1	18.15	18.47	4.59
4	10	1	6.53	6.81	14.19
4	11	1	3.65	3.74	11.32
4	12	1	1.97*	2.27	0.78
4	13	1	5.11	4.79	13.79
4	14	1	1.16*	0.71	1.48
4	15	1	4.30	4.06	10.39
4	16	1	2.79*	2.67	0.96
4	17	1	1.65*	0.94	0.37
4	18	1	3.46*	4.42	1.05
4	19	1	2.24*	1.36	0.54
4	19	0	2.67*	0.72	1.17
4	18	0	1.68*	1.37	0.36
4	17	0	1.75*	1.75	2.42
4	16	0	1.90*	2.15	0.60
4	15	0	1.84*	1.11	0.67
4	14	0	8.24	8.73	13.64
4	13	0	2.97	3.44	7 80
4	12	0	4.17	4.98	11.79
4	11	0	4.75	5.24	14 47
4	10	0	9.14	8.86	13.80
4	9	0	10.36	12.07	11.08
4	8	0	25.30	26.17	2.74
4	7	0	15.00	15.29	6.09
4	6	0	2.47*	3.44	1.77
4	5	0	9.50	9.93	14.29
4	4	0	18.43	19.75	4.69
4	3	0	12.54	12.85	9.25
4	2	0	5.46	5.62	21.17
4	1	0	3.47	3.30	15.72
4	0	0	5.49	5.10	20.05
5	0	0	1.45*	0.98	0.47
5	1	0	2.91*	2.61	1.70
5	2	0	8.49	7.85	14.07
5	3	0	7.61	7.28	15.63
5	4	0	1.99*	3.18	0.72
5	5	0	6.29	6.69	15.81

h	k	l	Fo	Fc	weight
5	6	0	7.11	8.27	14 37
5	7	0	5.91	5.85	14.37
5	8	0	21.76	22.72	3.30
5	9	0	6.18	6.06	13.98
5	10	0	5.80	6.63	13.32
5	11	0	1.50*	0.44	0.45
5	12	0	8.58	8.71	13.30
5	13	0	8.15	7.96	13.56
5	14	0	1.52*	0.40	0.43
5	15	0	5.97	5.81	10.58
5	16	0	2.99*	2.95	0.93
5	17	0	4.02	3.99	6.56
5	18	0	3.30	2.28	5.00
5	18	1	1.68*	0.29	0.34
5	17	1	10.26	9.04	9.39
5	16	1	6.67	5.81	9.38
5	15	1	4.08	4.43	7.35
5	14	1	1.50*	0.16	0.38
5	13	1	1.30*	2.87	0.31
5	12	1	1.60*	1.57	0.39
5	11	1	5.85	5.96	12.57
5	10	1	17.86	19.19	4.28
5	9	1	16.91	16.97	5.19
5	8	1	2.61	2.36	5.33
5	7	1	8.51	8.68	13.29
5	6	1	1.96*	0.63	0.77
5	5	1	2.07*	1.53	1.23
5	4	1	2.16*	0.15	1.23
5	3	1	1.79*	2.41	0.69
5	2	1	7.58	8.15	14.60
5	1	1	1.49*	0.98	0.45
5	0	2	8.61	8.04	15.34
5	1	2	1.40*	1.38	0.51
5	2	2	7.84	7.58	16.02
5	3	2	2.71*	0.83	1.85
5	4	2	2.35*	1.92	1.29
5	5	2	4.17	5.11	10.27
5	6	2	9.74	9.91	12.46
5	7	2	20.90	20.86	3.43
5	8	2	18.25	18.28	4.36
5	9	2	2.97	2.27	6.90
5	10	2	4.70	4.72	12.21
5	11	2	0.89*	1.19	0.19
5	12	2	7.49	7.24	12.69
5	13	2	1.99*	2.28	0.68
5	14	2	6.79	6.21	11.30
5	15	2	2.71*	3.95	0.74
5	16	2	5.30	4.87	9.67
5	17	2	1.71*	0.41	0.34
5	17	3	1.70*	0.20	0.34
5	16	3	3.73	3.72	6.51
5	15	3	4.69	3.36	9.13
5	14	3	0.69*	2.83	0.05
5	13	3	3.71	2.92	9.15
5	12	3	1.58*	1.92	0.40
5	11	3	1.85*	2.73	3.27
5	10	3	8.25	8.51	12.78
5	9	3	8.73	9.08	13.44

h	k	l	Fo	Fc	weight
5	8	3	1.58*	2.12	0.58
5	7	3	2.80*	3.02	1.34
5	6	3	17.13	18.86	4.45
5	5	3	21.41	21.67	3.18
5	4	3	5.71	5.86	14.87
5	3	3	5.82	5.12	14.70
5	2	3	2.31*	1.13	1.17
5	1	3	12.47	13.91	8.41
5	0	4	26.69	27.18	2.48
5	1	4	5.51	5.10	13.83
5	2	4	4.70	5.32	11.44
5	3	4	16.07	16.71	5.73
5	4	4	3.53	3.50	8.15
5	5	4	5.92	5.95	13.53
5	6	4	8.13	8.36	12.74
5	7	4	20.26	20.49	3.71
5	8	4	2.38*	3.04	0.73
5	9	4	2.66*	2.87	1.09
5	10	4	2.56*	2.84	1.16
5	11	4	4.07	4.03	9.60
5	12	4	3.36*	2.42	1.28
5	13	4	3.08*	2.31	1.56
5	14	4	1.64*	1.06	0.37
5	15	4	0.73*	0.34	0.08
5	16	4	2.88*	3.65	0.59
5	15	5	1.28*	0.02	0.20
5	14	5	2.40*	2.06	0.72
5	13	5	2.23*	1.60	0.74
5	12	5	4.49	4.32	9.88
5	11	5	1.56*	0.56	0.41
5	10	5	2.08*	0.97	0.63
5	9	5	1.58*	1.71	0.42
5	8	5	1.13*	0.57	1.25
5	7	5	5.71	5.68	13.22
5	6	5	10.25	9.97	11.25
5	5	5	19.45	19.34	3.86
5	4	5	8.75	8.45	13.13
5	3	5	2.86	3.33	7.34
5	2	5	13.55	13.81	7.05
5	1	5	5.49	5.48	13.74
5	0	6	2.27*	0.07	1.34
5	1	6	6.88	6.91	15.39
5	2	6	9.99	10.02	12.71
5	3	6	11.56	11.41	9.44
5	4	6	13.85	13.66	6.91
5	5	6	2.07*	2.82	0.60
5	6	6	5.10	5.22	10.64
5	7	6	3.75	3.30	9.21
5	8	6	2.36*	1.67	1.15
5	9	6	0.38*	0.93	0.14
5	10	6	2.45*	2.22	0.69
5	11	6	2.86*	2.66	1.21
5	12	6	1.61*	0.21	0.39
5	13	6	1.02*	1.40	0.12
5	14	6	1.66*	0.67	0.33
5	13	7	6.39	5.85	9.76
5	12	7	3.10	2.65	4.88
5	11	7	1.59*	0.58	0.40

h	k	l	Fo	Fc	weight 14
5	10	7	1.78*	2.57	0.32
5	9	7	1.54*	0.51	0 36
5	8	7	7.16	6.98	12.11
5	7	7	2.91*	2.26	1.30
5	6	7	6.31	6.13	13.86
5	5	7	6.72	6.90	12.78
5	4	7	1.31*	2.23	1.58
5	3	7	4.82	4.78	10.71
5	2	7	4.36	3.92	11.22
5	1	7	1.37*	1.05	1.67
5	0	8	4.83	4.17	10.49
5	1	8	4.76	4.84	10.95
5	2	8	3.37*	4.26	1.28
5	3	8	1.57*	1.27	0.41
5	4	8	9.55	9.19	11.67
5	5	8	2.70*	5.28	0.59
5	6	8	9.77	9.33	9.93
5	7	8	2.30*	2.74	0.71
5	8	8	1.68*	0.21	0.35
5	9	8	6.26	5.74	10 45
5	10	8	6.45	6.06	9.93
5	11	8	3.94	3.69	7 01
5	12	8	2.13*	1.37	0.53
5	10	9	1.74*	1.15	0.33
5	9	9	4.99	4.37	8.19
5	8	9	7.50	7.31	9.62
5	7	9	6.77	6.37	10.39
5	6	9	4.40	4.35	9.02
5	5	9	1.70*	1.99	0.35
5	4	9	3.06	3.09	4.82
5	3	9	2.68	2.37	5.08
5	2	9	0.97*	2.62	0.10
5	1	9	3.47	2.55	8.86
5	0	10	1.89*	0.25	0.49
5	1	10	5.64	5.05	10.62
5	2	10	3.73	3.25	6.98
5	3	10	2.50*	0.85	0.79
5	4	10	2.29*	0.25	0.79
5	5	10	4.92	4.84	8.02
5	6	10	1.81*	1.64	0.45
5	7	10	1.78*	0.04	2.22
5	8	10	3.38*	3.83	0.85
5	4	11	1.97*	1.80	2.04
5	3	11	8.14	7.63	10.44
5	2	11	3.77	3.59	6.00
5	1	11	3.68	3.65	5.22
6	1	9	7.22	6.78	9.99
6	2	9	2.66*	3.61	0.55
6	3	9	2.77*	1.57	0.77
6	4	9	7.96	7.59	10.22
6	5	9	1.76*	0.92	0.32
6	6	8	3.26*	2.64	1.14
6	7	8	1.65*	3.68	0.20
6	6	8	1.72*	0.58	0.34
6	5	8	2.89*	2.94	0.80
6	4	8	1.73*	0.44	0.33
6	3	8	1.43*	1.29	0.20
6	2	8	6.69	6.32	11.05

h	k	l	Fo	Fc	weight
6	1	8	1.62*	0.53	0.38
6	0	8	7.05	7.23	10.32
6	1	7	7.63	7.29	11.89
6	2	7	4.91	4.78	10.47
6	3	7	3.19	3.72	5.81
6	4	7	2.59*	1.37	0.84
6	5	7	1.56*	1.93	0.37
6	6	7	1.64*	1.02	0.37
6	7	7	6.71	6.38	10.64
6	8	7	1.81*	2.52	0.30
6	9	7	2.84*	1.23	1.03
6	10	7	8.59	7.90	9.56
6	12	6	11.46	10.33	8.12
6	11	6	2.21*	2.81	0.35
6	10	6	1.26*	1.54	0.16
6	8	6	3.34*	2.98	1.22
6	8	6	7.28	7.20	11.07
6	7	6	2.49*	3.28	0.56
6	6	6	1.18*	0.96	0.24
6	5	6	1.65*	1.60	0.37
6	4	6	4.13	4.28	8.38
6	3	6	1.54*	0.84	0.42
6	2	6	1.63*	0.37	0.38
6	1	6	2.08*	0.55	0.90
6	0	6	3.22*	3.72	1.31
6	1	5	1.58*	1.40	2.11
6	2	5	2.30*	0.66	1.02
6	3	5	0.64*	1.78	0.07
6	4	5	7.77	8.10	12.13
6	5	5	6.75	7.35	11.97
6	6	5	6.30	6.33	12.53
6	7	5	2.32*	2.08	0.96
6	8	5	1.52*	0.01	0.34
6	9	5	2.85*	0.37	1.66
6	10	5	2.99*	2.29	0.86
6	11	5	1.74*	0.07	0.33
6	12	5	1.77*	1.87	0.32
6	13	5	2.37*	1.98	0.42
6	14	4	1.83*	0.76	0.32
6	13	4	1.03*	0.84	0.13
6	12	4	2.86	2.56	6.06
6	11	4	4.00	4.39	7.24
6	10	4	1.82*	1.08	0.50
6	9	4	2.13*	1.96	3.32
6	8	4	4.35	4.73	8.45
6	7	4	6.16	6.02	13.13
6	6	4	5.14	5.34	10.89
6	5	4	1.61*	0.82	0.39
6	4	4	15.33	15.55	6.24
6	3	4	0.88*	1.64	0.12
6	2	4	8.57	8.46	12.63
6	1	4	14.50	14.17	6.86
6	0	4	2.22*	1.28	0.96
6	1	3	5.05	5.31	9.92
6	2	3	18.26	18.65	4.32
6	3	3	9.82	9.66	11.41
6	4	3	5.11	5.09	10.58
6	5	3	11.32	11.86	9.42
6	6	3	18.24	18.52	4.08
6	7	3	1.29*	0.43	1.46
6	8	3	7.01	7.67	11.49
6	9	3	2.46*	0.82	1.28
6	10	3	1.67*	0.53	0.36
6	11	3	1.48*	1.80	1.60
6	12	3	4.19	4.39	7.75
6	13	3	4.05	3.36	6.81
6	14	3	5.40	5.92	7.13
6	15	3	3.19*	3.12	0.70
6	15	2	5.19	5.05	6.71
6	14	2	1.82*	2.35	0.30
6	13	2	2.82*	2.34	0.92
6	12	2	0.97*	1.59	0.17
6	11	2	2.60*	2.27	1.23
6	10	2	1.65*	1.33	0.37
6	9	2	1.62*	0.18	0.38
6	8	2	1.86*	1.84	3.05
6	7	2	1.68*	3.46	0.36
6	6	2	14.09	14.98	7.52
6	5	2	4.24	4.63	10.80
6	4	2	12.11	12.78	8.94
6	3	2	12.11	12.54	8.56
6	2	2	3.05	3.70	5.39
6	1	2	1.62*	1.32	0.38
6	0	2	19.62	19.51	4.01
6	1	1	2.54*	3.14	0.88
6	2	1	6.44	6.42	12.59
6	3	1	1.39*	2.16	1.40
6	4	1	2.56*	2.81	4.68
6	5	1	4.76	4.96	10.38
6	6	1	5.61	4.73	12.89
6	7	1	1.65*	0.72	0.37
6	8	1	12.50	12.99	8.39
6	9	1	1.46*	0.94	0.47
6	10	1	2.89*	2.59	1.12
6	11	1	0.66*	0.33	0.06
6	12	1	1.35*	1.58	0.32
6	13	1	1.70*	0.57	0.35
6	14	1	5.42	5.67	8.42
6	15	1	4.82	4.67	6.92
6	16	1	2.25*	2.49	0.51
6	16	0	5.56	5.38	8.63
6	15	0	2.89*	0.79	1.35
6	14	0	1.41*	2.92	0.19
6	13	0	5.14	4.72	9.96
6	12	0	3.59	3.68	7.11
6	11	0	5.62	5.99	11.63
6	10	0	4.46	4.94	9.26
6	9	0	1.39*	1.35	0.32
6	8	0	5.89	6.18	11.53
6	7	0	9.91	10.31	11.09
6	6	0	18.40	18.24	4.25
6	5	0	11.62	12.25	9.80
6	4	0	12.99	13.94	7.46
6	3	0	6.10	6.40	12.23
6	2	0	2.08*	1.70	3.01
6	1	0	1.24*	0.72	0.22
6	0	0	2.78*	2.25	1.12
7	0	0	1.77*	3.20	0.32
7	1	0	13.30	14.14	6.99
7	2	0	2.31*	3.51	0.66
7	3	0	14.58	15.13	6.57
7	4	0	9.12	9.79	10.52
7	5	0	8.83	9.04	11.63
7	6	0	6.23	6.17	11.49
7	7	0	1.64*	1.45	0.37
7	8	0	13.60	13.89	6.71
7	9	0	3.68	2.50	7.33
7	10	0	2.57*	1.91	0.75
7	11	0	2.71*	1.32	0.88
7	12	0	4.56	4.13	8.61
7	13	0	1.80*	0.70	0.31
7	14	0	4.77	4.24	7.33
7	13	1	3.05*	0.89	1.01
7	12	1	3.24*	1.50	1.05
7	11	1	3.77	2.97	7.05
7	10	1	1.66*	1.88	0.36
7	9	1	5.35	5.46	8.65
7	8	1	0.95*	3.14	0.11
7	7	1	3.91	4.38	6.78
7	6	1	4.41	4.94	7.98
7	5	1	3.34*	2.83	1.31
7	4	1	4.22	4.83	7.64
7	3	1	3.94	3.40	6.95
7	2	1	1.98*	2.76	0.36
7	1	1	19.96	20.94	3.60
7	0	2	7.37	7.36	11.52
7	1	2	7.07	6.59	11.05
7	2	2	5.11	5.60	8.36
7	3	2	3.62	4.40	5.56
7	4	2	9.24	9.01	11.42
7	5	2	5.51	5.07	10.22
7	6	2	5.87	5.78	10.35
7	7	2	1.90*	0.29	0.59
7	8	2	9.55	8.87	10.31
7	9	2	2.69*	0.09	1.03
7	10	2	5.11	5.26	7.55
7	11	2	3.14*	2.43	1.01
7	12	2	1.86*	1.81	0.29
7	13	2	2.01*	3.15	0.25
7	12	3	1.98*	1.58	0.37
7	11	3	1.80*	1.30	0.43
7	10	3	5.44	5.20	8.73
7	9	3	1.81*	0.71	0.31
7	8	3	3.51	2.72	6.19
7	7	3	2.28*	1.39	0.90
7	6	3	1.72*	1.89	0.34
7	5	3	1.77*	3.33	0.38
7	4	3	3.39*	4.58	1.08
7	3	3	3.02*	2.62	1.31
7	2	3	10.21	10.21	10.51
7	1	3	8.09	8.45	11.31
7	0	4	11.28	11.63	9.24
7	1	4	5.03	4.98	9.56
7	2	4	3.81	3.88	6.82
7	3	4	1.08*	0.87	0.86
7	4	4	2.36*	2.42	0.59
7	5	4	1.74*	0.27	0.33
7	6	4	1.72*	0.53	0.34
7	7	4	2.35*	2.60	3.27
7	8	4	1.89*	2.91	0.33
7	9	4	5.46	5.40	7.88
7	10	4	4.99	5.17	7.28
7	11	4	2.80*	0.26	1.06
7	10	5	1.31*	0.36	0.19
7	9	5	3.32*	2.90	1.04
7	8	5	1.79*	0.74	0.46
7	7	5	1.25*	0.68	0.23
7	6	5	2.02*	0.62	0.48
7	5	5	1.73*	1.78	0.34
7	4	5	3.43*	3.58	1.11
7	3	5	2.51*	2.68	3.92
7	2	5	4.55	4.59	8.95
7	1	5	1.76*	0.09	0.32
7	0	6	8.24	8.35	9.34
7	1	6	2.47*	4.46	0.46
7	2	6	1.05*	1.32	0.65
7	3	6	2.59*	1.74	0.90
7	4	6	4.73	4.17	7.73
7	5	6	3.64	3.14	5.88
7	6	6	1.67*	0.04	0.36
7	7	6	1.29*	0.57	0.18
7	8	6	1.81*	0.11	0.31
7	5	7	2.37*	1.18	0.56
7	4	7	2.68*	3.69	0.44
7	3	7	3.14*	1.10	0.96
7	2	7	4.14	3.82	6.74
7	1	7	4.80	5.57	7.63
8	1	5	2.48*	2.12	0.51
8	2	5	2.12*	1.30	0.36
8	3	5	3.53*	5.03	0.65
8	6	4	1.99*	1.97	0.32
8	5	4	2.47*	1.61	0.56
8	4	4	3.54*	3.28	1.00
8	3	4	1.20*	0.50	0.69
8	2	4	2.77*	2.38	3.07
8	1	4	3.01*	2.90	0.90
8	0	4	2.00*	3.22	0.25
8	1	3	6.70	6.84	8.80
8	2	3	7.27	7.57	8.76
8	3	3	1.79*	1.67	0.31
8	4	3	3.82*	5.02	1.01
8	5	3	3.37	3.74	4.64
8	6	3	2.43*	1.89	0.53
8	7	3	2.68*	2.84	0.69
8	8	3	5.50	5.73	6.91
8	9	2	1.29*	1.53	0.16
8	8	2	1.69*	2.21	0.28
8	7	2	1.26*	0.47	0.17
8	6	2	2.79*	1.52	0.76
8	5	2	1.75*	2.62	0.26
8	4	2	3.39*	1.73	1.14
8	3	2	1.81*	1.52	0.30

h	k	l	Fo	Fc	weight
8	2	2	2.71*	2.25	0.58
8	1	2	6.49	6.64	8.87
8	0	2	12.61	12.36	7.65
8	1	1	4.52	3.52	7.10
8	2	1	9.15	8.89	9.71
8	3	1	4.37	3.75	6.68
8	4	1	1.96*	0.19	0.39
8	5	1	2.21*	3.96	0.40
8	6	1	1.96*	0.44	0.26
8	7	1	4.76	5.07	6.71
8	8	1	1.88*	0.83	0.28
8	9	1	3.37*	2.32	0.90
8	10	1	1.87*	2.69	0.28
8	11	0	1.06*	0.48	0.09
8	10	0	1.95*	1.24	0.39
8	9	0	6.32	6.34	8.22
8	8	0	2.15*	2.11	0.51
8	7	0	5.07	5.10	7.97
8	6	0	3.34*	0.80	1.32
8	5	0	3.16*	2.18	0.95
8	4	0	7.43	7.85	10.06
8	3	0	2.96*	3.01	0.72
8	2	0	5.63	5.56	8.48
8	1	0	11.37	10.87	8.18
8	0	0	18.40	18.66	3.92
9	0	0	4.90	4.61	5.78
9	1	0	2.00*	0.63	0.25
9	2	0	4.90	4.40	6.13
9	3	0	2.66*	2.19	0.47
9	4	0	1.66*	2.78	0.17
9	5	0	1.96*	0.85	0.26
9	6	0	1.97*	0.64	0.26
9	4	1	7.11	6.58	8.22
9	3	1	2.01*	2.27	0.25
9	2	1	1.49*	2.73	0.16
9	1	1	1.49*	1.75	0.15

3516 reflections

6,7-dimethyl-4aβ,5,8,8aβ-tetrahydronaphthoquin-1α,4α-diol

h	k	l	Fo	Fc	weight
0	0	-8	6.25*	4.44	0.23
0	0	-6	2.87*	1.74	0.12
0	0	-4	80.83	77.44	0.34
0	0	-2	66.08	65.74	0.53
1	0	-8	3.29*	1.42	0.09
1	0	-6	22.59	22.31	8.49
1	0	-4	12.71	12.72	15.44
1	0	-2	11.78	11.70	24.53
1	0	0	20.77	21.62	3.89
1	0	2	44.01	45.37	1.03
1	0	4	51.64	51.62	0.71
1	0	6	10.81	10.96	5.63
1	0	8	3.61*	0.56	0.08
2	0	-8	30.90	30.85	3.06
2	0	-6	3.22*	5.03	0.21
2	0	-4	32.21	32.43	2.07
2	0	-2	4.59*	2.13	0.58
2	0	0	92.50	100.77	0.02
2	0	2	87.17	88.78	0.31
2	0	4	134.81	129.64	0.13
2	0	6	12.04	11.98	6.02
2	0	8	10.52	11.65	3.38
3	0	-8	21.94	22.43	7.67
3	0	-6	11.84	12.89	9.01
3	0	-4	17.62	17.30	14.05
3	0	-2	22.25	22.49	5.57
3	0	0	2.58*	2.15	0.15
3	0	2	19.06	19.17	7.05
3	0	4	28.14	27.10	3.11
3	0	6	11.46	12.56	5.27
3	0	8	14.62	15.53	4.68
4	0	-8	22.93	22.80	6.12
4	0	-6	18.20	17.65	10.36
4	0	-4	53.41	49.16	0.68
4	0	-2	57.99	57.93	0.64
4	0	0	72.12	76.40	0.44
4	0	2	4.62	4.56	4.25
4	0	4	4.43*	1.51	0.29
4	0	6	6.97*	6.51	0.29
4	0	8	7.51*	12.08	0.15
5	0	-8	18.51	18.79	7.91
5	0	-6	2.96*	4.46	0.11
5	0	-4	21.82	20.81	6.74
5	0	-2	56.94	55.15	0.65
5	0	0	46.93	46.97	0.88
5	0	2	42.35	41.57	0.91
5	0	4	1.90*	5.43	0.03
5	0	6	3.53*	0.56	0.11
6	0	-8	3.27*	0.61	0.09
6	0	-6	12.17	12.13	8.77
6	0	-4	11.98	11.71	13.04
6	0	-2	14.31	14.53	16.13
6	0	0	113.64	114.23	0.18
6	0	2	28.05	26.94	3.29
6	0	4	43.71	44.08	1.09
6	0	6	2.32*	1.21	0.07
7	0	-8	4.80*	4.10	0.19
7	0	-6	5.04*	3.12	0.26
7	0	-4	9.95	10.42	10.26
7	0	-2	18.36	18.68	9.95
7	0	0	11.54	10.70	12.20
7	0	2	2.60*	1.89	0.08
7	0	4	48.07	48.65	0.95
7	0	6	3.71*	3.72	0.07
8	0	-8	21.35	20.59	7.19
8	0	-6	6.49	5.68	3.83
8	0	-4	6.34*	9.36	0.35
8	0	-2	36.55	36.58	1.55
8	0	0	3.57*	6.81	0.16
8	0	2	3.82*	1.93	0.17
8	0	4	31.02	31.03	3.81
8	0	6	2.50*	2.34	0.03
9	0	-8	4.07*	4.60	0.10
9	0	-6	2.87*	2.55	0.07
9	0	-4	40.60	41.06	1.26
9	0	-2	58.80	57.58	0.54
9	0	0	15.64	15.60	9.99
9	0	2	28.15	28.46	4.21
9	0	4	8.83	8.95	3.37
10	0	-8	8.46	8.10	3.08
10	0	-6	3.45*	0.73	0.14
10	0	-4	12.72	13.14	7.41
10	0	-2	5.56	5.83	2.89
10	0	0	19.29	18.88	8.93
10	0	2	5.60	7.33	1.86
10	0	4	1.72*	4.70	0.01
11	0	-8	14.82	14.75	5.50
11	0	-6	5.06*	2.58	0.21
11	0	-4	25.20	24.35	4.73
11	0	-2	3.52*	5.05	0.91
11	0	0	32.07	34.39	2.55
11	0	2	24.17	24.76	7.21
11	0	4	3.76*	2.44	0.07
12	0	-8	3.78*	5.71	0.07
12	0	-6	2.35*	2.99	0.03
12	0	-4	24.96	24.47	5.35
12	0	-2	3.45*	5.01	0.08
12	0	0	16.66	16.36	6.44
12	0	2	4.22*	2.78	0.13
13	0	-6	14.93	14.98	5.08
13	0	-4	4.06*	1.29	0.13
13	0	-2	5.71*	8.74	0.15
13	0	0	6.36*	6.10	0.31
14	0	-6	15.24	14.86	5.03
14	0	-4	6.01*	0.54	0.29
14	0	-2	15.16	14.87	5.85
14	0	0	5.93*	1.88	0.23
0	1	-8	3.57*	1.56	0.08
0	1	-8	12.78	12.80	5.54
0	1	-7	3.64*	0.88	0.13
0	1	-6	32.68	30.85	2.58
0	1	-5	11.65	11.53	12.65
0	1	-4	93.80	89.27	0.26
0	1	-3	9.01	8.95	12.85
0	1	-2	29.34	30.90	1.92
0	1	-1	111.32	118.10	0.01
1	1	-9	5.45*	2.51	0.26
1	1	-8	6.75*	6.99	0.28
1	1	-7	6.87	6.04	3.74
1	1	-6	13.72	14.21	9.72
1	1	-5	2.64*	1.69	0.14
1	1	-4	38.09	38.71	1.13
1	1	-3	27.85	27.29	2.65
1	1	-2	7.29	7.60	12.58
1	1	-1	62.92	64.39	0.60
1	1	0	22.62	23.49	3.40
1	1	1	5.15	5.65	9.40
1	1	2	6.42	6.74	6.95
1	1	3	72.23	73.58	0.43
1	1	4	6.01*	6.21	0.42
1	1	5	8.68	8.70	5.68
1	1	6	5.71*	6.70	0.19
1	1	7	3.39*	0.22	0.06
1	1	8	7.72*	5.10	0.24
1	1	9	3.97*	3.82	0.07
2	1	-9	16.26	16.40	6.19
2	1	-8	7.04*	8.58	0.26
2	1	-7	15.84	15.66	9.00
2	1	-6	3.05*	2.07	0.11
2	1	-5	16.79	17.00	10.31
2	1	-4	28.70	28.64	2.96
2	1	-3	6.52	6.27	8.18
2	1	-2	78.98	79.97	0.38
2	1	-1	17.41	17.88	8.11
2	1	0	108.14	118.36	0.01
2	1	1	41.48	44.51	1.18
2	1	2	43.60	43.02	1.02
2	1	3	38.42	36.04	1.67
2	1	4	21.53	21.12	7.15
2	1	5	3.89*	0.28	0.18
2	1	6	6.61	6.57	2.60
2	1	7	15.14	16.00	5.89
2	1	8	2.91*	4.27	0.05
3	1	-9	7.57*	8.20	0.23
3	1	-8	4.43*	0.13	0.14
3	1	-7	13.43	13.21	7.65
3	1	-6	3.22*	2.60	0.17
3	1	-5	34.02	33.98	1.72
3	1	-4	8.48	9.07	11.38
3	1	-3	24.72	25.61	3.66
3	1	-2	1.84*	1.46	0.08
3	1	-1	25.07	25.86	3.32
3	1	0	15.25	14.89	14.22
3	1	1	3.50*	1.23	0.29
3	1	2	24.70	25.80	3.57
3	1	3	2.18*	1.85	0.08
3	1	4	14.71	14.15	12.31
3	1	5	9.13	10.67	5.57
3	1	6	2.08*	6.44	0.02
3	1	7	11.06	11.81	4.83
3	1	8	3.67*	2.00	0.07
4	1	-9	7.94	7.59	2.59
4	1	-8	52.30	54.19	0.84
4	1	-7	16.55	17.31	9.38
4	1	-6	10.05	9.76	8.70
4	1	-5	23.41	21.80	4.35
4	1	-4	22.66	22.04	4.99
4	1	-3	3.11*	3.38	2.39
4	1	-2	16.36	16.44	11.87
4	1	-1	65.62	68.19	0.52
4	1	0	53.04	54.17	0.75
4	1	1	3.80*	2.20	0.33
4	1	2	13.89	12.96	15.68
4	1	3	4.03	4.65	2.47
4	1	4	4.79*	3.18	0.31
4	1	5	2.80*	2.98	0.07
4	1	6	4.81*	6.98	1.21
4	1	7	4.94*	3.47	0.15
4	1	8	3.88*	1.54	0.07
5	1	-9	3.78*	5.31	0.10
5	1	-8	17.64	18.07	7.41
5	1	-7	5.43*	3.81	0.29
5	1	-6	11.70	11.09	10.35
5	1	-5	11.90	12.10	11.97
5	1	-4	29.73	27.15	2.82
5	1	-3	100.16	88.70	0.23
5	1	-2	17.31	17.31	10.64
5	1	-1	25.40	26.11	3.58
5	1	0	2.94*	1.06	0.20
5	1	1	23.40	23.57	5.16
5	1	2	18.10	17.94	10.84
5	1	3	5.48	4.42	3.88
5	1	4	12.30	10.84	7.80
5	1	5	3.42*	0.17	0.09
5	1	6	8.12	8.92	3.55
5	1	7	3.70*	3.19	0.07
6	1	-9	20.04	18.85	6.42
6	1	-8	8.24	8.60	3.67
6	1	-7	3.14*	4.05	0.10
6	1	-6	3.05*	3.99	0.10
6	1	-5	12.83	12.80	10.81
6	1	-4	12.29	11.81	12.85
6	1	-3	20.55	20.99	6.41
6	1	-2	12.74	13.23	15.82
6	1	-1	65.66	66.10	0.49
6	1	0	44.96	44.29	0.88
6	1	1	34.15	35.39	1.75
6	1	2	5.05	5.55	3.71
6	1	3	36.71	36.73	1.86
6	1	4	17.70	18.02	9.04
6	1	5	4.04*	2.33	0.12
6	1	6	4.92*	1.53	0.14
6	1	7	6.34*	1.39	0.25
7	1	-9	7.62	8.22	2.40
7	1	-8	4.81*	1.12	0.25
7	1	-7	1.83*	1.96	0.30
7	1	-6	3.00*	1.39	0.11
7	1	-5	10.80	10.94	8.86
7	1	-4	12.27	13.10	12.48
7	1	-3	10.23	10.23	11.29
7	1	-2	12.86	12.59	13.15
7	1	-1	12.91	13.10	13.19

h	k	l	Fo	Fc	weight
7	1	0	1.17*	1.65	0.03
7	1	1	2.85*	2.42	0.12
7	1	2	11.87	11.67	9.00
7	1	3	32.22	31.73	2.87
7	1	4	3.29*	2.03	0.09
7	1	5	9.53	10.12	4.38
7	1	6	2.41*	0.16	0.04
8	1	-9	6.72*	5.76	0.26
8	1	-8	10.44	9.68	5.00
8	1	-7	8.62	8.23	4.80
8	1	-6	8.29	7.78	4.91
8	1	-5	12.09	12.03	9.24
8	1	-4	1.30*	1.86	0.02
8	1	-3	4.85*	5.11	0.33
8	1	-2	17.24	17.40	11.04
8	1	-1	20.58	19.91	8.55
8	1	0	19.12	17.88	9.89
8	1	1	19.07	18.36	11.08
8	1	2	18.23	18.02	9.77
8	1	3	22.69	22.59	7.58
8	1	4	37.57	37.60	1.84
8	1	5	7.74	7.76	2.68
8	1	6	3.54*	0.21	0.08
9	1	-9	2.49*	5.24	0.03
9	1	-8	3.77*	7.47	0.07
9	1	-7	3.38*	0.64	0.09
9	1	-6	4.47*	8.31	0.13
9	1	-5	13.50	13.61	8.13
9	1	-4	5.23	3.66	3.09
9	1	-3	22.76	22.42	6.09
9	1	-2	5.96	5.83	3.58
9	1	-1	3.97*	3.64	0.22
9	1	0	2.92*	0.62	0.12
9	1	1	5.44*	2.40	0.27
9	1	2	31.38	31.06	3.69
9	1	3	3.10*	2.16	0.06
9	1	4	7.14*	6.75	0.31
9	1	5	1.74*	7.79	0.01
10	1	-9	3.33*	0.32	0.09
10	1	-8	22.97	23.47	6.66
10	1	-7	3.47*	2.83	0.75
10	1	-6	9.53	9.48	5.09
10	1	-5	6.28*	6.59	0.39
10	1	-4	24.85	25.38	4.72
10	1	-3	18.42	17.84	9.76
10	1	-2	11.06	11.47	7.33
10	1	-1	6.14*	7.06	0.33
10	1	0	3.16*	1.88	0.10
10	1	1	19.62	19.43	7.88
10	1	2	5.93	5.77	2.30
10	1	3	14.50	14.11	6.06
10	1	4	6.65*	4.25	0.23
11	1	-8	4.28*	2.63	0.09
11	1	-7	3.39*	2.16	0.09
11	1	-6	3.49*	1.56	0.08
11	1	-5	3.33*	2.79	0.09
11	1	-4	24.72	24.34	5.89
11	1	-3	26.15	26.32	4.24
11	1	-2	5.74*	5.00	0.31
11	1	-1	3.66*	1.12	0.14
11	1	0	11.71	11.86	5.16
11	1	1	21.26	21.75	7.20
11	1	2	3.69*	4.00	0.07
11	1	3	3.83*	0.35	0.10
11	1	4	2.54*	2.35	0.03
12	1	-8	1.80*	4.83	0.02
12	1	-7	3.81*	1.34	0.07
12	1	-6	15.34	15.16	6.10
12	1	-5	13.61	13.54	5.93
12	1	-4	15.61	15.88	7.45
12	1	-3	6.82*	5.64	0.34
12	1	-2	3.34*	3.62	0.09
12	1	-1	3.54*	4.20	0.10
12	1	0	12.20	13.44	4.85
12	1	1	3.66*	1.38	0.07
12	1	2	4.88*	0.28	0.17
12	1	3	3.85*	4.00	0.61
13	1	-7	5.35*	5.48	0.11
13	1	-6	14.43	14.06	4.95
13	1	-5	3.56*	0.75	0.08
13	1	-4	10.68	10.43	4.30
13	1	-3	3.24*	0.07	0.10
13	1	-2	3.53*	0.79	0.08
13	1	-1	3.73*	5.53	0.09
13	1	0	14.35	14.43	5.59
13	1	1	2.48*	5.37	0.04
14	1	-6	1.80*	5.41	0.02
14	1	-5	3.94*	5.51	0.07
14	1	-4	4.26*	6.06	0.09
14	1	-3	4.23*	1.18	0.17
14	1	-2	7.76*	9.96	0.22
14	1	-1	3.57*	0.65	0.08
14	1	0	5.66*	2.77	0.24
0	2	-9	3.57*	2.71	0.08
0	2	-8	5.85*	0.20	0.27
0	2	-7	18.41	17.58	9.13
0	2	-6	1.36*	0.62	0.02
0	2	-5	40.82	37.93	1.38
0	2	-4	9.62	9.24	11.65
0	2	-3	15.05	14.93	16.88
0	2	-2	1.37*	3.48	0.04
0	2	-1	17.79	18.40	8.48
0	2	0	63.01	65.55	0.60
1	2	-9	3.48*	2.29	0.08
1	2	-8	3.52*	3.46	0.08
1	2	-7	6.05*	5.79	0.31
1	2	-6	25.86	25.37	4.08
1	2	-5	18.92	18.52	13.29
1	2	-4	6.24	6.47	7.24
1	2	-3	15.25	15.18	13.25
1	2	-2	2.50*	1.75	0.16
1	2	-1	70.61	72.68	0.48
1	2	0	69.26	73.91	0.50
1	2	1	1.19*	3.76	0.05
1	2	2	30.52	31.00	2.44
1	2	3	21.05	20.92	7.32
1	2	4	30.05	30.22	2.63
1	2	5	3.04*	0.18	0.11
1	2	6	1.39*	2.15	0.01
1	2	7	5.89*	5.51	0.17
1	2	8	2.34*	3.58	0.03
1	2	9	5.83	4.97	1.15
2	2	-9	3.65*	0.48	0.07
2	2	-8	6.52*	7.59	0.27
2	2	-7	2.52*	1.91	0.05
2	2	-6	9.75	9.79	7.84
2	2	-5	15.14	15.49	14.39
2	2	-4	25.53	25.61	4.08
2	2	-3	2.46*	1.59	0.17
2	2	-2	10.91	10.64	18.91
2	2	-1	149.32	159.26	0.01
2	2	0	8.93	9.08	19.67
2	2	1	13.12	13.66	21.99
2	2	2	21.21	21.46	6.09
2	2	3	39.81	38.25	1.06
2	2	4	36.36	35.27	1.61
2	2	5	3.25*	1.95	0.09
2	2	6	14.59	14.00	7.57
2	2	7	10.47	11.81	3.98
2	2	8	11.52	10.86	4.08
3	2	-9	3.29*	4.00	0.54
3	2	-8	4.44*	8.39	0.09
3	2	-7	6.16	7.28	2.57
3	2	-6	6.45	7.90	4.03
3	2	-5	11.78	12.01	13.15
3	2	-4	19.84	19.91	7.82
3	2	-3	28.44	28.52	2.43
3	2	-2	43.70	45.22	1.04
3	2	-1	61.52	63.58	0.60
3	2	0	11.58	11.54	17.90
3	2	1	3.26*	2.88	0.22
3	2	2	29.90	28.61	2.31
3	2	3	18.91	17.85	11.23
3	2	4	13.50	12.49	11.66
3	2	5	3.24*	2.58	0.10
3	2	6	12.80	12.45	6.09
3	2	7	3.70*	1.07	0.07
3	2	8	3.89*	2.96	0.07
4	2	-9	36.01	36.55	2.44
4	2	-8	9.83	10.46	4.12
4	2	-7	17.06	17.94	8.90
4	2	-6	1.33*	5.39	0.02
4	2	-5	2.76*	1.50	0.13
4	2	-4	18.87	17.34	7.92
4	2	-3	2.44*	4.00	0.15
4	2	-2	63.09	66.64	0.55
4	2	-1	44.76	45.19	0.98
4	2	0	15.75	16.05	14.72
4	2	1	2.63*	1.78	0.14
4	2	2	15.77	15.49	16.46
4	2	3	21.61	20.91	7.62
4	2	4	8.91	10.11	6.00
4	2	5	6.45*	6.63	0.34
4	2	6	3.55*	1.05	0.08
4	2	7	7.57*	4.71	0.25
4	2	8	4.01*	0.61	0.06
5	2	-9	15.03	15.00	5.50
5	2	-8	6.68*	7.72	0.25
5	2	-7	31.44	31.15	2.87
5	2	-6	2.33*	0.46	0.10
5	2	-5	1.24*	0.21	0.03
5	2	-4	26.37	25.18	3.70
5	2	-3	38.24	37.13	1.67
5	2	-2	17.06	17.86	9.66
5	2	-1	10.07	10.52	13.92
5	2	0	41.07	42.40	1.05
5	2	1	10.07	10.07	12.66
5	2	2	12.43	12.14	11.78
5	2	3	3.06*	1.97	0.11
5	2	4	5.25*	6.34	0.23
5	2	5	24.88	24.91	5.41
5	2	6	2.74*	0.30	0.05
5	2	7	5.39*	9.20	0.12
6	2	-9	12.76	12.25	4.83
6	2	-8	4.20*	4.69	0.11
6	2	-7	17.27	17.49	8.87
6	2	-6	5.14*	5.30	0.34
6	2	-5	57.40	57.70	0.57
6	2	-4	10.72	10.84	11.66
6	2	-3	5.90	4.03	5.57
6	2	-2	2.63*	1.56	0.17
6	2	-1	23.06	22.79	4.42
6	2	0	2.65*	1.82	0.14
6	2	1	5.10	4.43	4.41
6	2	2	22.23	22.12	8.34
6	2	3	16.84	16.46	11.15
6	2	4	10.94	11.31	5.54
6	2	5	3.36*	0.81	0.09
6	2	6	4.82*	5.70	1.21
6	2	7	3.94*	2.11	0.08
7	2	-9	7.29*	7.58	0.27
7	2	-8	5.57*	6.59	0.22
7	2	-7	3.98*	0.13	0.17
7	2	-6	3.72*	7.08	0.11
7	2	-5	22.89	22.42	6.39
7	2	-4	11.20	11.59	10.69
7	2	-3	24.71	23.10	5.85
7	2	-2	16.68	16.55	10.40
7	2	-1	57.99	57.24	0.58
7	2	0	12.30	11.96	12.89
7	2	1	14.10	14.22	13.05
7	2	2	19.60	19.17	7.45
7	2	3	11.11	11.29	6.75
7	2	4	16.21	16.37	8.27
7	2	5	8.58	8.16	3.70
7	2	6	3.82*	0.79	0.13
8	2	-8	2.46*	2.21	0.05
8	2	-8	3.25*	1.49	0.09
8	2	-7	13.93	13.49	7.32
8	2	-6	15.64	16.69	8.59
8	2	-5	15.31	15.21	10.48
8	2	-4	0.97*	0.40	0.14

h	k	l	Fo	Fc	weight
8	2	-3	17.50	16.86	12.85
8	2	-2	41.73	40.95	1.33
8	2	-1	31.90	28.21	2.29
8	2	0	8.01	7.60	6.33
8	2	1	1.33*	1.80	0.03
8	2	2	17.52	18.15	9.50
8	2	3	44.98	45.30	1.02
8	2	4	20.01	19.39	8.01
8	2	5	3.52*	3.64	0.08
8	2	6	3.88*	4.33	0.07
9	2	-9	11.07	10.18	4.22
9	2	-8	6.02*	1.97	0.30
9	2	-7	4.85	4.08	1.62
9	2	-6	5.60*	0.09	0.34
9	2	-5	5.03	5.12	2.09
9	2	-4	8.23	7.64	5.67
9	2	-3	11.17	10.80	8.40
9	2	-2	29.33	28.88	2.85
9	2	-1	8.75	8.71	6.61
9	2	0	11.41	11.41	8.19
9	2	1	27.09	26.94	3.55
9	2	2	3.39*	3.94	0.09
9	2	3	38.12	38.93	1.83
9	2	4	3.68*	1.45	0.07
9	2	5	8.08	8.66	2.72
10	2	-9	16.76	16.88	5.02
10	2	-8	20.36	20.48	6.35
10	2	-7	3.25*	2.52	0.09
10	2	-6	5.14*	5.86	0.28
10	2	-5	6.31*	8.07	0.32
10	2	-4	3.53*	8.66	0.09
10	2	-3	27.53	26.96	3.59
10	2	-2	13.10	12.82	8.22
10	2	-1	11.29	11.20	6.92
10	2	0	3.55*	2.64	0.11
10	2	1	4.96*	3.60	0.28
10	2	2	3.44*	3.58	0.08
10	2	3	21.44	21.99	6.77
10	2	4	5.45	4.71	1.28
11	2	-8	2.48*	3.22	0.03
11	2	-7	5.80*	2.50	0.32
11	2	-6	3.35*	3.25	0.09
11	2	-5	9.78	10.21	4.79
11	2	-4	14.16	13.16	7.20
11	2	-3	9.93	10.21	4.58
11	2	-2	2.10*	3.12	0.04
11	2	-1	3.35*	3.77	0.09
11	2	0	3.40*	1.62	0.09
11	2	1	10.38	10.53	4.55
11	2	2	11.39	11.42	4.64
11	2	3	4.21*	0.05	1.07
11	2	4	1.80*	0.73	0.02
12	2	-8	1.80*	1.28	0.02
12	2	-7	3.87*	3.46	0.10
12	2	-6	13.32	13.14	5.06
12	2	-5	24.40	24.28	7.57
12	2	-4	11.33	11.70	5.28
12	2	-3	5.66*	6.03	0.22
12	2	-2	4.97*	0.20	0.31
12	2	-1	3.35*	2.42	0.09
12	2	0	11.75	11.36	4.71
12	2	1	11.57	12.20	4.42
12	2	2	3.74*	1.60	0.07
12	2	3	5.41*	2.34	0.15
13	2	-7	3.78*	2.92	0.07
13	2	-6	11.51	11.97	4.20
13	2	-5	4.48*	5.74	0.10
13	2	-4	5.26*	7.22	0.18
13	2	-3	2.86*	5.49	0.06
13	2	-2	3.28*	1.06	0.09
13	2	-1	3.65*	0.24	0.08
13	2	0	3.82*	7.01	0.06
13	2	1	16.08	14.92	5.81
14	2	-6	3.12*	0.39	0.07
14	2	-5	5.58*	1.68	0.25
14	2	-4	4.27*	3.79	0.09
14	2	-3	3.40*	3.79	0.09
14	2	-2	4.60*	2.81	0.13
14	2	-1	5.92	5.90	1.41
14	2	0	1.80*	0.36	0.02
0	3	-9	3.52*	4.23	0.08
0	3	-8	11.89	11.99	4.80
0	3	-7	3.19*	2.95	0.10
0	3	-6	3.37*	0.50	0.15
0	3	-5	3.05*	5.17	0.11
0	3	-4	21.11	19.76	8.33
0	3	-3	22.68	22.80	5.64
0	3	-2	18.58	18.05	9.31
0	3	-1	65.10	67.44	0.55
1	3	-9	2.46*	2.46	0.04
1	3	-8	5.33*	6.79	0.19
1	3	-7	5.33*	0.85	0.28
1	3	-6	42.90	44.16	1.16
1	3	-5	5.04*	4.54	0.48
1	3	-4	3.28*	3.08	0.26
1	3	-3	17.27	17.07	12.54
1	3	-2	64.86	65.41	0.54
1	3	-1	23.75	24.63	3.65
1	3	0	22.20	22.62	5.36
1	3	1	6.29	5.17	8.88
1	3	2	2.70*	2.16	0.14
1	3	3	31.07	30.88	2.16
1	3	4	23.73	24.23	4.99
1	3	5	19.55	19.04	11.44
1	3	6	1.40*	1.38	0.01
1	3	7	4.21*	5.25	0.82
1	3	8	11.15	11.19	3.46
1	3	9	5.06*	1.55	0.15
2	3	-9	5.62	6.10	1.32
2	3	-8	1.96*	0.83	0.26
2	3	-7	51.59	51.60	0.60
2	3	-6	3.28*	2.65	0.13
2	3	-5	9.76	9.38	9.83
2	3	-4	13.99	14.10	15.81
2	3	-3	6.50	6.85	7.64
2	3	-2	117.87	122.63	0.17
2	3	-1	53.74	56.06	0.76
2	3	0	126.00	135.58	0.01
2	3	1	38.43	39.14	1.26
2	3	2	19.28	18.75	7.08
2	3	3	117.00	115.32	0.17
2	3	4	7.19	7.08	5.39
2	3	5	5.43*	2.40	0.35
2	3	6	4.08*	3.82	0.12
2	3	7	4.71*	1.93	0.16
2	3	8	11.46	11.86	3.83
3	3	-9	5.40*	2.87	0.16
3	3	-8	7.71	7.72	3.33
3	3	-7	4.61*	1.77	0.19
3	3	-6	5.17*	1.68	0.59
3	3	-5	20.47	19.42	9.86
3	3	-4	8.58	8.40	10.70
3	3	-3	6.10	5.59	7.04
3	3	-2	85.46	84.10	0.32
3	3	-1	11.34	11.27	17.55
3	3	0	13.52	13.60	19.72
3	3	1	13.41	13.53	18.84
3	3	2	66.92	67.77	0.48
3	3	3	19.46	18.69	9.78
3	3	4	14.97	14.56	10.74
3	3	5	4.32*	2.82	0.18
3	3	6	2.98*	3.32	0.05
3	3	7	3.62*	0.14	0.08
3	3	8	5.22*	1.58	0.15
4	3	-9	4.37*	4.54	1.09
4	3	-8	5.47*	7.57	0.19
4	3	-7	4.84*	4.13	0.25
4	3	-6	15.21	15.29	10.22
4	3	-5	2.75*	0.91	0.17
4	3	-4	17.35	17.44	9.67
4	3	-3	26.89	27.05	3.15
4	3	-2	32.16	33.48	2.20
4	3	-1	3.03*	2.87	0.22
4	3	0	40.60	43.92	1.10
4	3	1	24.98	25.18	4.46
4	3	2	59.18	59.46	0.58
4	3	3	7.72	8.41	6.69
4	3	4	5.98*	6.58	0.36
4	3	5	3.48*	1.66	0.11
4	3	6	8.44	9.13	3.38
4	3	7	6.43*	4.64	0.34
4	3	8	5.05*	0.82	0.14
5	3	-9	11.03	10.84	4.23
5	3	-8	7.75	7.41	3.61
5	3	-7	2.80*	2.95	0.13
5	3	-6	2.78*	1.27	0.13
5	3	-5	24.98	24.20	4.85
5	3	-4	14.89	14.86	13.16
5	3	-3	26.19	25.78	4.01
5	3	-2	3.38*	2.72	0.28
5	3	-1	11.68	11.39	16.74
5	3	0	16.73	16.65	11.36
5	3	1	3.39*	3.80	2.13
5	3	2	33.26	31.71	2.35
5	3	3	11.67	12.06	8.95
5	3	4	7.91	7.91	4.20
5	3	5	3.51*	0.15	0.08
5	3	6	16.31	18.31	6.77
5	3	7	3.62*	1.24	0.08
6	3	-9	21.30	21.60	6.31
6	3	-8	10.19	8.91	5.31
6	3	-7	3.35*	2.38	0.09
6	3	-6	16.01	15.92	9.89
6	3	-5	2.65*	0.37	0.14
6	3	-4	15.35	14.46	13.88
6	3	-3	12.08	11.01	13.65
6	3	-2	1.10*	0.49	0.03
6	3	-1	5.54	5.96	6.04
6	3	0	9.18	8.47	11.45
6	3	1	4.37*	4.71	0.42
6	3	2	7.63	7.63	5.65
6	3	3	13.27	12.96	9.51
6	3	4	10.15	10.47	5.70
6	3	5	17.49	17.29	7.69
6	3	6	5.73*	2.59	0.22
6	3	7	3.92*	0.59	0.07
7	3	-9	10.47	9.54	4.11
7	3	-8	5.12*	1.32	0.20
7	3	-7	5.25*	0.70	0.25
7	3	-6	1.95*	2.76	0.39
7	3	-5	15.71	15.73	11.43
7	3	-4	10.75	10.89	9.21
7	3	-3	2.95*	3.68	0.21
7	3	-2	8.44	8.38	8.83
7	3	-1	16.27	16.38	13.80
7	3	0	2.94*	7.49	0.09
7	3	1	15.75	15.29	11.77
7	3	2	11.30	10.90	7.93
7	3	3	27.43	27.29	4.59
7	3	4	20.41	19.97	8.57
7	3	5	11.93	11.66	5.09
7	3	6	3.62*	1.81	0.08
8	3	-9	6.06*	1.57	0.29
8	3	-8	3.67*	2.28	0.07
8	3	-7	12.87	12.66	6.23
8	3	-6	9.00	8.92	5.03
8	3	-5	2.39*	1.08	0.07
8	3	-4	3.65*	5.00	1.53
8	3	-3	13.06	13.20	9.96
8	3	-2	5.02*	5.67	0.43
8	3	-1	19.78	19.23	9.15
8	3	0	4.46*	4.15	0.44
8	3	1	3.13*	0.12	0.10
8	3	2	14.45	14.65	8.42
8	3	3	33.31	33.18	2.56
8	3	4	8.71	9.22	3.35
8	3	5	3.36*	2.12	0.07
8	3	6	6.18*	1.90	0.25
9	3	-9	3.97*	4.74	0.10
9	3	-8	6.05*	5.58	0.18
9	3	-7	6.94	7.98	2.81
9	3	-6	11.23	11.22	6.12

h	k	l	Fo	Fc	weight
9	3	-5	6.01	6.09	2.81
9	3	-4	19.00	18.74	10.15
9	3	-3	26.29	25.35	4.07
9	3	-2	7.00	7.26	5.33
9	3	-1	4.46*	2.68	0.23
9	3	0	11.05	11.88	8.22
9	3	1	19.05	18.49	8.83
9	3	2	10.95	10.55	5.15
9	3	3	5.19*	4.47	0.17
9	3	4	3.65*	3.54	0.07
9	3	5	2.33*	0.43	0.30
10	3	-8	3.53*	5.56	0.58
10	3	-7	8.62	8.98	3.56
10	3	-6	4.41*	3.16	0.18
10	3	-5	9.94	9.82	5.17
10	3	-4	13.56	12.97	8.22
10	3	-3	12.97	13.03	8.01
10	3	-2	5.49*	3.81	0.34
10	3	-1	8.36	8.22	5.20
10	3	0	10.50	10.46	6.13
10	3	1	15.71	16.40	7.59
10	3	2	3.32*	1.87	0.09
10	3	3	15.28	15.55	5.87
10	3	4	3.87*	0.47	0.11
11	3	-8	3.95*	5.53	0.06
11	3	-7	7.14*	4.73	0.26
11	3	-6	6.05*	6.67	0.29
11	3	-5	17.81	17.51	7.63
11	3	-4	13.47	13.40	6.75
11	3	-3	10.02	9.65	5.20
11	3	-2	4.74*	5.81	0.19
11	3	-1	5.02*	0.65	0.23
11	3	0	5.30	6.34	1.73
11	3	1	3.18*	0.29	0.06
11	3	2	5.23*	3.95	0.19
11	3	3	1.73*	0.41	0.02
12	3	-7	5.50*	2.98	0.17
12	3	-6	9.68	9.98	3.78
12	3	-5	18.65	18.98	6.69
12	3	-4	5.54*	5.44	0.20
12	3	-3	3.58*	2.36	0.08
12	3	-2	6.71	6.80	2.80
12	3	-1	7.13	7.07	2.97
12	3	0	16.72	16.71	6.44
12	3	1	6.28*	5.16	0.28
12	3	2	3.75*	3.43	0.07
13	3	-7	3.58*	1.82	0.08
13	3	-6	3.49*	2.64	0.08
13	3	-5	6.13*	7.77	0.18
13	3	-4	6.03*	1.77	0.28
13	3	-3	4.40*	6.55	0.12
13	3	-2	5.26*	3.93	0.18
13	3	-1	3.76*	0.25	0.11
13	3	0	17.77	17.77	5.60
13	3	1	3.50*	3.14	0.08
14	3	-5	6.53	8.48	1.92
14	3	-4	3.60*	1.25	0.08
14	3	-3	4.27*	1.74	0.15
14	3	-2	14.72	14.12	5.67
14	3	-1	8.96	9.79	2.74
0	4	-9	3.56*	1.83	0.08
0	4	-8	5.93*	5.13	0.18
0	4	-7	13.31	13.85	6.52
0	4	-6	23.02	22.63	9.10
0	4	-5	34.45	34.77	1.60
0	4	-4	14.83	14.68	15.36
0	4	-3	39.15	39.96	1.11
0	4	-2	22.63	22.48	5.14
0	4	-1	14.90	15.14	19.42
0	4	0	200.39	217.41	0.00
1	4	-9	5.53*	6.70	0.19
1	4	-8	3.28*	1.10	0.09
1	4	-7	6.76	6.68	2.95
1	4	-6	26.45	26.86	4.52
1	4	-5	2.16*	3.25	0.07
1	4	-4	2.68*	4.09	0.14
1	4	-3	68.95	68.31	0.46
1	4	-2	49.90	48.89	0.83
1	4	-1	56.17	58.98	0.70
1	4	0	15.83	16.21	15.34
1	4	1	9.73	10.15	13.28
1	4	2	3.46*	1.02	0.29
1	4	3	2.57*	1.21	0.15
1	4	4	8.27	7.07	7.45
1	4	5	20.36	20.25	7.06
1	4	6	3.68*	2.92	0.07
1	4	7	6.17	5.78	1.85
1	4	8	3.97*	5.16	0.06
1	4	9	11.84	11.02	3.29
2	4	-9	1.73*	3.21	0.02
2	4	-8	20.55	20.48	8.03
2	4	-7	5.13*	2.72	0.24
2	4	-6	27.81	27.47	3.29
2	4	-5	2.76*	5.63	0.10
2	4	-4	12.54	12.50	14.78
2	4	-3	38.74	36.83	1.14
2	4	-2	19.80	19.78	7.65
2	4	-1	172.47	182.16	0.00
2	4	0	47.96	50.70	0.80
2	4	1	48.66	49.45	0.86
2	4	2	11.55	12.22	15.30
2	4	3	25.63	25.60	3.66
2	4	4	69.33	66.05	0.43
2	4	5	6.58	7.23	3.05
2	4	6	1.46*	2.24	0.02
2	4	7	5.92*	0.48	0.30
2	4	8	2.19*	2.13	0.21
3	4	-9	13.64	14.29	5.05
3	4	-8	11.07	11.12	5.09
3	4	-7	36.27	36.79	1.67
3	4	-6	38.96	38.80	1.32
3	4	-5	5.39*	4.43	0.54
3	4	-4	18.95	19.60	9.28
3	4	-3	5.27	5.78	5.45
3	4	-2	79.75	79.77	0.36
3	4	-1	40.48	41.26	1.13
3	4	0	5.19	6.20	5.26
3	4	1	12.17	12.04	16.22
3	4	2	2.63*	1.88	0.14
3	4	3	20.03	18.86	9.55
3	4	4	14.02	15.05	9.83
3	4	5	12.33	12.16	7.15
3	4	6	19.78	19.58	8.16
3	4	7	7.63*	8.01	0.27
3	4	8	4.09*	3.29	0.06
4	4	-9	2.43*	3.28	0.03
4	4	-8	5.29*	3.61	0.22
4	4	-7	3.34*	1.84	0.09
4	4	-6	4.91*	1.86	0.31
4	4	-5	12.34	12.13	10.67
4	4	-4	2.44*	6.06	1.12
4	4	-3	2.43*	1.40	0.17
4	4	-2	15.24	15.25	14.46
4	4	-1	43.64	46.50	0.99
4	4	0	57.35	60.21	0.64
4	4	1	23.64	23.81	4.34
4	4	2	2.81*	3.92	0.13
4	4	3	31.10	30.17	2.41
4	4	4	7.17	6.85	4.45
4	4	5	3.52*	4.20	0.08
4	4	6	10.96	12.10	4.23
4	4	7	3.58*	4.08	0.08
4	4	8	3.62*	2.30	0.08
5	4	-9	7.66	8.01	2.22
5	4	-8	3.58*	1.98	0.08
5	4	-7	5.75*	6.53	0.29
5	4	-6	4.97*	1.70	0.25
5	4	-5	10.22	9.48	8.66
5	4	-4	13.71	13.68	14.01
5	4	-3	24.68	23.56	4.82
5	4	-2	5.97	5.08	6.71
5	4	-1	9.74	10.19	13.42
5	4	0	12.75	12.80	15.29
5	4	1	6.07	6.57	6.11
5	4	2	14.08	14.44	13.31
5	4	3	29.21	29.34	2.87
5	4	4	2.96*	2.91	0.11
5	4	5	5.98*	3.18	0.27
5	4	6	4.13*	3.66	0.91
5	4	7	4.57*	3.57	0.10
6	4	-9	4.23*	1.33	0.12
6	4	-8	6.84*	8.56	0.33
6	4	-7	12.06	12.21	6.84
6	4	-6	13.77	13.82	9.13
6	4	-5	6.00*	4.73	0.44
6	4	-4	3.88*	0.12	0.41
6	4	-3	31.94	31.95	1.87
6	4	-2	5.15*	4.89	0.47
6	4	-1	13.48	13.41	14.18
6	4	0	24.03	23.66	6.76
6	4	1	16.89	17.06	11.63
6	4	2	2.98*	1.78	0.11
6	4	3	7.78	7.48	4.56
6	4	4	27.93	28.04	3.92
6	4	5	24.74	24.77	7.20
6	4	6	4.72*	4.60	0.12
6	4	7	8.63	8.68	2.54
7	4	-9	3.01*	2.17	0.06
7	4	-8	8.01	9.65	2.92
7	4	-7	4.33*	2.83	0.18
7	4	-6	3.21*	4.51	0.14
7	4	-5	9.79	8.72	7.05
7	4	-4	6.63	6.04	6.09
7	4	-3	13.83	12.82	13.23
7	4	-2	19.15	19.46	9.44
7	4	-1	60.30	60.05	0.54
7	4	0	2.86*	2.79	0.12
7	4	1	22.58	22.52	5.99
7	4	2	3.56*	4.87	0.16
7	4	3	20.54	20.10	9.23
7	4	4	3.65*	4.91	0.08
7	4	5	3.97*	0.71	0.15
7	4	6	2.45*	4.51	0.03
8	4	-9	6.59*	5.52	0.21
8	4	-8	8.74	8.74	3.18
8	4	-7	12.67	13.03	6.52
8	4	-6	9.19	8.54	4.99
8	4	-5	5.05*	5.78	0.33
8	4	-4	5.90	6.61	3.78
8	4	-3	10.25	9.56	7.91
8	4	-2	6.51	6.70	4.88
8	4	-1	29.05	29.37	2.97
8	4	0	3.92*	5.50	0.17
8	4	1	33.37	32.42	2.48
8	4	2	15.90	15.72	8.76
8	4	3	4.25*	3.69	0.14
8	4	4	4.21*	8.70	0.08
8	4	5	3.46*	0.03	0.08
8	4	6	3.85*	0.95	0.06
9	4	-9	7.16*	6.33	0.23
9	4	-8	7.08	6.58	2.43
9	4	-7	16.76	17.02	7.16
9	4	-6	9.22	9.05	5.11
9	4	-5	3.85*	3.19	0.27
9	4	-4	16.61	17.08	9.81
9	4	-3	4.44	3.72	2.00
9	4	-2	18.51	19.12	9.12
9	4	-1	4.52*	5.66	0.31
9	4	0	2.86*	1.65	0.90
9	4	1	6.46	6.49	2.96
9	4	2	3.44*	0.67	0.08
9	4	3	34.69	35.26	2.79
9	4	4	4.92*	5.69	1.25
9	4	5	3.57*	0.15	0.08
10	4	-8	3.00*	4.23	0.07
10	4	-7	7.36*	9.85	0.25
10	4	-6	3.86*	6.76	0.09
10	4	-5	5.46*	3.81	0.27
10	4	-4	5.30*	1.89	0.39
10	4	-3	32.38	32.29	2.37
10	4	-2	3.51*	3.11	0.18
10	4	-1	10.16	10.45	5.56

h	k	l	Fo	Fc	weight
10	4	0	5.90*	6.78	0.33
10	4	1	6.22	6.20	2.65
10	4	2	3.88*	5.53	0.09
10	4	3	1.66*	6.59	0.01
10	4	4	3.67*	1.12	0.07
11	4	-8	1.49*	0.55	0.13
11	4	-7	3.39*	0.13	0.10
11	4	-6	13.92	14.03	5.94
11	4	-5	27.25	26.60	4.46
11	4	-4	12.29	12.69	6.10
11	4	-3	20.06	20.37	8.77
11	4	-2	4.78*	2.29	0.27
11	4	-1	3.31*	1.06	0.09
11	4	0	11.68	12.55	5.86
11	4	1	2.78*	2.24	0.06
11	4	2	3.33*	6.07	0.07
11	4	3	6.27*	5.52	0.28
12	4	-7	3.52*	1.45	0.08
12	4	-6	8.83	8.93	3.02
12	4	-5	8.59	7.77	3.21
12	4	-4	1.94*	0.89	0.27
12	4	-3	1.59*	2.97	0.02
12	4	-2	5.04*	6.41	0.25
12	4	-1	3.60*	4.21	0.11
12	4	0	5.69*	1.81	0.33
12	4	1	3.58*	0.90	0.08
12	4	2	3.45*	2.11	0.61
13	4	-6	3.67*	0.20	0.07
13	4	-5	6.65	6.34	2.10
13	4	-4	1.69*	9.17	0.01
13	4	-3	4.10*	0.94	0.14
13	4	-2	3.46*	1.48	0.08
13	4	-1	15.08	15.29	5.80
13	4	0	6.81	7.41	1.92
13	4	1	1.78*	2.49	0.02
14	4	-5	3.57*	5.70	0.07
14	4	-4	3.53*	5.40	0.05
14	4	-3	3.92*	0.75	0.08
14	4	-2	10.43	11.13	3.64
14	4	-1	5.34*	3.51	0.29
0	5	-9	3.10*	1.10	0.07
0	5	-8	3.63*	3.88	0.08
0	5	-7	11.29	11.98	5.69
0	5	-6	3.23*	5.19	0.10
0	5	-5	22.94	22.97	8.01
0	5	-4	18.00	17.43	9.93
0	5	-3	20.67	21.24	7.09
0	5	-2	22.52	22.91	4.69
0	5	-1	21.60	21.93	6.54
1	5	-9	12.61	12.17	4.41
1	5	-8	3.61*	6.27	0.08
1	5	-7	9.80	10.36	5.33
1	5	-6	20.59	20.59	7.83
1	5	-5	2.85*	6.14	0.14
1	5	-4	22.60	22.06	5.29
1	5	-3	5.69	5.49	6.18
1	5	-2	49.39	51.15	0.82
1	5	-1	81.71	85.21	0.35
1	5	0	5.07*	3.52	0.52
1	5	1	11.22	10.87	17.04
1	5	2	5.40	5.56	5.23
1	5	3	52.33	48.38	0.71
1	5	4	2.77*	2.24	0.13
1	5	5	24.62	23.67	6.29
1	5	6	9.23	8.62	4.50
1	5	7	6.06*	6.80	0.18
1	5	8	8.50	8.44	2.45
2	5	-9	11.40	12.28	3.49
2	5	-8	10.08	10.57	4.41
2	5	-7	33.78	33.95	2.57
2	5	-6	22.43	22.50	5.56
2	5	-5	14.80	14.57	11.78
2	5	-4	10.49	11.31	12.82
2	5	-3	40.40	38.88	1.05
2	5	-2	39.05	38.10	1.16
2	5	-1	6.64	7.09	7.40
2	5	0	21.96	22.99	5.10
2	5	1	3.63*	3.81	0.31
2	5	2	2.73*	2.42	0.13
2	5	3	3.75*	0.78	0.25
2	5	4	20.17	20.66	6.61
2	5	5	5.05	4.91	2.11
2	5	6	1.48*	4.47	0.02
2	5	7	4.53*	2.02	0.14
2	5	8	3.83*	3.24	0.07
3	5	-9	9.41	9.63	3.18
3	5	-8	12.78	13.18	5.75
3	5	-7	59.70	59.82	0.49
3	5	-6	3.65*	3.83	0.15
3	5	-5	21.55	22.46	7.61
3	5	-4	8.48	8.48	9.45
3	5	-3	82.49	80.24	0.33
3	5	-2	44.26	42.68	0.94
3	5	-1	6.26	6.84	7.28
3	5	0	15.40	15.31	11.87
3	5	1	6.40	5.83	7.71
3	5	2	29.63	29.01	2.80
3	5	3	5.02*	5.81	0.39
3	5	4	3.04*	2.03	0.11
3	5	5	11.54	11.23	6.15
3	5	6	4.57*	6.64	0.10
3	5	7	4.35*	9.21	0.10
3	5	8	1.77*	0.34	0.02
4	5	-9	4.24*	2.68	0.11
4	5	-8	33.25	32.85	2.39
4	5	-7	6.85*	7.89	0.32
4	5	-6	12.21	11.65	7.82
4	5	-5	26.23	27.10	3.64
4	5	-4	33.11	30.77	1.80
4	5	-3	52.14	50.41	0.71
4	5	-2	2.52*	0.32	0.16
4	5	-1	15.81	16.14	17.14
4	5	0	18.80	19.88	9.37
4	5	1	7.03	6.36	7.68
4	5	2	18.47	18.57	9.44
4	5	3	7.21	6.94	5.16
4	5	4	3.13*	2.83	0.10
4	5	5	3.40*	1.01	0.09
4	5	6	24.78	24.81	6.35
4	5	7	4.78*	2.88	0.12
5	5	-9	7.82	8.50	2.34
5	5	-8	2.29*	2.90	0.04
5	5	-7	2.61*	1.05	0.07
5	5	-6	5.94*	4.76	0.41
5	5	-5	12.31	12.24	9.69
5	5	-4	1.72*	5.03	0.04
5	5	-3	55.08	52.82	0.63
5	5	-2	3.28*	3.95	0.23
5	5	-1	2.15*	1.07	0.13
5	5	0	24.72	25.06	4.00
5	5	1	1.62*	2.38	0.04
5	5	2	19.83	19.49	8.87
5	5	3	10.01	11.17	6.99
5	5	4	8.78	8.79	4.42
5	5	5	5.24*	1.65	0.23
5	5	6	9.13	8.72	3.34
5	5	7	4.93*	0.92	0.11
6	5	-9	2.46*	2.16	0.04
6	5	-8	3.40*	3.72	0.09
6	5	-7	12.11	12.49	6.28
6	5	-6	17.41	17.94	9.55
6	5	-5	18.32	18.30	10.62
6	5	-4	29.97	29.47	3.01
6	5	-3	15.51	15.96	14.06
6	5	-2	8.02	7.42	8.64
6	5	-1	13.58	13.58	14.21
6	5	0	27.80	26.95	3.42
6	5	1	25.38	25.07	4.05
6	5	2	6.84	7.39	4.53
6	5	3	22.62	22.86	6.54
6	5	4	5.89*	7.41	0.31
6	5	5	48.38	47.29	0.90
6	5	6	5.59*	3.58	0.19
7	5	7	4.17*	2.16	0.06
7	5	-9	10.91	10.78	3.94
7	5	-8	1.65*	0.15	0.03
7	5	-7	2.92*	2.67	0.56
7	5	-6	4.37*	2.51	0.27
7	5	-5	3.61*	1.61	1.51
7	5	-4	22.54	22.94	5.94
7	5	-3	4.95	4.36	3.60
7	5	-2	21.99	22.37	8.40
7	5	-1	2.55*	1.69	0.15
7	5	0	15.43	15.72	11.17
7	5	1	2.98*	0.84	0.11
7	5	2	3.06*	3.80	0.12
7	5	3	18.12	18.32	8.86
7	5	4	5.76*	5.80	0.29
7	5	5	24.37	24.41	6.92
7	5	6	3.66*	0.27	0.07
8	5	-9	3.08*	4.28	0.05
8	5	-8	13.86	13.98	5.80
8	5	-7	21.91	22.07	8.14
8	5	-6	15.09	15.22	7.60
8	5	-5	30.34	30.69	3.03
8	5	-4	2.99*	0.18	0.11
8	5	-3	23.33	23.34	5.56
8	5	-2	11.05	10.64	9.38
8	5	-1	16.13	16.02	10.99
8	5	0	4.21*	5.87	0.19
8	5	1	3.15*	0.18	0.10
8	5	2	11.47	12.29	6.09
8	5	3	19.25	19.25	8.30
8	5	4	22.15	22.15	6.87
8	5	5	5.66*	9.42	0.11
8	5	-8	3.60*	5.59	0.08
8	5	-7	4.86*	11.41	0.09
8	5	-6	5.77*	5.12	0.19
8	5	-5	10.77	11.61	6.13
8	5	-4	3.49*	2.13	0.11
8	5	-3	38.10	36.62	1.30
8	5	-2	12.45	12.17	8.06
8	5	-1	2.40*	0.19	0.08
8	5	0	11.01	11.63	5.46
8	5	1	3.41*	4.29	0.88
8	5	2	9.76	9.80	5.61
8	5	3	10.45	10.30	4.51
8	5	4	6.84*	9.06	0.20
8	5	5	5.62*	2.16	0.18
9	5	-8	7.57	7.28	2.72
9	5	-7	5.26*	9.44	0.11
9	5	-6	4.28*	6.95	1.12
9	5	-5	3.71*	6.31	0.07
9	5	-4	20.13	20.17	8.00
9	5	-3	26.03	26.56	5.11
9	5	-2	8.79	8.18	4.60
9	5	-1	5.68*	3.47	0.32
9	5	0	10.78	10.66	5.80
9	5	1	25.72	26.49	4.96
9	5	2	16.15	15.90	6.76
9	5	3	4.74*	2.29	0.18
9	5	4	3.05*	0.71	0.06
9	5	5	2.53*	1.02	0.03
10	5	-8	2.53*	1.02	0.03
10	5	-7	6.41*	5.80	0.31
10	5	-6	13.46	12.57	5.81
10	5	-5	11.33	11.23	4.89
10	5	-4	8.63	8.77	3.89
10	5	-3	6.74	5.78	2.79
10	5	-2	3.00*	0.35	0.11
10	5	-1	4.64*	3.07	0.20
10	5	0	6.11*	2.87	0.35
10	5	1	29.11	29.38	3.22
10	5	2	3.37*	1.76	0.08
10	5	3	4.62*	5.44	0.85
11	5	-7	1.77*	4.32	0.02
11	5	-6	9.85	8.31	3.78
11	5	-5	9.90	9.58	4.05
11	5	-4	9.61	10.72	3.78
11	5	-3	15.10	15.10	6.75
11	5	-2	3.56*	3.22	0.08
11	5	-1	3.99*	0.38	0.14
11	5	0	5.89*	0.71	0.24

h	k	l	Fo	Fc	weight
12	5	1	3.77*	1.65	0.07
12	5	2	0.86*	3.65	0.04
13	5	-6	3.94*	5.14	0.06
13	5	-5	20.25	19.64	6.44
13	5	-4	8.46	7.57	3.75
13	5	-3	3.58*	2.96	0.08
13	5	-2	5.26	5.85	1.34
13	5	-1	8.89	9.74	3.24
13	5	0	15.89	15.40	5.40
13	5	1	5.94*	4.24	0.21
14	5	-5	4.41*	6.78	0.08
14	5	-4	3.08*	1.31	0.07
14	5	-3	3.96*	4.07	0.10
14	5	-2	3.48*	2.37	0.08
14	5	-1	3.66*	3.52	0.07
0	6	-8	3.48*	3.74	0.08
0	6	-7	6.80*	5.52	0.34
0	6	-6	3.29*	3.50	0.09
0	6	-5	34.02	35.19	2.04
0	6	-4	25.91	26.31	4.16
0	6	-3	10.75	10.85	12.23
0	6	-2	42.02	43.88	1.01
0	6	-1	27.36	26.60	3.47
0	6	0	41.04	41.66	1.09
1	6	-9	3.99*	5.43	0.08
1	6	-8	3.41*	2.54	0.09
1	6	-7	11.60	11.77	5.82
1	6	-6	3.76*	6.51	0.11
1	6	-5	19.27	19.35	8.57
1	6	-4	8.48	8.36	8.61
1	6	-3	13.38	13.56	15.32
1	6	-2	32.75	32.69	2.07
1	6	-1	113.69	120.04	0.19
1	6	0	29.92	30.14	2.41
1	6	1	11.72	11.57	16.33
1	6	2	18.44	17.93	10.14
1	6	3	2.26*	1.68	0.09
1	6	4	8.94	8.41	6.87
1	6	5	37.58	36.64	1.33
1	6	6	3.70*	4.60	0.71
1	6	7	4.13*	2.44	0.97
1	6	8	7.05*	7.06	0.26
2	6	-9	9.21	9.53	2.81
2	6	-8	18.10	18.15	6.82
2	6	-7	15.83	16.60	7.45
2	6	-6	3.98*	3.55	0.24
2	6	-5	21.53	21.22	8.42
2	6	-4	4.60*	5.19	0.36
2	6	-3	43.13	43.19	0.93
2	6	-2	22.43	21.95	6.39
2	6	-1	3.85*	4.11	0.27
2	6	0	20.06	20.38	9.14
2	6	1	3.46*	6.75	0.24
2	6	2	7.52	6.97	8.28
2	6	3	10.08	10.27	10.47
2	6	4	3.38*	3.07	0.19
2	6	5	12.73	12.41	7.34
2	6	6	28.20	27.77	4.04
2	6	7	13.20	13.92	5.18
2	6	8	5.79*	2.60	0.17
3	6	-9	3.04*	4.88	0.04
3	6	-8	6.04	6.07	2.05
3	6	-7	11.71	11.80	5.59
3	6	-6	18.23	18.88	8.81
3	6	-5	16.48	16.24	10.95
3	6	-4	10.89	10.96	11.38
3	6	-3	60.13	56.85	0.56
3	6	-2	45.63	45.40	0.88
3	6	-1	18.21	18.38	9.58
3	6	0	4.73*	0.97	0.54
3	6	1	27.50	28.98	3.19
3	6	2	5.47	5.45	5.34
3	6	3	6.02	5.53	4.65
3	6	4	3.47*	6.02	0.08
3	6	5	4.05*	4.14	0.15
3	6	6	7.31	8.33	2.65
3	6	7	1.66*	6.00	0.02
3	6	8	3.82*	1.23	0.07
4	6	-9	7.05	7.74	2.06
4	6	-8	4.62*	1.48	0.21
4	6	-7	23.16	23.60	8.08
4	6	-6	11.50	11.54	7.13
4	6	-5	22.94	22.81	6.44
4	6	-4	40.36	38.62	1.39
4	6	-3	6.59	6.63	6.88
4	6	-2	2.57*	7.07	0.15
4	6	-1	30.79	33.81	2.07
4	6	0	13.66	13.60	15.86
4	6	1	8.35	8.57	9.26
4	6	2	11.45	11.52	11.02
4	6	3	47.95	48.25	0.73
4	6	4	4.96*	1.32	0.32
4	6	5	13.20	13.33	6.43
4	6	6	6.67*	5.85	0.21
4	6	7	4.52*	3.17	0.16
5	6	-9	18.88	18.94	5.84
5	6	-8	11.22	11.41	4.57
5	6	-7	6.72	6.88	3.17
5	6	-6	4.94*	3.05	0.49
5	6	-5	13.04	12.75	9.30
5	6	-4	25.37	25.35	4.57
5	6	-3	24.01	23.28	4.94
5	6	-2	15.27	14.65	9.50
5	6	-1	2.24*	4.64	0.09
5	6	0	13.34	13.62	13.87
5	6	1	2.83*	0.17	0.12
5	6	2	8.99	9.05	7.41
5	6	3	5.01*	4.09	0.26
5	6	4	3.78*	0.13	0.15
5	6	5	7.97	8.50	3.17
5	6	6	5.21*	5.42	0.17
5	6	7	6.10*	5.26	0.14
6	6	-9	7.26*	8.55	0.20
6	6	-8	8.47	8.31	3.76
6	6	-7	3.09*	2.86	0.10
6	6	-6	3.24*	0.67	0.13
6	6	-5	17.13	17.45	10.19
6	6	-4	12.36	11.89	10.24
6	6	-3	29.00	28.67	2.52
6	6	-2	2.57*	3.95	0.15
6	6	-1	26.94	27.11	3.52
6	6	0	20.42	20.07	8.65
6	6	1	4.87*	0.92	0.55
6	6	2	3.24*	0.29	0.13
6	6	3	3.14*	1.16	0.11
6	6	4	36.02	36.52	2.05
6	6	5	24.61	24.69	5.48
6	6	6	5.11*	0.83	0.20
7	6	-9	6.40*	10.06	0.15
7	6	-8	12.77	12.73	5.27
7	6	-7	12.59	12.96	6.26
7	6	-6	5.13*	2.32	0.24
7	6	-5	13.09	13.55	8.14
7	6	-4	9.92	9.15	8.46
7	6	-3	16.34	15.53	12.42
7	6	-2	3.78*	2.22	0.33
7	6	-1	33.60	33.11	1.61
7	6	0	5.60*	2.86	0.38
7	6	1	10.77	9.58	8.73
7	6	2	3.02*	0.22	0.11
7	6	3	3.37*	4.73	0.09
7	6	4	21.04	21.71	7.71
7	6	5	3.32*	6.24	0.06
7	6	6	2.21*	2.16	0.20
8	6	-9	3.73*	1.99	0.07
8	6	-8	5.09*	1.58	0.20
8	6	-7	7.52	8.45	2.96
8	6	-6	6.08*	8.95	0.29
8	6	-5	13.13	13.56	7.31
8	6	-4	14.14	13.95	9.54
8	6	-3	10.49	11.23	7.02
8	6	-2	2.99*	3.30	0.11
8	6	-1	3.53*	1.30	0.18
8	6	0	5.45*	8.04	0.28
8	6	1	3.98*	1.98	0.22
8	6	2	2.08*	0.05	0.03
8	6	3	24.55	24.96	5.99
8	6	4	7.47	7.94	2.42
8	6	5	6.69*	3.06	0.35
9	6	-8	1.73*	2.94	0.02
9	6	-7	3.53*	4.17	0.08
9	6	-6	15.92	16.09	7.57
9	6	-5	8.72	9.22	4.45
9	6	-4	13.33	14.18	7.52
9	6	-3	14.88	14.83	8.83
9	6	-2	20.58	20.01	8.35
9	6	-1	3.18*	4.07	0.10
9	6	0	3.12*	1.62	0.10
9	6	1	3.36*	2.05	0.09
9	6	2	5.50	6.13	1.81
9	6	3	3.79*	3.47	0.07
9	6	4	3.57*	3.46	0.08
9	6	5	2.54*	0.07	0.04
10	6	-8	15.22	15.22	5.13
10	6	-7	3.30*	1.63	0.09
10	6	-6	10.38	10.68	4.36
10	6	-5	25.63	26.01	5.51
10	6	-4	20.94	21.52	8.42
10	6	-3	20.01	20.00	7.84
10	6	-2	5.54*	7.94	0.25
10	6	-1	5.77*	1.33	0.39
10	6	0	10.24	10.68	5.65
10	6	1	3.83*	0.74	0.11
10	6	2	2.81*	2.38	0.06
10	6	3	5.87*	7.64	0.23
10	6	4	4.36*	0.46	0.13
11	6	-7	4.58*	2.73	0.22
11	6	-6	3.64*	1.05	0.08
11	6	-5	13.47	13.22	6.32
11	6	-4	4.18*	3.49	0.13
11	6	-3	37.73	38.13	1.88
11	6	-2	5.82*	0.50	0.34
11	6	-1	3.57*	0.94	0.08
11	6	0	6.59*	3.92	0.34
11	6	1	4.35*	5.55	0.11
11	6	2	3.67*	2.69	0.07
11	6	3	5.02*	1.52	0.16
12	6	-7	8.26	8.02	2.71
12	6	-6	6.10	6.70	1.62
12	6	-5	14.94	15.04	5.70
12	6	-4	16.67	17.98	6.46
12	6	-3	10.01	9.47	4.53
12	6	-2	3.52*	3.54	0.08
12	6	-1	6.39*	8.75	0.22
12	6	0	3.67*	2.87	0.07
12	6	1	4.23*	4.90	0.12
12	6	2	3.84*	0.54	0.07
13	6	-6	12.02	12.58	4.39
13	6	-5	3.69*	1.65	0.07
13	6	-4	3.83*	4.14	0.79
13	6	-3	2.96*	0.27	0.07
13	6	-2	3.51*	2.87	0.08
13	6	-1	4.24*	0.75	0.17
13	6	0	3.56*	1.90	0.08
14	6	-4	5.92	3.42	1.93
14	6	-3	3.62*	2.65	0.08
14	6	-2	4.75*	2.60	0.13
0	7	-8	3.83*	3.49	0.07
0	7	-7	10.55	10.41	5.08
0	7	-6	9.56	8.51	5.60
0	7	-5	7.20	6.78	4.67
0	7	-4	11.91	11.67	10.56
0	7	-3	24.34	23.71	6.05
0	7	-2	14.00	14.29	16.09
0	7	-1	54.56	55.39	0.68
1	7	-8	9.04	9.24	3.81
1	7	-7	11.59	11.78	6.42
1	7	-6	54.92	57.04	0.55
1	7	-5	28.86	29.02	3.27
1	7	-4	21.46	21.42	7.33
1	7	-3	9.42	9.36	11.13
1	7	-2	88.50	87.79	0.29

h	k	l	Fo	Fc	weight
1	7	-1	19.10	19.10	11.30
1	7	0	7.91	8.30	10.31
1	7	1	40.42	40.31	1.04
1	7	2	8.79	8.52	10.32
1	7	3	8.79	9.35	9.22
1	7	4	3.83*	4.86	0.19
1	7	5	29.80	30.47	2.95
1	7	6	15.80	15.92	7.03
1	7	7	16.15	15.72	6.11
1	7	8	13.98	12.83	4.37
2	7	-9	3.90*	3.74	0.07
2	7	-8	3.54*	3.16	0.08
2	7	-7	3.42*	5.74	0.09
2	7	-6	8.32	8.73	4.16
2	7	-5	3.52*	0.60	0.20
2	7	-4	16.73	16.75	13.54
2	7	-3	41.62	41.33	0.94
2	7	-2	27.90	28.16	2.26
2	7	-1	2.52*	2.64	0.14
2	7	0	9.49	9.72	12.75
2	7	1	22.46	23.54	5.87
2	7	2	2.69*	1.10	0.14
2	7	3	3.22*	2.41	0.15
2	7	4	3.05*	1.63	0.11
2	7	5	8.68	9.33	4.04
2	7	6	3.75*	3.17	0.07
2	7	7	15.00	15.79	5.04
2	7	8	3.85*	1.88	0.08
3	7	-9	3.97*	3.46	0.12
3	7	-8	13.65	12.96	5.88
3	7	-7	18.82	19.18	7.78
3	7	-6	3.29*	1.45	0.09
3	7	-5	6.68	7.06	4.62
3	7	-4	9.15	9.48	8.66
3	7	-3	18.83	18.83	9.89
3	7	-2	80.70	82.12	0.34
3	7	-1	16.24	16.04	13.03
3	7	0	56.41	54.85	0.63
3	7	1	2.80*	5.33	0.13
3	7	2	2.63*	6.94	0.08
3	7	3	3.89*	5.64	0.17
3	7	4	5.92*	1.94	0.40
3	7	5	5.07*	3.54	0.18
3	7	6	14.45	14.63	6.01
3	7	7	8.00	9.48	2.35
3	7	8	3.73*	3.73	0.07
4	7	-8	10.65	11.72	3.74
4	7	-7	14.76	15.18	7.32
4	7	-6	10.63	10.56	5.67
4	7	-5	3.21*	3.36	0.10
4	7	-4	2.18*	2.83	0.70
4	7	-3	56.77	56.44	0.60
4	7	-2	5.78	5.17	5.36
4	7	-1	43.84	45.46	0.90
4	7	0	3.73*	4.33	0.24
4	7	1	4.04*	1.10	0.37
4	7	2	28.52	29.13	2.49
4	7	3	4.82*	6.16	0.20
4	7	4	16.06	16.34	8.48
4	7	5	12.26	11.80	6.16
4	7	6	17.34	17.01	6.68
4	7	7	4.25*	4.18	0.10
5	7	-8	3.83*	0.36	0.07
5	7	-7	12.59	13.05	5.85
5	7	-6	5.05*	0.56	0.23
5	7	-5	10.53	11.13	7.21
5	7	-4	2.23*	3.81	0.07
5	7	-3	44.81	43.07	0.82
5	7	-2	3.55*	5.49	0.19
5	7	-1	11.24	11.97	11.27
5	7	0	17.14	17.67	13.53
5	7	1	37.26	37.35	1.52
5	7	2	2.58*	1.77	0.10
5	7	3	3.63*	2.78	0.14
5	7	4	2.39*	1.37	0.43
5	7	5	22.04	22.03	7.86
5	7	6	26.33	27.00	5.58
5	7	7	4.03*	0.56	0.06
6	7	-8	1.78*	6.37	0.02
6	7	-7	5.30*	1.67	0.31
6	7	-6	1.48*	1.44	0.03
6	7	-5	3.17*	4.99	0.10
6	7	-4	7.20	8.51	4.65
6	7	-3	7.78	9.14	6.12
6	7	-2	14.14	14.66	12.92
6	7	-1	18.35	17.74	10.48
6	7	0	10.75	10.56	8.81
6	7	1	17.57	17.73	9.47
6	7	2	16.49	17.07	9.46
6	7	3	17.83	17.78	9.03
6	7	4	5.28*	7.96	0.14
6	7	5	6.48*	7.26	0.17
6	7	6	9.14	8.12	3.27
7	7	-9	5.39*	0.16	0.20
7	7	-8	11.30	11.68	4.23
7	7	-7	3.19*	2.73	0.10
7	7	-6	9.81	9.61	5.77
7	7	-5	25.00	24.78	4.30
7	7	-4	25.52	25.50	5.08
7	7	-3	4.39*	5.81	0.26
7	7	-2	34.13	33.80	1.56
7	7	-1	22.61	22.64	6.46
7	7	0	9.87	10.07	7.30
7	7	1	6.92	6.78	3.77
7	7	2	3.29*	0.86	0.09
7	7	3	10.76	12.17	5.43
7	7	4	8.34	8.24	3.55
7	7	5	16.86	15.81	6.18
7	7	6	2.53*	1.42	0.04
8	7	-8	5.69	4.75	1.54
8	7	-7	4.31*	1.92	0.16
8	7	-6	3.46*	4.49	0.09
8	7	-5	4.67*	0.59	0.29
8	7	-4	8.12	8.52	4.52
8	7	-3	22.67	22.70	6.31
8	7	-2	14.23	14.43	8.84
8	7	-1	1.94*	0.94	0.05
8	7	0	7.51	8.51	4.27
8	7	1	6.81	6.52	3.12
8	7	2	8.13	9.28	3.40
8	7	3	3.43*	5.33	0.08
8	7	4	12.01	12.12	4.32
8	7	5	5.57	5.95	1.33
8	7	-8	9.59	8.68	3.24
9	7	-7	3.44*	0.33	0.08
9	7	-6	3.18*	0.23	0.10
9	7	-5	5.72*	5.13	0.32
9	7	-4	10.36	10.52	5.92
9	7	-3	11.81	11.49	6.66
9	7	-2	9.50	8.88	5.96
9	7	-1	10.63	10.60	6.10
9	7	0	3.60*	5.33	0.10
9	7	1	9.46	9.62	4.75
9	7	2	23.22	23.33	6.17
9	7	3	2.33*	4.88	0.03
9	7	4	3.84*	3.77	0.07
10	7	-8	11.15	10.94	4.18
10	7	-7	3.68*	1.02	0.07
10	7	-6	4.01*	0.20	0.10
10	7	-5	4.48*	2.92	0.23
10	7	-4	28.22	28.36	3.58
10	7	-3	6.06*	3.44	0.32
10	7	-2	8.98	9.71	4.34
10	7	-1	6.79*	7.33	0.24
10	7	0	5.89*	4.96	0.21
10	7	1	22.89	22.81	8.05
10	7	2	9.10	9.27	3.29
10	7	3	6.43*	6.72	0.22
10	7	4	4.03*	5.28	0.07
11	7	-7	3.61*	0.02	0.08
11	7	-6	6.06	6.52	1.87
11	7	-5	10.73	10.32	4.15
11	7	-4	3.31*	1.45	0.09
11	7	-3	9.47	9.55	4.08
11	7	-2	3.16*	1.73	0.10
11	7	-1	5.04	5.81	1.50
11	7	0	7.08*	5.87	0.25
11	7	1	24.17	23.33	6.86
11	7	2	3.88*	3.59	0.07
11	7	3	5.85	5.90	1.33
11	7	-6	7.13	7.99	1.74
12	7	-5	11.79	13.00	3.94
12	7	-4	6.27*	7.48	0.23
12	7	-3	9.33	9.98	3.77
12	7	-2	6.21*	7.87	0.21
12	7	-1	4.10*	2.96	0.11
12	7	0	19.58	19.28	6.48
12	7	1	2.47*	6.03	0.03
13	7	-5	5.92	6.36	1.62
13	7	-4	6.98*	7.10	0.27
13	7	-3	3.56*	0.70	0.08
13	7	-2	3.01*	1.79	0.05
13	7	-1	4.64*	4.13	0.15
13	7	0	3.09*	5.67	0.04
0	8	-8	4.24*	0.74	0.17
0	8	-7	3.60*	3.07	0.08
0	8	-6	15.48	15.96	7.26
0	8	-5	12.47	12.28	8.50
0	8	-4	16.98	17.19	9.99
0	8	-3	13.96	14.22	13.33
0	8	-2	17.26	17.42	13.43
0	8	-1	26.15	26.84	3.81
0	8	0	12.60	12.67	14.62
1	8	-8	9.22	8.46	3.62
1	8	-7	14.46	15.29	6.15
1	8	-6	58.23	60.80	0.50
1	8	-5	7.24	7.41	4.01
1	8	-4	12.81	12.63	10.18
1	8	-3	30.70	30.40	2.47
1	8	-2	17.93	16.94	9.05
1	8	-1	25.96	25.07	3.92
1	8	0	26.11	26.92	3.19
1	8	1	11.01	11.08	13.35
1	8	2	14.75	14.96	14.55
1	8	3	12.89	13.29	11.79
1	8	4	2.29*	2.34	0.07
1	8	5	36.41	37.16	1.70
1	8	6	3.71*	4.49	0.07
1	8	7	6.14*	4.52	0.24
2	8	8	4.66*	3.24	0.08
2	8	-8	5.87*	6.49	0.17
2	8	-7	8.52	8.97	3.83
2	8	-6	12.08	11.65	6.81
2	8	-5	6.13*	8.78	0.33
2	8	-4	22.48	22.76	6.11
2	8	-3	17.11	16.92	13.89
2	8	-2	47.26	46.45	0.80
2	8	-1	17.84	17.74	8.51
2	8	0	5.39	6.27	5.23
2	8	1	2.78*	0.63	0.13
2	8	2	4.73*	0.28	0.46
2	8	3	11.86	11.93	9.14
2	8	4	3.31*	0.98	0.09
2	8	5	6.51	6.63	2.67
2	8	6	14.58	15.26	5.84
2	8	7	6.04*	2.70	0.20
2	8	8	3.91*	0.75	0.07
3	8	-9	2.77*	0.01	0.39
3	8	-8	3.49*	3.01	0.08
3	8	-7	7.22*	7.47	0.29
3	8	-6	31.75	30.62	2.77
3	8	-5	2.38*	5.61	0.06
3	8	-4	33.84	33.36	2.10
3	8	-3	13.27	13.93	12.98
3	8	-2	63.29	62.43	0.51
3	8	-1	38.53	39.85	1.55
3	8	0	2.57*	1.55	0.15
3	8	1	26.80	28.16	3.44
3	8	2	10.28	10.42	9.23
3	8	3	28.58	28.12	4.04
3	8	4	10.40	10.71	5.60
3	8	5	1.50*	5.01	0.01
3	8	6	11.46	11.37	4.95
3	8	7	10.81	10.49	3.62
4	8	-9	3.54*	0.77	0.08
4	8	-8	3.71*	3.34	0.07
4	8	-7	19.68	19.89	7.56
4	8	-6	3.34*	3.10	0.87
4	8	-5	2.77*	0.18	0.11
4	8	-4	2.93*	2.68	0.12
4	8	-3	10.67	10.80	10.15
4	8	-2	7.44	7.42	7.52
4	8	-1	6.07	6.66	5.72
4	8	0	7.53	8.13	7.83
4	8	1	25.02	25.24	4.19
4	8	2	20.01	19.99	7.38
4	8	3	1.35*	0.33	0.02
4	8	4	3.47*	1.25	0.08
4	8	5	21.41	21.38	8.05
4	8	6	12.47	13.10	4.41
4	8	7	8.99	9.01	2.85
5	8	-9	4.41*	8.71	0.08
5	8	-8	3.48*	2.84	0.08
5	8	-7	5.02*	4.83	0.21
5	8	-6	8.80	9.34	4.46
5	8	-5	11.39	10.96	7.68
5	8	-4	6.09*	7.31	0.30
5	8	-3	10.02	9.26	7.90
5	8	-2	5.90	6.92	4.27
5	8	-1	14.99	15.03	13.79
5	8	0	13.40	14.08	12.06
5	8	1	9.43	9.70	7.65
5	8	2	8.49	8.02	5.48
5	8	3	5.04	5.17	1.97
5	8	4	6.45	7.43	2.23
5	8	5	4.22*	7.79	0.10
5	8	6	2.61*	4.94	0.30
6	8	-8	13.47	13.03	5.11
6	8	-7	3.37*	0.47	0.09
6	8	-6	11.92	12.81	6.12
6	8	-5	21.70	22.20	9.43
6	8	-4	19.71	18.95	9.90
6	8	-3	20.78	20.99	6.34
6	8	-2	2.90*	1.84	0.12
6	8	-1	26.60	26.48	4.34
6	8	0	2.24*	1.59	0.07
6	8	1	4.63*	4.36	0.28
6	8	2	11.06	11.86	7.00
6	8	3	3.29*	2.10	0.09
6	8	4	15.62	15.02	6.84
6	8	5	11.10	9.98	4.35
6	8	6	6.07*	6.16	0.17
7	8	-8	4.22*	2.40	0.13
7	8	-7	5.63*	2.05	0.23
7	8	-6	18.80	19.12	8.04
7	8	-5	15.27	15.79	8.11
7	8	-4	9.31	9.36	5.67
7	8	-3	9.13	8.23	6.13
7	8	-2	5.02*	1.71	0.36
7	8	-1	8.19	8.50	5.07
7	8	0	4.38	5.14	2.18
7	8	1	5.06*	4.17	0.39
7	8	2	3.44*	0.20	0.08
7	8	3	3.07*	4.20	0.06
7	8	4	5.37*	4.13	0.17
7	8	5	2.96*	8.49	0.04
8	8	-8	6.05*	4.19	0.20
8	8	-7	6.70	6.27	2.46
8	8	-6	2.73*	3.51	0.05
8	8	-5	20.24	20.04	8.29
8	8	-4	4.12*	2.29	0.27
8	8	-3	13.19	13.43	7.73
8	8	-2	22.07	22.08	6.59
8	8	-1	5.07*	5.58	0.31
8	8	0	2.02*	0.11	0.06
8	8	1	6.71	6.56	3.21
8	8	2	11.24	11.83	5.25
8	8	3	7.88	7.30	3.25
8	8	4	11.38	11.70	4.23
8	8	5	6.84	7.85	1.79
9	8	-8	6.42	5.54	1.87
9	8	-7	2.39*	4.74	0.04
9	8	-6	7.33	6.36	2.94
9	8	-5	6.61*	6.37	0.27
9	8	-4	12.38	12.36	7.02
9	8	-3	17.51	17.16	8.71
9	8	-2	38.62	37.57	2.02
9	8	-1	3.15*	3.48	0.10
9	8	0	3.54*	1.59	0.08
9	8	1	3.35*	0.75	0.09
9	8	2	9.95	10.18	3.97
9	8	3	3.83*	6.82	0.07
9	8	4	3.70*	0.81	0.07
10	8	-7	6.52	8.34	1.71
10	8	-6	5.00*	4.97	0.16
10	8	-5	13.50	12.70	6.20
10	8	-4	3.14*	1.58	0.10
10	8	-3	9.15	9.09	4.17
10	8	-2	6.87	7.31	2.77
10	8	-1	5.14*	2.95	0.26
10	8	0	5.69*	1.42	0.26
10	8	1	4.29*	5.22	0.10
10	8	2	5.03*	1.06	0.17
10	8	3	13.86	13.19	5.03
11	8	-7	2.52*	1.30	0.04
11	8	-6	12.06	11.77	4.77
11	8	-5	15.42	14.82	6.23
11	8	-4	13.86	14.43	5.64
11	8	-3	5.34	4.98	1.67
11	8	-2	5.35*	3.67	0.41
11	8	-1	7.90	7.74	3.38
11	8	0	11.04	10.95	4.55
11	8	1	5.88*	5.46	0.23
11	8	2	15.69	15.56	5.30
12	8	-6	10.21	10.79	3.34
12	8	-5	3.87*	5.44	0.10
12	8	-4	5.84	7.21	1.78
12	8	-3	11.51	12.94	4.34
12	8	-2	4.77*	2.98	0.18
12	8	-1	3.42*	1.36	0.09
12	8	0	3.87*	0.07	0.13
12	8	1	4.08*	5.10	0.06
13	8	-5	3.61*	6.54	0.08
13	8	-4	8.12*	7.77	0.24
13	8	-3	3.90*	3.43	0.07
13	8	-2	6.40	6.12	1.96
13	8	-1	6.90*	8.70	0.20
0	9	-8	1.76*	5.40	0.01
0	9	-7	17.91	17.79	6.61
0	9	-6	23.25	23.06	6.53
0	9	-5	3.39*	3.89	0.85
0	9	-4	6.95	6.53	4.16
0	9	-3	12.24	11.67	10.85
0	9	-2	30.66	30.94	2.50
0	9	-1	28.33	27.63	3.44
1	9	-8	3.68*	2.54	0.07
1	9	-7	19.27	19.17	7.71
1	9	-6	40.88	39.83	1.47
1	9	-5	6.72	7.70	3.31
1	9	-4	8.76	8.75	6.68
1	9	-3	12.09	12.11	9.95
1	9	-2	40.65	40.13	1.41
1	9	-1	14.64	14.28	13.94
1	9	0	13.93	13.77	13.84
1	9	1	8.63	8.01	8.74
1	9	2	11.59	11.47	10.94
1	9	3	1.28*	0.83	0.02
1	9	4	10.59	9.93	7.38
1	9	5	12.94	12.35	6.67
1	9	6	22.37	21.95	7.74
1	9	7	6.04*	5.90	0.22
1	9	8	4.19*	1.15	0.06
2	9	-8	1.73*	4.97	0.02
2	9	-7	11.16	11.02	4.46
2	9	-6	15.27	15.76	6.62
2	9	-5	11.25	11.58	6.75
2	9	-4	35.08	35.65	1.95
2	9	-3	26.53	25.69	3.22
2	9	-2	20.82	20.49	8.25
2	9	-1	8.10	8.22	9.66
2	9	0	24.36	24.36	4.36
2	9	1	26.71	27.17	3.32
2	9	2	13.54	13.46	10.80
2	9	3	12.08	11.91	8.36
2	9	4	10.61	9.75	6.03
2	9	5	16.50	16.66	7.04
2	9	6	4.52*	2.80	0.14
2	9	7	10.60	10.20	3.69
3	9	-8	12.13	12.88	4.65
3	9	-7	9.22	9.61	3.84
3	9	-6	4.77*	1.82	0.23
3	9	-5	14.62	15.18	8.41
3	9	-4	19.00	18.39	11.19
3	9	-3	8.36	2.65	3.65
3	9	-2	41.16	40.65	1.37
3	9	-1	10.36	10.05	11.35
3	9	0	19.04	19.25	7.53
3	9	1	9.72	10.50	8.94
3	9	2	5.86*	8.48	0.40
3	9	3	14.90	14.08	9.47
3	9	4	11.14	12.15	5.79
3	9	5	6.85*	7.85	0.28
3	9	6	4.33*	3.26	0.12
3	9	7	3.92*	0.40	0.07
4	9	-8	5.15*	2.16	0.21
4	9	-7	11.03	10.70	4.76
4	9	-6	10.37	10.35	5.12
4	9	-5	3.29*	1.66	0.09
4	9	-4	3.01*	2.57	0.11
4	9	-3	6.63	5.19	5.15
4	9	-2	7.81	6.71	6.26
4	9	-1	15.18	16.04	13.60
4	9	0	23.28	22.72	5.33
4	9	1	25.02	24.80	5.07
4	9	2	3.72*	4.00	1.52
4	9	3	18.82	18.84	9.37
4	9	4	23.85	24.88	4.82
4	9	5	9.03	8.20	3.77
4	9	6	28.86	28.57	4.57
4	9	7	4.02*	1.75	0.06
5	9	-8	15.74	15.46	5.66
5	9	-7	5.37*	5.56	0.24
5	9	-6	18.93	18.51	8.51
5	9	-5	6.46*	8.48	0.27
5	9	-4	16.93	16.53	10.06
5	9	-3	11.46	10.31	9.70
5	9	-2	22.26	23.68	6.62
5	9	-1	2.54*	2.62	0.12
5	9	0	3.86*	3.84	0.20
5	9	1	2.88*	0.33	0.12
5	9	2	4.57*	1.84	0.26
5	9	3	5.62*	2.53	0.45
5	9	4	10.24	11.00	4.49
5	9	5	1.63*	0.39	0.02
5	9	6	21.59	21.73	6.22
6	9	-8	4.90*	1.53	0.21
6	9	-7	13.69	13.71	6.11
6	9	-6	3.33*	1.80	0.09
6	9	-5	3.89*	3.66	0.19
6	9	-4	7.46	8.01	3.78
6	9	-3	11.01	9.99	7.64
6	9	-2	20.58	19.95	8.17
6	9	-1	1.33*	0.41	0.02
6	9	0	4.45*	3.24	0.32
6	9	1	14.27	13.68	8.61
6	9	2	3.21*	7.77	0.06
6	9	3	3.42*	0.97	0.09
6	9	4	1.59*	4.46	0.02
6	9	5	11.86	11.35	4.52
6	9	6	3.99*	5.28	0.06
7	9	-8	3.67*	2.01	0.07
7	9	-7	12.63	12.83	5.16

h	k	l	Fo	Fc	weight
7	9	-6	7.36	7.12	3.31
7	9	-5	3.19*	1.68	0.10
7	9	-4	24.15	24.54	6.17
7	9	-3	3.15*	7.12	0.07
7	9	-2	22.14	22.22	8.36
7	9	-1	6.77	6.68	3.67
7	9	0	1.89*	5.14	0.04
7	9	1	8.82	9.64	5.06
7	9	2	3.36*	0.70	0.09
7	9	3	6.70	6.57	2.79
7	9	4	7.20*	9.47	0.19
7	9	5	3.64*	0.25	0.08
8	9	-8	3.45*	1.21	0.08
8	9	-7	18.15	18.58	6.28
8	9	-6	9.13	8.45	3.78
8	9	-5	5.89*	6.43	0.27
8	9	-4	16.28	15.49	8.51
8	9	-3	24.47	24.82	4.54
8	9	-2	10.93	10.84	6.26
8	9	-1	4.08*	3.55	1.38
8	9	0	7.12	8.41	3.16
8	9	1	3.70*	1.92	0.11
8	9	2	19.51	19.50	7.72
8	9	3	10.97	10.70	4.60
8	9	4	5.42*	3.67	0.15
9	9	-7	5.45*	4.50	0.21
9	9	-6	5.46	6.83	1.63
9	9	-5	3.64*	3.46	0.99
9	9	-4	22.04	21.86	5.94
9	9	-3	24.91	24.98	5.19
9	9	-2	3.53*	3.36	0.08
9	9	-1	4.79*	3.97	0.23
9	9	0	3.77*	5.82	0.11
9	9	1	13.35	13.11	6.40
9	9	2	22.22	22.00	7.12
9	9	3	5.11*	5.82	0.13
9	9	4	16.36	16.72	4.85
10	9	-7	11.84	11.35	4.37
10	9	-6	11.14	11.17	4.28
10	9	-5	3.53*	1.02	0.08
10	9	-4	4.11*	5.36	1.19
10	9	-3	10.91	11.20	5.06
10	9	-2	3.65*	5.98	0.07
10	9	-1	7.69	6.74	3.97
10	9	0	4.26*	2.00	0.18
10	9	1	3.66*	0.07	0.07
10	9	2	11.33	10.74	3.98
10	9	3	5.02*	1.27	0.15
11	9	-6	12.47	12.55	4.40
11	9	-5	3.74*	5.44	0.71
11	9	-4	3.40*	0.94	0.09
11	9	-3	2.33*	0.93	0.03
11	9	-2	3.46*	4.45	0.08
11	9	-1	3.49*	2.61	0.08
11	9	0	13.78	14.33	5.52
11	9	1	12.84	14.22	4.15
11	9	2	3.09*	1.56	0.07
12	9	-5	3.82*	1.15	0.07
12	9	-4	3.87*	3.24	0.11
12	9	-3	3.66*	2.15	0.07
12	9	-2	6.82	6.64	2.20
12	9	-1	3.64*	1.66	0.08
12	9	0	13.04	12.64	4.38
13	9	-4	3.63*	5.81	0.08
13	9	-3	3.71*	0.73	0.07
13	9	-2	3.51*	0.18	0.08
0	10	-8	3.11*	4.34	0.05
0	10	-7	3.64*	3.49	0.08
0	10	-6	4.74*	4.75	0.21
0	10	-5	3.50*	7.12	0.08
0	10	-4	9.84	9.95	6.54
0	10	-3	18.72	18.11	7.54
0	10	-2	32.03	30.76	2.27
0	10	-1	22.14	21.57	6.54
0	10	0	32.02	32.87	2.33
1	10	-8	6.40*	3.44	0.25
1	10	-7	5.26*	0.44	0.19
1	10	-6	8.49	7.75	3.96
1	10	-5	25.03	25.57	7.12
1	10	-4	10.37	10.43	6.65
1	10	-3	2.80*	0.56	0.12
1	10	-2	3.06*	1.79	0.14
1	10	-1	29.93	29.20	3.07
1	10	0	38.60	38.13	1.46
1	10	1	2.74*	1.07	0.13
1	10	2	21.68	21.21	5.58
1	10	3	6.47	7.30	3.17
1	10	4	20.37	20.14	6.37
1	10	5	22.62	22.83	6.59
1	10	6	4.24*	1.57	0.12
1	10	7	4.83*	1.94	0.14
2	10	-8	2.07*	0.99	0.23
2	10	-7	11.71	11.75	4.99
2	10	-6	24.98	24.10	7.00
2	10	-5	1.91*	4.14	0.28
2	10	-4	11.61	11.92	7.53
2	10	-3	18.65	18.09	11.64
2	10	-2	3.55*	2.72	0.22
2	10	-1	26.63	27.63	3.91
2	10	0	6.63	6.68	5.65
2	10	1	9.44	9.27	7.97
2	10	2	13.69	14.05	9.80
2	10	3	4.91*	3.47	0.24
2	10	4	14.23	14.06	7.41
2	10	5	19.34	18.89	8.07
2	10	6	6.74*	8.76	0.24
2	10	7	9.40	9.09	2.78
3	10	-8	6.36	5.45	1.87
3	10	-7	5.70*	1.96	0.29
3	10	-6	6.38*	6.99	0.26
3	10	-5	6.06	6.94	2.61
3	10	-4	3.23*	0.57	0.10
3	10	-3	29.13	28.04	2.88
3	10	-2	30.72	30.42	2.84
3	10	-1	23.01	22.43	5.59
3	10	0	10.55	10.20	6.72
3	10	1	11.01	10.80	9.06
3	10	2	15.74	15.79	9.41
3	10	3	3.19*	2.43	0.10
3	10	4	26.20	26.02	4.68
3	10	5	11.10	11.77	4.71
3	10	6	3.63*	0.84	0.08
3	10	7	3.56*	3.77	0.06
4	10	-8	2.47*	3.32	0.04
4	10	-7	4.66*	2.70	0.16
4	10	-6	8.93	8.72	3.97
4	10	-5	14.00	14.36	7.60
4	10	-4	6.55*	7.49	0.35
4	10	-3	18.07	17.87	9.64
4	10	-2	21.74	21.44	5.65
4	10	-1	2.77*	3.54	0.13
4	10	0	10.81	10.66	7.90
4	10	1	13.95	13.91	9.84
4	10	2	3.37*	2.80	0.13
4	10	3	10.57	10.50	6.02
4	10	4	16.07	15.35	7.51
4	10	5	3.90*	6.04	0.07
4	10	6	7.07*	6.66	0.26
5	10	-8	6.56*	7.76	0.19
5	10	-7	3.39*	1.91	0.09
5	10	-6	5.86*	2.45	0.45
5	10	-5	6.48*	5.69	0.38
5	10	-4	32.42	32.55	2.40
5	10	-3	8.63	8.71	5.55
5	10	-2	2.78*	0.42	0.13
5	10	-1	5.81	6.39	3.08
5	10	0	13.35	12.64	9.46
5	10	1	4.75*	8.42	0.18
5	10	2	6.77	7.50	2.90
5	10	3	11.18	10.38	5.56
5	10	4	5.22*	4.42	0.21
5	10	5	18.81	18.06	6.78
6	10	6	4.01*	1.78	0.06
6	10	-8	3.70*	3.85	0.07
6	10	-7	3.34*	2.27	0.07
6	10	-6	4.20*	1.93	0.14
6	10	-5	3.71*	3.32	0.11
6	10	-4	3.84*	7.91	0.09
6	10	-3	22.56	23.26	10.06
6	10	-2	9.14	9.28	5.41
6	10	-1	10.47	10.51	6.80
6	10	0	2.41*	0.82	0.06
6	10	1	3.92*	3.84	1.23
6	10	2	18.39	18.12	8.48
6	10	3	3.52*	3.86	0.08
6	10	4	3.43*	1.72	0.08
6	10	5	9.94	9.82	3.06
7	10	-8	5.35*	7.72	0.20
7	10	-7	5.36*	4.98	0.16
7	10	-6	2.80*	0.42	0.07
7	10	-5	11.12	11.80	5.73
7	10	-4	5.86	5.58	2.44
7	10	-3	3.31*	0.96	0.09
7	10	-2	16.32	16.86	8.82
7	10	-1	3.22*	0.12	0.10
7	10	0	10.03	10.17	5.66
7	10	1	10.56	10.82	5.16
7	10	2	9.49	9.01	4.85
7	10	3	2.27*	3.32	0.04
7	10	4	2.92*	0.40	0.05
7	10	5	5.89*	5.86	0.14
8	10	-7	8.88	9.20	3.19
8	10	-6	13.18	14.47	5.65
8	10	-5	3.54*	1.59	0.11
8	10	-4	17.42	16.76	8.14
8	10	-3	3.18*	0.05	0.10
8	10	-2	23.48	23.27	6.04
8	10	-1	12.12	12.06	6.36
8	10	0	3.30*	2.19	0.09
8	10	1	3.10*	3.98	0.08
8	10	2	11.20	11.75	5.07
8	10	3	1.67*	3.10	0.02
8	10	4	11.61	11.13	3.95
9	10	-7	5.27*	4.19	0.13
9	10	-6	6.08*	7.06	0.30
9	10	-5	8.80	9.10	4.09
9	10	-4	5.72*	4.99	0.28
9	10	-3	3.40*	0.59	0.09
9	10	-2	34.14	34.79	2.04
9	10	-1	8.72	8.80	3.87
9	10	0	4.17*	4.77	0.12
9	10	1	16.22	16.58	6.63
9	10	2	13.42	13.40	5.11
9	10	3	3.72*	0.49	0.07
10	10	-7	3.11*	0.90	0.05
10	10	-6	5.75*	3.52	0.15
10	10	-5	14.57	14.10	6.10
10	10	-4	4.93*	2.28	0.23
10	10	-3	14.78	15.24	6.10
10	10	-2	12.92	13.25	5.48
10	10	-1	3.63*	4.00	0.09
10	10	0	3.29*	4.82	0.07
10	10	1	4.13*	3.96	0.10
10	10	2	12.74	12.83	4.33
11	10	-6	3.83*	1.43	0.07
11	10	-5	3.42*	1.57	0.09
11	10	-4	12.96	13.66	4.85
11	10	-3	11.28	12.20	4.38
11	10	-2	6.29*	4.56	0.29
11	10	-1	5.35*	2.76	0.35
11	10	0	4.83*	0.31	1.19
11	10	1	2.05*	1.64	0.24
12	10	-5	8.57	8.34	2.60
12	10	-4	3.46*	1.09	0.08
12	10	-3	6.06*	0.17	0.24
12	10	-2	3.75*	2.95	0.07
12	10	-1	4.32*	2.14	0.13
12	10	0	7.17*	6.85	0.28
0	11	-7	3.75*	1.88	0.07
0	11	-6	3.62*	6.31	0.08
0	11	-5	4.46*	2.58	1.36
0	11	-4	6.76*	9.98	0.23

h	k	l	Fo	Fc	weight
0	11	-3	12.04	12.11	7.90
0	11	-2	9.85	9.58	7.38
0	11	-1	9.14	9.68	6.68
1	11	-7	3.50*	0.16	0.08
1	11	-6	2.98*	2.70	0.61
1	11	-5	17.03	16.50	8.17
1	11	-4	11.08	10.61	7.15
1	11	-3	9.19	8.69	5.76
1	11	-2	4.90*	3.71	0.38
1	11	-1	20.64	20.48	7.26
1	11	0	4.22*	1.68	0.25
1	11	1	19.18	18.67	11.30
1	11	2	11.99	11.38	8.19
1	11	3	9.63	8.73	6.11
1	11	4	20.83	21.31	9.04
1	11	5	24.41	24.87	5.59
1	11	6	19.59	19.53	6.80
1	11	7	4.94*	7.14	0.09
2	11	-8	3.52*	2.89	0.08
2	11	-7	2.39*	6.34	0.03
2	11	-6	6.95*	5.87	0.33
2	11	-5	9.23	9.01	5.02
2	11	-4	5.53*	5.39	0.25
2	11	-3	4.09*	2.98	0.22
2	11	-2	15.19	16.15	10.48
2	11	-1	14.94	14.37	10.79
2	11	0	2.92*	3.54	0.12
2	11	1	4.72*	0.36	0.33
2	11	2	33.45	33.93	2.47
2	11	3	4.47*	2.03	0.20
2	11	4	2.11*	3.30	0.03
2	11	5	2.23*	6.15	0.03
2	11	6	3.60*	1.33	0.08
2	11	7	5.33*	7.28	0.08
3	11	-8	5.06*	2.89	0.16
3	11	-7	15.49	16.49	5.67
3	11	-6	9.81	9.93	4.23
3	11	-5	3.26*	1.74	0.09
3	11	-4	7.67	7.10	4.55
3	11	-3	31.37	31.53	3.00
3	11	-2	3.26*	3.08	1.09
3	11	-1	10.65	11.19	7.26
3	11	0	3.22*	2.40	0.08
3	11	1	3.18*	1.91	0.10
3	11	2	12.69	12.61	8.02
3	11	3	3.06*	0.58	0.11
3	11	4	2.16*	4.64	0.28
3	11	5	11.47	10.95	4.67
3	11	6	3.72*	3.49	0.07
4	11	-8	14.81	14.43	4.48
4	11	-7	3.37*	2.77	0.09
4	11	-6	4.22*	6.82	0.11
4	11	-5	3.52*	3.53	0.08
4	11	-4	20.79	20.63	7.58
4	11	-3	9.87	9.81	6.20
4	11	-2	16.04	15.52	9.91
4	11	-1	5.85*	7.86	0.33
4	11	0	5.23*	6.06	0.21
4	11	1	20.17	19.87	8.28
4	11	2	9.40	8.70	5.35
4	11	3	6.32*	1.99	0.34
4	11	4	3.57*	5.09	0.08
4	11	5	3.48*	5.10	0.08
4	11	6	4.09*	0.05	0.06
5	11	-8	17.14	17.02	5.28
5	11	-7	4.49*	2.22	0.11
5	11	-6	4.83*	4.49	0.16
5	11	-5	3.40*	3.93	0.09
5	11	-4	15.59	15.76	8.21
5	11	-3	29.17	28.57	4.17
5	11	-2	5.73*	5.87	0.37
5	11	-1	3.02*	1.39	0.11
5	11	0	3.17*	1.13	0.10
5	11	1	7.65	8.77	3.71
5	11	2	9.83	10.27	5.64
5	11	3	4.07*	0.54	0.10
5	11	4	12.68	12.40	4.93
5	11	5	5.38*	2.52	0.20
5	11	6	6.48*	5.69	0.20
6	11	-8	4.77*	3.33	0.18
6	11	-7	4.52*	8.69	0.10
6	11	-6	6.91*	7.60	0.28
6	11	-5	6.03*	6.41	0.27
6	11	-4	6.00*	5.89	0.21
6	11	-3	2.06*	1.95	0.04
6	11	-2	8.04	8.33	4.60
6	11	-1	13.02	12.95	7.76
6	11	0	4.89*	6.43	0.17
6	11	1	4.32*	5.20	1.49
6	11	2	4.34*	4.84	1.29
6	11	3	6.36*	3.29	0.36
6	11	4	3.73*	5.32	0.07
6	11	5	4.30*	5.48	0.12
7	11	-7	3.44*	2.64	0.08
7	11	-6	3.16*	0.45	0.10
7	11	-5	3.55*	1.64	0.15
7	11	-4	4.10*	2.77	1.22
7	11	-3	3.35*	2.13	0.11
7	11	-2	10.70	9.53	5.76
7	11	-1	7.28	6.30	3.84
7	11	0	5.18*	3.97	0.22
7	11	1	3.75*	4.61	0.10
7	11	2	1.58*	2.51	0.17
7	11	3	5.21*	0.62	0.17
7	11	4	10.24	9.72	3.29
8	11	-7	2.14*	0.24	0.22
8	11	-6	3.47*	0.41	0.08
8	11	-5	5.39*	7.03	0.16
8	11	-4	10.07	11.34	4.68
8	11	-3	20.78	22.07	7.60
8	11	-2	4.85*	6.52	0.16
8	11	-1	12.49	13.06	5.74
8	11	0	8.22	8.15	3.73
8	11	1	3.56*	4.54	0.09
8	11	2	25.06	24.75	5.59
8	11	3	6.39*	3.58	0.28
8	11	4	11.12	11.29	3.57
9	11	-7	3.61*	0.01	0.08
9	11	-6	5.55	6.22	1.39
9	11	-5	7.73	6.92	2.46
9	11	-4	1.63*	4.48	0.03
9	11	-3	25.30	25.28	5.69
9	11	-2	5.74*	1.60	0.34
9	11	-1	6.77*	8.68	0.26
9	11	0	6.06*	2.36	0.31
9	11	1	5.24*	3.53	0.28
9	11	2	4.52*	3.29	0.12
9	11	3	6.66	7.70	1.63
10	11	-6	7.08*	7.78	0.23
10	11	-5	3.56*	0.38	0.08
10	11	-4	4.76*	4.34	0.18
10	11	-3	5.25*	4.89	0.18
10	11	-2	10.04	9.55	3.92
10	11	-1	6.44*	1.15	0.38
10	11	0	10.28	10.07	4.02
10	11	1	22.35	22.62	6.54
10	11	2	9.87	10.71	2.90
11	11	-5	3.07*	6.98	0.04
11	11	-4	3.54*	2.82	0.08
11	11	-3	7.30*	7.52	0.27
11	11	-2	3.46*	1.86	0.08
11	11	-1	3.80*	2.92	0.07
11	11	0	6.33*	6.46	0.21
11	11	1	16.66	16.54	4.93
12	11	-4	7.20*	4.76	0.28
12	11	-3	3.64*	1.38	0.08
12	11	-2	3.33*	0.66	0.09
12	11	-1	3.75*	2.06	0.07
0	12	-7	3.70*	1.15	0.07
0	12	-6	3.33*	4.46	0.64
0	12	-5	11.74	11.49	5.65
0	12	-4	11.20	11.58	5.94
0	12	-3	20.77	20.36	9.85
0	12	-2	7.04	6.83	4.11
0	12	-1	6.44*	8.76	0.35
0	12	0	33.59	33.93	2.50
1	12	-7	8.54	8.53	2.79
1	12	-6	10.40	10.01	4.14
1	12	-5	9.81	10.36	4.36
1	12	-4	3.92*	0.44	0.13
1	12	-3	4.49*	2.02	0.28
1	12	-2	4.34*	3.07	0.23
1	12	-1	31.60	30.85	2.57
1	12	0	28.60	28.64	3.83
1	12	1	3.27*	3.34	0.09
1	12	2	5.20*	5.69	0.20
1	12	3	3.35*	2.07	0.09
1	12	4	4.28*	0.77	0.14
1	12	5	30.62	29.86	3.32
1	12	6	10.07	9.66	3.21
1	12	7	8.19	6.82	2.70
2	12	-7	3.62*	0.16	0.08
2	12	-6	4.01*	2.65	0.11
2	12	-5	3.41*	3.76	0.09
2	12	-4	5.73*	5.68	0.36
2	12	-3	18.43	17.96	9.73
2	12	-2	12.62	11.29	8.97
2	12	-1	14.61	15.60	9.16
2	12	0	10.64	10.81	7.33
2	12	1	13.89	13.01	8.37
2	12	2	13.77	13.65	8.26
2	12	3	6.40*	4.02	0.31
2	12	4	3.36*	2.06	0.09
2	12	5	13.05	12.28	5.12
2	12	6	11.65	10.94	4.52
3	12	-7	1.73*	5.36	0.02
3	12	-6	14.94	15.45	5.87
3	12	-5	9.68	10.71	4.21
3	12	-4	3.93*	5.59	0.12
3	12	-3	13.32	13.21	8.07
3	12	-2	26.78	26.08	4.21
3	12	-1	8.46	8.74	5.38
3	12	0	5.99	5.29	3.66
3	12	1	3.22*	1.20	0.10
3	12	2	11.86	11.66	6.78
3	12	3	3.36*	6.52	0.08
3	12	4	14.62	14.52	6.72
3	12	5	15.18	15.09	5.75
3	12	6	12.39	11.38	4.31
4	12	-7	8.69	8.67	3.08
4	12	-6	2.84*	1.70	0.06
4	12	-5	9.62	9.84	4.57
4	12	-4	18.34	17.95	8.63
4	12	-3	3.31*	1.92	0.09
4	12	-2	14.57	13.82	8.75
4	12	-1	2.56*	5.23	0.56
4	12	0	9.00	8.56	5.32
4	12	1	5.17*	6.10	0.21
4	12	2	2.96*	2.52	0.10
4	12	3	2.67*	0.57	0.06
4	12	4	2.09*	0.32	0.23
4	12	5	3.47*	2.55	0.08
4	12	6	8.79	9.22	2.24
5	12	-7	12.23	12.37	4.41
5	12	-6	3.69*	2.18	0.07
5	12	-5	5.47*	6.37	0.20
5	12	-4	3.30*	1.79	0.09
5	12	-3	15.05	15.18	8.06
5	12	-2	13.79	14.37	8.03
5	12	-1	14.43	14.32	8.18
5	12	0	17.00	17.34	8.28
5	12	1	3.39*	1.06	0.09
5	12	2	14.28	14.29	7.19
5	12	3	3.53*	5.40	0.08
5	12	4	10.78	10.01	4.49
5	12	5	6.75*	7.15	0.26
6	12	-7	3.03*	5.30	0.05
6	12	-6	3.65*	2.81	0.08
6	12	-5	2.78*	3.34	0.10
6	12	-4	4.50*	4.11	1.40
6	12	-3	10.21	10.35	5.40
6	12	-2	11.11	10.28	6.58

h	k	l	Fo	Fc	weight
6	12	-1	2.96*	0.67	0.07
6	12	0	5.97*	4.92	0.29
6	12	1	3.47*	0.33	0.08
6	12	2	8.11	7.29	3.73
6	12	3	13.16	12.72	5.61
6	12	4	3.73*	0.31	0.07
6	12	5	8.52	8.57	2.64
7	12	-7	3.40*	2.39	0.09
7	12	-6	6.12*	8.21	0.25
7	12	-5	6.16	6.39	1.98
7	12	-4	6.72*	2.51	0.34
7	12	-3	3.47*	0.61	0.08
7	12	-2	12.94	13.57	6.75
7	12	-1	31.02	31.45	2.68
7	12	0	3.46*	3.02	0.08
7	12	1	3.52*	4.81	0.08
7	12	2	7.46*	7.30	0.23
7	12	3	21.85	20.57	6.81
7	12	4	15.65	15.70	4.80
8	12	-7	7.19*	9.28	0.21
8	12	-6	10.90	10.16	4.49
8	12	-5	3.66*	4.29	0.07
8	12	-4	2.81*	5.53	0.06
8	12	-3	4.78*	1.74	0.19
8	12	-2	17.61	17.83	7.37
8	12	-1	11.96	11.18	6.14
8	12	0	3.42*	0.86	0.09
8	12	1	4.01*	4.99	0.10
8	12	2	9.94	9.84	3.42
8	12	3	3.66*	0.75	0.07
9	12	-6	9.76	9.82	3.39
9	12	-5	8.16	7.95	2.93
9	12	-4	3.44*	1.80	0.08
9	12	-3	11.29	11.02	4.68
9	12	-2	12.11	12.06	4.88
9	12	-1	10.52	10.86	4.06
9	12	0	6.22*	7.58	0.19
9	12	1	3.40*	3.91	0.10
9	12	2	7.22*	7.64	0.21
10	12	-5	6.34*	4.47	0.27
10	12	-4	5.17*	4.63	0.16
10	12	-3	10.24	10.25	3.81
10	12	-2	7.31	7.62	2.47
10	12	-1	4.51*	3.10	0.16
10	12	0	9.35	8.94	3.47
10	12	1	1.77*	5.03	0.02
11	12	-4	3.46*	2.34	0.08
11	12	-3	8.39	9.47	2.70
11	12	-2	3.52*	1.23	0.08
11	12	-1	3.66*	2.13	0.07
11	12	0	5.08*	6.42	0.18
0	13	-6	11.99	11.85	4.74
0	13	-5	10.28	11.34	3.87
0	13	-4	6.38*	8.38	0.26
0	13	-3	5.73	6.58	2.24
0	13	-2	14.76	15.08	8.22
0	13	-1	4.22*	1.51	0.21
1	13	-7	3.55*	0.94	0.08
1	13	-6	20.42	20.54	6.20
1	13	-5	3.60*	4.12	0.08
1	13	-4	8.28	9.06	3.39
1	13	-3	5.12*	6.05	0.19
1	13	-2	23.60	24.24	5.03
1	13	-1	3.14*	1.84	0.12
1	13	0	4.43*	3.53	0.20
1	13	1	13.33	13.28	7.39
1	13	2	12.77	12.78	6.92
1	13	3	3.63*	3.59	0.08
1	13	4	3.55*	3.12	0.08
1	13	5	2.85*	3.23	0.04
1	13	6	6.00	6.73	1.36
2	13	-7	13.52	12.37	4.96
2	13	-6	6.07*	3.37	0.27
2	13	-5	12.21	12.08	5.48
2	13	-4	3.76*	4.26	0.12
2	13	-3	2.96*	3.38	0.08
2	13	-2	4.77*	3.80	0.24
2	13	-1	24.87	24.77	5.66
2	13	0	9.16	8.17	5.53
2	13	1	5.36*	1.68	0.23
2	13	2	5.09*	0.49	0.25
2	13	3	7.83	9.01	3.27
2	13	4	5.03*	3.17	0.21
2	13	5	3.34*	4.22	0.06
2	13	6	7.25*	6.22	0.23
3	13	-7	14.41	14.50	5.15
3	13	-6	4.72*	5.19	1.14
3	13	-5	6.81*	9.80	0.24
3	13	-4	3.37*	1.80	0.09
3	13	-3	3.51*	3.88	0.08
3	13	-2	20.61	20.61	6.27
3	13	-1	18.01	18.38	8.72
3	13	0	3.21*	3.12	0.09
3	13	1	10.51	11.61	5.15
3	13	2	5.89*	2.31	0.30
3	13	3	6.17	4.76	2.50
3	13	4	1.62*	2.26	0.02
3	13	5	8.76	9.48	2.76
3	13	6	7.39*	7.43	0.18
4	13	-7	3.49*	0.95	0.08
4	13	-6	6.31*	8.00	0.20
4	13	-5	3.42*	0.12	0.09
4	13	-4	10.33	11.09	5.07
4	13	-3	17.01	17.28	8.06
4	13	-2	23.43	23.52	5.91
4	13	-1	9.59	10.79	4.83
4	13	0	1.47*	3.55	0.02
4	13	1	2.88*	2.03	0.10
4	13	2	18.62	19.14	7.91
4	13	3	10.32	10.59	4.55
4	13	4	4.98*	3.29	0.16
4	13	5	3.59*	0.58	0.08
5	13	-7	1.78*	0.26	0.02
5	13	-6	2.40*	2.33	0.03
5	13	-5	2.82*	0.33	0.06
5	13	-4	3.51*	2.39	0.08
5	13	-3	1.53*	6.19	0.01
5	13	-2	3.50*	4.12	0.08
5	13	-1	15.59	15.52	7.41
5	13	0	24.73	24.51	5.67
5	13	1	2.17*	2.14	0.03
5	13	2	5.68*	2.60	0.23
5	13	3	13.60	14.14	5.58
5	13	4	5.65*	3.00	0.21
5	13	5	3.57*	0.85	0.07
6	13	-7	3.59*	1.41	0.08
6	13	-6	5.95*	2.57	0.30
6	13	-5	3.56*	3.97	0.08
6	13	-4	7.54	8.07	3.14
6	13	-3	12.56	13.08	5.86
6	13	-2	6.15*	3.96	0.29
6	13	-1	4.60*	3.81	0.14
6	13	0	5.79*	2.61	0.21
6	13	1	8.52	8.83	3.53
6	13	2	9.74	9.86	3.83
6	13	3	13.41	13.70	4.94
6	13	4	6.07*	6.98	0.17
7	13	-6	4.61*	3.16	0.12
7	13	-5	7.80	8.14	2.75
7	13	-4	3.47*	1.29	0.08
7	13	-3	11.14	11.55	5.65
7	13	-2	29.73	30.41	3.36
7	13	-1	5.29	5.58	1.55
7	13	0	5.76*	5.21	0.33
7	13	1	5.40*	6.42	0.20
7	13	2	17.55	17.26	5.97
7	13	3	6.89	8.26	1.72
8	13	-6	4.69*	2.55	0.15
8	13	-5	4.20*	6.05	0.10
8	13	-4	3.49*	2.48	0.08
8	13	-3	3.29*	4.13	0.06
8	13	-2	5.40*	4.56	0.16
8	13	-1	3.66*	3.77	0.07
8	13	0	3.57*	1.54	0.08
8	13	1	6.96	6.59	2.52
8	13	2	7.55*	6.80	0.28
8	13	3	10.21	10.04	3.07
9	13	-5	3.51*	3.93	0.08
9	13	-4	2.97*	0.11	0.08
9	13	-3	6.82	6.02	2.25
9	13	-2	2.38*	1.48	0.05
9	13	-1	3.77*	0.25	0.13
9	13	0	3.42*	3.90	0.07
9	13	1	13.55	13.12	4.78
9	13	2	10.45	10.44	3.23
10	13	-5	2.83*	3.47	0.40
10	13	-4	2.78*	4.23	0.37
10	13	-3	5.52*	1.52	0.20
10	13	-2	3.69*	0.27	0.07
10	13	-1	3.79*	4.01	0.07
10	13	0	3.64*	1.87	0.08
11	13	-2	7.76	7.98	2.19
0	14	-6	4.65*	1.48	0.16
0	14	-5	11.85	10.22	4.66
0	14	-4	4.81*	6.60	0.11
0	14	-3	2.47*	4.95	0.41
0	14	-2	7.23	7.14	2.95
0	14	-1	13.61	13.59	7.07
0	14	0	3.40*	1.52	0.09
1	14	-6	6.28*	2.50	0.22
1	14	-5	7.98	9.33	2.53
1	14	-4	3.56*	3.82	0.10
1	14	-3	15.73	16.24	7.25
1	14	-2	7.52	8.19	3.36
1	14	-1	14.26	13.61	7.71
1	14	0	3.43*	2.49	0.09
1	14	1	22.33	22.17	6.09
1	14	2	3.64*	3.01	0.08
1	14	3	3.11*	3.57	0.07
1	14	4	9.71	8.69	3.85
1	14	5	2.39*	5.90	0.02
1	14	6	5.33*	0.72	0.20
2	14	-6	5.48*	6.78	0.17
2	14	-5	10.44	10.43	4.60
2	14	-4	3.40*	2.37	0.09
2	14	-3	9.69	9.36	4.78
2	14	-2	3.35*	3.24	0.10
2	14	-1	28.16	29.11	3.69
2	14	0	23.41	23.38	4.82
2	14	1	17.84	16.93	8.49
2	14	2	2.16*	0.08	0.04
2	14	3	5.24*	5.83	0.23
2	14	4	8.62	8.79	3.33
2	14	5	9.10	8.96	2.84
3	14	-6	10.67	11.07	4.01
3	14	-5	6.42*	5.84	0.23
3	14	-4	11.57	11.03	6.10
3	14	-3	4.63*	5.46	0.16
3	14	-2	10.41	10.42	5.18
3	14	-1	20.00	19.74	9.18
3	14	0	3.64*	5.36	0.08
3	14	1	4.80*	1.87	0.18
3	14	2	4.92*	1.19	0.19
3	14	3	7.21	7.28	2.44
3	14	4	10.82	11.13	3.86
4	14	-6	3.42*	0.03	0.09
4	14	-5	6.88	6.45	2.34
4	14	-4	3.49*	0.16	0.08
4	14	-3	5.18*	3.82	0.25
4	14	-2	1.53*	4.49	0.01
4	14	-1	12.94	12.95	6.07
4	14	0	15.24	15.41	7.32
4	14	1	8.23	7.73	3.45
4	14	2	3.34*	1.59	0.09
4	14	3	16.85	16.82	6.28
4	14	4	15.82	15.82	5.30
4	14	5	3.58*	5.41	0.05
5	14	-6	7.41*	8.54	0.28
5	14	-5	4.44*	5.78	0.12
5	14	-4	9.68	9.71	4.40
5	14	-3	7.61	6.78	3.69

h	k	l	Fo	Fc	weight
5	14	-2	13.16	13.33	6.54
5	14	-1	21.76	22.41	6.08
5	14	0	1.56*	6.39	0.02
5	14	1	4.76*	3.56	0.21
5	14	2	3.53*	1.60	0.08
5	14	3	1.68*	0.86	0.02
5	14	4	5.54*	0.47	0.22
6	14	-6	3.54*	0.58	0.08
6	14	-5	8.25	7.70	3.02
6	14	-4	4.04*	7.15	0.09
6	14	-3	2.80*	3.28	0.07
6	14	-2	14.47	14.70	5.83
6	14	-1	19.89	20.30	7.98
6	14	0	3.51*	2.16	0.08
6	14	1	10.40	10.51	4.18
6	14	2	3.27*	0.29	0.09
6	14	3	6.24*	4.44	0.26
6	14	4	12.31	10.97	4.49
7	14	-6	4.00*	9.01	0.06
7	14	-5	9.58	8.71	3.52
7	14	-4	3.49*	3.42	0.08
7	14	-3	13.48	13.59	5.27
7	14	-2	16.59	15.72	6.41
7	14	-1	17.91	17.45	6.64
7	14	0	5.94*	6.22	0.21
7	14	1	4.11*	3.82	0.10
7	14	2	5.45*	1.30	0.29
7	14	3	8.27	7.84	2.37
8	14	-5	3.77*	1.63	0.07
8	14	-4	3.87*	3.10	0.07
8	14	-3	5.08*	3.98	0.14
8	14	-2	6.23	7.20	1.79
8	14	-1	11.28	11.43	4.04
8	14	0	8.73	8.25	2.91
8	14	1	9.01	9.29	2.97
8	14	2	3.79*	6.89	0.07
9	14	-5	1.80*	4.56	0.01
9	14	-4	4.67*	3.46	0.11
9	14	-3	3.48*	4.24	0.08
9	14	-2	14.33	14.30	5.21
9	14	-1	3.86*	1.31	0.07
9	14	0	5.27*	3.91	0.18
9	14	1	9.33	10.30	2.47
10	14	-3	3.58*	1.08	0.08
10	14	-2	3.61*	2.72	0.08
10	14	-1	3.59*	3.33	0.07
0	15	-5	3.81*	2.50	0.07
0	15	-4	9.99	10.42	3.61
0	15	-3	12.79	12.00	6.15
0	15	-2	17.24	17.87	7.13
0	15	-1	3.40*	1.67	0.09
1	15	-6	6.94*	1.00	0.25
1	15	-5	7.25	6.41	2.44
1	15	-4	5.62	5.91	1.59
1	15	-3	1.59*	4.02	0.02
1	15	-2	4.67*	1.75	0.17
1	15	-1	5.53*	8.18	0.17
1	15	0	16.45	16.85	7.12
1	15	1	3.29*	1.81	0.09
1	15	2	15.37	14.92	7.18
1	15	3	10.45	10.83	3.92
1	15	4	14.14	14.62	5.10
1	15	5	3.70*	0.55	0.07
2	15	-6	5.92*	4.08	0.21
2	15	-5	5.13*	0.64	0.20
2	15	-4	6.58*	10.56	0.21
2	15	-3	14.15	13.71	6.40
2	15	-2	3.49*	5.62	0.09
2	15	-1	3.54*	5.04	0.08
2	15	0	1.54*	0.19	0.02
2	15	1	3.69*	2.45	0.07
2	15	2	12.86	12.99	5.63
2	15	3	14.57	13.89	5.61
2	15	4	5.37	6.09	1.33
2	15	5	6.42	6.87	1.62
3	15	-6	3.67*	0.80	0.07
3	15	-5	5.67*	7.70	0.13
3	15	-4	1.65*	5.70	0.01
3	15	-3	6.80*	8.03	0.27
3	15	-2	6.65	7.37	2.66
3	15	-1	6.68	6.51	2.37
3	15	0	13.45	13.30	6.27
3	15	1	3.38*	4.56	0.09
3	15	2	6.65*	7.72	0.27
3	15	3	5.76*	10.87	0.15
3	15	4	7.32*	7.78	0.27
3	15	5	6.24*	2.24	0.21
4	15	-6	6.44*	1.49	0.27
4	15	-5	2.43*	1.72	0.05
4	15	-4	8.26	9.14	3.31
4	15	-3	1.62*	3.50	0.02
4	15	-2	9.70	9.65	4.72
4	15	-1	7.39	7.91	2.85
4	15	0	16.22	16.63	6.96
4	15	1	10.15	9.39	4.18
4	15	2	6.84	7.69	2.05
4	15	3	3.61*	1.50	0.08
4	15	4	4.31*	2.63	0.11
5	15	-6	3.74*	1.90	0.07
5	15	-5	4.24*	2.40	0.13
5	15	-4	4.44*	9.37	0.09
5	15	-3	1.64*	3.66	0.02
5	15	-2	14.17	13.59	6.31
5	15	-1	3.69*	1.41	0.07
5	15	0	9.97	9.46	4.29
5	15	1	1.64*	1.97	0.02
5	15	2	6.07*	5.13	0.22
5	15	3	8.14	7.29	2.72
5	15	4	6.98*	7.34	0.20
6	15	-5	2.48*	4.52	0.02
6	15	-4	3.49*	2.02	0.08
6	15	-3	3.06*	1.17	0.11
6	15	-2	21.67	22.09	6.80
6	15	-1	5.20*	2.81	0.17
6	15	0	3.72*	5.42	0.07
6	15	1	7.31	7.52	2.51
6	15	2	15.07	14.78	5.40
6	15	3	8.75	7.81	2.74
7	15	-5	5.03*	4.32	0.16
7	15	-4	5.12*	6.20	1.27
7	15	-3	2.41*	2.64	0.30
7	15	-2	4.47*	4.26	0.11
7	15	-1	5.34*	0.51	0.30
7	15	0	12.41	12.34	4.66
7	15	1	3.57*	1.32	0.08
7	15	2	3.54*	0.97	0.08
8	15	-4	5.67*	3.56	0.17
8	15	-3	4.40*	3.90	0.89
8	15	-2	6.25*	3.83	0.26
8	15	-1	5.75*	1.29	0.18
8	15	0	4.95*	5.77	0.12
8	15	1	3.49*	1.19	0.08
9	15	-3	10.44	9.89	4.20
9	15	-2	3.08*	5.28	0.04
9	15	-1	10.68	10.89	3.40
0	16	-5	7.12*	3.82	0.26
0	16	-4	2.42*	5.84	0.03
0	16	-3	4.41*	4.47	1.10
0	16	-2	2.29*	1.10	0.07
0	16	-1	3.64*	5.45	0.08
0	16	0	27.44	27.82	4.65
1	16	-5	11.22	11.08	3.63
1	16	-4	3.41*	3.58	0.07
1	16	-3	3.82*	1.52	0.07
1	16	-2	3.74*	6.15	0.07
1	16	-1	3.91*	2.45	0.16
1	16	0	10.78	11.57	4.22
1	16	1	19.38	19.29	7.77
1	16	2	3.47*	0.78	0.08
1	16	3	4.06*	3.46	0.99
1	16	4	4.24*	1.39	0.10
1	16	5	8.32	8.26	2.24
2	16	-5	3.73*	1.06	0.07
2	16	-4	6.14*	3.06	0.21
2	16	-3	3.62*	1.92	0.08
2	16	-2	16.38	15.79	6.54
2	16	-1	16.45	15.77	6.63
2	16	0	11.52	12.53	4.88
2	16	1	3.70*	1.27	0.07
2	16	2	3.14*	1.60	0.10
2	16	3	3.39*	5.71	0.05
2	16	4	15.70	15.11	5.20
3	16	-5	3.20*	3.77	0.47
3	16	-4	5.12*	8.41	0.18
3	16	-3	10.85	11.18	4.00
3	16	-2	3.54*	4.16	0.08
3	16	-1	15.77	16.31	6.04
3	16	0	14.66	15.10	6.20
3	16	1	2.84*	2.16	0.06
3	16	2	6.03*	4.95	0.17
3	16	3	8.28	8.68	2.42
3	16	4	7.70	6.88	2.38
4	16	-5	3.60*	0.30	0.08
4	16	-4	6.65*	5.40	0.20
4	16	-3	7.89	9.63	2 54
4	16	-2	5.22*	4.79	0.18
4	16	-1	6.76*	5.44	0.28
4	16	0	7.05	6.66	2.34
4	16	1	8.02	8.10	2.79
4	16	2	3.66*	1.22	0.07
4	16	3	3.94*	0.84	0.06
5	16	-5	15.16	14.74	5.51
5	16	-4	6.60	5.42	2.01
5	16	-3	3.59*	4.24	0.08
5	16	-2	3.83*	3.96	0.06
5	16	-1	19.98	20.29	6.50
5	16	0	19.41	19.92	6.67
5	16	1	5.10*	0.84	0.24
5	16	2	3.68*	1.19	0.07
5	16	3	3.58*	6.50	0.06
6	16	-4	12.14	12.47	4.25
6	16	-3	3.64*	3.01	0.08
6	16	-2	3.82*	1.68	0.13
6	16	-1	3.81*	0.54	0.11
6	16	0	2.42*	2.76	0.03
6	16	1	6.03	5.84	1.67
6	16	2	7.34*	6.79	0.28
7	16	-4	5.93*	2.74	0.29
7	16	-3	1.76*	0.06	0.02
7	16	-2	4.61*	0.48	0.21
7	16	-1	10.20	11.21	3.55
7	16	0	4.09*	5.06	0.71
7	16	1	12.59	12.71	4.02
8	16	-3	3.77*	0.42	0.07
8	16	-2	6.31	7.23	1.74
8	16	-1	6.07	5.61	1.73
0	17	-4	5.32*	6.40	0.17
0	17	-3	3.65*	2.45	0.08
0	17	-2	2.91*	2.11	0.07
0	17	-1	4.69*	1.77	0.13
1	17	-4	9.17	9.92	2.89
1	17	-3	9.61	8.80	3.97
1	17	-2	3.57*	2.91	0.08
1	17	-1	5.25*	4.78	0.21
1	17	0	6.82*	7.06	0.24
1	17	1	5.00*	7.15	0.09
1	17	2	3.60*	1.47	0.08
1	17	3	6.48*	10.51	0.16
1	17	4	5.36*	0.68	0.20
2	17	-4	3.83*	0.38	0.07
2	17	-3	3.43*	0.73	0.10
2	17	-2	3.51*	2.81	0.08
2	17	-1	3.28*	1.20	0.09
2	17	0	14.91	15.39	5.71
2	17	1	5.12*	6.27	1.12
2	17	2	3.46*	2.71	0.08
2	17	3	3.65*	1.63	0.08
3	17	-4	3.74*	4.93	0.07
3	17	-3	2.98*	2.80	0.06
3	17	-2	3.79*	6.71	0.08
3	17	-1	7.90	8.79	2.52
3	17	0	6.83*	7.38	0.19

h	k	l	Fo	Fc	weight
3	17	1	14.03	14.83	5.00
3	17	2	3.66*	3.89	0.07
3	17	3	3.79*	1.74	0.07
4	17	-4	6.15*	1.83	0.23
4	17	-3	8.01	8.22	2.65
4	17	-2	15.07	15.41	5.42
4	17	-1	4.81*	7.34	0.14
4	17	0	6.41	6.46	1.82
4	17	1	5.46*	3.02	0.26
4	17	2	7.47*	9.72	0.24
5	17	-4	3.61*	0.35	0.08
5	17	-3	3.59*	4.14	0.08
5	17	-2	3.50*	1.49	0.08
5	17	-1	10.82	11.41	3.55
5	17	0	6.50*	7.02	0.20
5	17	1	3.73*	0.61	0.07
5	17	2	5.95*	2.40	0.21
6	17	-3	9.53	10.06	2.90
6	17	-2	3.53*	0.31	0.07
6	17	-1	3.63*	0.44	0.08
6	17	0	5.88*	4.64	0.16
6	17	1	14.11	13.13	4.79
7	17	-2	3.68*	2.51	0.07
7	17	-1	3.77*	0.76	0.07
0	18	-3	3.45*	4.66	0.08
0	18	-2	8.46	8.19	2.79
0	18	-1	11.76	10.59	4.76
0	18	0	17.59	17.16	5.68
1	18	-3	3.34*	4.21	0.56
1	18	-2	3.90*	1.02	0.07
1	18	-1	3.85*	1.84	0.08
1	18	0	6.66*	6.66	0.23
1	18	1	3.46*	1.96	0.08
1	18	2	5.82*	3.84	0.22
1	18	3	7.61*	7.70	0.20
2	18	-3	4.35*	0.25	0.13
2	18	-2	4.02*	3.33	0.06
2	18	-1	8.78	9.27	2.90
2	18	0	7.33*	6.58	0.25
2	18	1	4.27*	2.33	0.12
2	18	2	3.96*	0.70	0.11
3	18	-3	3.74*	2.96	0.07
3	18	-2	3.41*	4.55	0.64
3	18	-1	6.52*	4.82	0.30
3	18	0	3.90*	3.83	0.12
3	18	1	3.47*	2.66	0.08
3	18	2	1.78*	3.75	0.02
4	18	-3	3.90*	0.84	0.07
4	18	-2	9.86	9.86	3.08
4	18	-1	2.49*	3.34	0.03
4	18	0	3.68*	3.86	0.07
4	18	1	3.57*	1.08	0.08
5	18	-2	2.54*	1.24	0.04
5	18	-1	6.61	7.10	1.61
5	18	0	5.68*	2.84	0.19
0	19	-1	8.18	8.61	2.38
1	19	-1	3.91*	1.19	0.07
1	19	0	3.67*	1.09	0.07
1	19	1	4.03*	4.40	0.06
2	19	-1	3.44*	1.95	0.08
2	19	0	4.39*	3.41	0.14

2845 reflections

a twistane derivative (twistenone)

h	k	l	Fo	Fc	weight
0	0	2	0.91*	1.01	1.21
0	0	4	9.53	9.17	28.30
0	0	6	6.63	7.13	41.70
0	0	8	1.57*	1.08	0.41
1	0	7	1.67*	1.59	0.72
1	0	5	6.81	6.93	45.58
1	0	3	28.64	27.16	2.66
1	0	1	13.43	13.74	10.43
1	0	-1	53.58	56.10	0.86
1	0	-3	25.20	25.12	3.41
1	0	-5	8.81	8.50	51.22
1	0	-7	3.40	2.59	14.76
2	0	-8	6.18	5.89	25.45
2	0	-6	9.82	10.16	36.69
2	0	-4	29.08	28.37	2.54
2	0	-2	29.48	29.17	2.63
2	0	0	44.50	45.30	1.22
2	0	2	6.52	6.39	79.93
2	0	4	15.54	15.64	8.52
2	0	6	3.05	2.80	13.35
3	0	5	7.89	7.51	41.11
3	0	3	12.15	12.70	17.63
3	0	1	15.16	14.82	10.53
3	0	-1	42.47	42.32	1.31
3	0	-3	24.25	23.36	3.48
3	0	-5	8.46	8.11	54.43
3	0	-7	7.12	7.48	33.81
4	0	-8	1.64*	0.53	0.37
4	0	-6	1.46*	0.04	0.47
4	0	-4	16.95	16.90	7.76
4	0	-2	11.04	10.91	21.21
4	0	0	7.81	8.44	52.26
4	0	2	4.52	4.84	35.45
4	0	4	4.41	4.96	27.74
4	0	6	4.08	3.03	13.11
5	0	5	2.33*	1.64	0.78
5	0	3	1.28*	0.69	0.56
5	0	1	8.45	9.02	42.60
5	0	-1	2.44	2.11	15.92
5	0	-3	32.43	32.78	1.99
5	0	-5	10.85	11.49	22.38
5	0	-7	2.84*	2.50	1.50
6	0	-6	5.71	5.44	24.01
6	0	-4	1.39*	1.40	0.58
6	0	-2	3.93	3.90	25.41
6	0	0	13.09	13.33	18.66
6	0	2	1.51*	1.71	0.44
7	0	1	1.55*	0.38	0.42
7	0	-1	2.58*	1.00	1.65
7	0	-3	2.40*	0.07	1.49
7	0	-5	1.65*	1.83	0.37
8	0	-4	1.48*	3.47	0.31
8	0	-2	4.45	4.24	16.36
8	1	-1	2.65*	2.71	0.98
8	1	-2	1.93*	0.84	0.79
8	1	-3	1.40*	0.42	0.51
8	1	-4	2.42*	2.13	5.95
7	1	-6	1.63*	2.39	0.45
7	1	-5	0.99*	2.62	0.11
7	1	-4	1.37*	0.73	0.53
7	1	-3	2.58*	2.78	1.36
7	1	-2	4.61	4.32	20.05
7	1	-1	1.36*	1.08	0.84
7	1	0	2.26*	2.33	1.23
7	1	1	1.55*	1.17	0.42
7	1	2	3.19*	2.60	1.23
6	1	3	1.41*	2.58	0.32
6	1	2	1.46*	1.49	0.47
6	1	1	1.84*	2.74	0.42
6	1	0	1.41*	0.12	0.50
6	1	-1	8.55	8.37	45.23
6	1	-2	9.33	9.39	46.36
6	1	-3	9.75	9.89	32.59
6	1	-4	2.49	3.03	11.90
6	1	-5	1.30*	0.19	0.34
6	1	-6	1.50*	1.10	0.44
6	1	-7	1.60*	0.27	0.39
5	1	-8	4.96	4.86	15.36
5	1	-7	2.18*	0.56	1.45
5	1	-6	1.36*	1.09	0.54
5	1	-5	7.22	7.67	40.78
5	1	-4	3.47	3.64	21.83
5	1	-3	1.08*	2.53	0.27
5	1	-2	2.06*	3.09	1.08
5	1	-1	0.92*	1.34	0.36
5	1	0	2.85	2.60	16.76
4	1	1	7.63	7.57	48.08
4	1	2	3.15	3.21	17.76
4	1	3	1.69*	1.45	0.66
4	1	4	2.38*	1.70	1.30
4	1	5	4.10	3.40	12.97
4	1	6	2.56*	1.83	1.05
4	1	5	1.52*	1.15	0.43
4	1	4	1.45*	0.61	0.47
4	1	3	15.91	15.63	10.08
4	1	2	15.50	15.19	8.31
4	1	1	18.57	18.53	4.78
4	1	0	2.47	2.35	23.58
4	1	-1	6.59	6.25	69.72
4	1	-2	16.60	15.52	8.75
4	1	-3	0.49*	0.52	0.11
4	1	-4	7.33	7.56	56.32
4	1	-5	8.05	8.27	46.90
4	1	-6	9.82	10.04	31.06
4	1	-7	1.88*	1.10	0.79
4	1	-8	5.01	4.97	15.88
3	1	-8	1.58*	1.87	0.37
3	1	-7	3.03*	3.06	1.61
3	1	-6	7.44	7.21	42.93
3	1	-5	7.25	7.03	81.55
3	1	-4	7.59	7.92	55.42
3	1	-3	11.35	11.10	18.29
3	1	-2	3.28	3.38	46.24
3	1	-1	17.76	16.95	5.92
3	1	0	11.60	11.90	19.02
3	1	1	19.80	19.79	4.80
3	1	2	6.88	6.69	69.74
3	1	3	6.27	6.17	55.95
3	1	4	2.70*	3.88	1.49
3	1	5	1.67*	0.61	0.96
3	1	6	3.01*	2.83	1.74
2	1	5	2.44	2.64	6.32
2	1	6	3.92	4.25	19.22
2	1	5	8.37	8.71	45.74
2	1	4	4.06	4.36	36.59
2	1	3	6.10	5.87	67.72
2	1	2	29.43	29.19	2.55
2	1	1	4.04	4.21	86.62
2	1	0	47.61	48.53	1.07
2	1	-1	18.81	18.97	5.84
2	1	-2	3.80	3.69	78.39
2	1	-3	2.24	2.29	25.91
2	1	-4	7.11	7.35	68.33
2	1	-5	1.58*	1.78	6.29
2	1	-6	5.55	5.72	33.30
2	1	-7	1.39*	0.38	0.51
2	1	-8	2.18*	2.01	4.32
1	1	-8	1.71*	0.68	0.34
1	1	-7	2.04*	0.61	0.91
1	1	-6	16.12	16.31	7.20
1	1	-5	14.15	14.47	12.12
1	1	-4	13.01	12.27	15.24
1	1	-3	2.78	3.06	37.42
1	1	-2	19.25	18.72	5.64
1	1	-1	46.06	48.60	1.15
1	1	0	35.76	37.40	1.90
1	1	1	29.17	29.77	2.75
1	1	2	42.35	41.67	1.33
1	1	3	21.66	22.55	4.21
1	1	4	7.72	7.79	52.49
1	1	5	18.33	19.04	6.73
1	1	6	1.38*	2.98	0.47
1	1	7	2.26*	1.23	1.23
0	1	8	0.72*	1.19	0.08
0	1	7	2.63*	2.02	1.94
0	1	6	7.31	7.22	44.48
0	1	5	12.15	12.84	16.90
0	1	4	1.04*	1.51	0.83
0	1	3	18.76	18.66	5.44
0	1	2	23.79	23.97	3.93
0	1	1	7.90	7.33	32.95
0	2	0	6.71	7.10	45.27
0	2	1	72.83	76.89	0.03
0	2	2	15.08	14.68	8.18
0	2	3	10.57	10.41	26.28
0	2	4	3.41	3.32	41.89
0	2	5	4.49	4.05	40.16
0	2	6	6.35	6.41	40.66
0	2	7	1.14*	0.64	0.44
0	2	8	1.78*	2.30	0.47
1	2	7	1.53*	2.27	0.43
1	2	6	2.12	2.52	8.05
1	2	5	3.05	2.15	9.28
1	2	4	5.60	5.58	53.42
1	2	3	16.13	16.17	6.42
1	2	2	28.77	28.02	2.73
1	2	1	11.93	11.97	11.76
1	2	0	60.43	63.20	0.04
1	2	-1	8.89	8.95	25.66
1	2	-2	40.24	40.19	1.47
1	2	-3	6.48	6.22	86.19
1	2	-4	7.36	7.09	60.39
1	2	-5	1.39*	0.67	0.82
1	2	-6	6.88	6.67	39.77
1	2	-7	2.04*	0.43	1.17
1	2	-8	1.74*	0.74	0.33
2	2	-8	1.73*	0.07	0.45
2	2	-7	1.66*	1.76	0.41
2	2	-6	4.27	4.66	21.75
2	2	-5	2.44*	3.07	2.37
2	2	-4	8.21	6.31	67.15
2	2	-3	26.23	24.82	3.12
2	2	-2	40.74	-40.49	1.43
2	2	-1	31.27	31.06	2.37
2	2	0	12.53	12.45	10.25
2	2	1	6.58	6.55	83.81
2	2	2	22.07	22.82	4.12
2	2	3	16.12	16.15	8.93
2	2	4	3.19	3.60	20.40
2	2	5	7.06	7.35	46.17
2	2	6	3.94	4.26	18.17
2	2	7	3.20*	2.67	1.41
3	2	6	2.19*	2.68	0.88
3	2	5	1.25*	0.94	0.64
3	2	4	12.74	13.17	15.13
3	2	3	2.03*	0.23	2.19
3	2	2	5.28	5.39	60.76
3	2	1	8.46	8.50	41.98
3	2	0	35.44	34.68	1.82
3	2	-1	11.83	12.05	14.58
3	2	-2	8.47	8.39	40.65
3	2	-3	3.46	3.19	47.73
3	2	-4	11.26	10.67	23.95
3	2	-5	5.13	5.41	40.02
3	2	-6	5.77	5.70	36.00
3	2	-7	1.83*	2.96	0.69
3	2	-8	2.55*	1.02	1.13
4	2	-8	3.25	3.47	8.70
4	2	-7	1.50*	0.62	0.45
4	2	-6	4.76	4.81	28.85
4	2	-5	11.88	12.07	21.63
4	2	-4	1.66*	0.87	1.29
4	2	-3	7.65	7.98	60.03
4	2	-2	17.98	18.32	5.20
4	2	-1	13.33	12.78	11.00
4	2	0	3.05	3.46	30.43
4	2	1	6.65	6.36	65.03
4	2	2	1.21*	0.32	0.68
4	2	3	7.70	7.69	47.77
4	2	4	0.63*	0.71	0.10
4	2	5	3.06	3.18	11.82
4	2	6	2.57*	0.70	1.45

h	k	l	Fo	Fc	weight
5	2	5	3.47*	3.23	1.23
5	2	4	1.53*	1.29	0.43
5	2	3	1.57*	0.04	1.08
5	2	2	4.92	4.68	30.21
5	2	1	1.35*	0.40	0.55
5	2	0	7.75	7.71	46.28
5	2	-1	1.42*	1.77	1.15
5	2	-2	17.70	17.92	7.19
5	2	-3	2.26*	2.13	1.65
5	2	-4	12.18	12.80	17.61
5	2	-5	1.39*	1.42	0.52
5	2	-6	1.55*	1.21	0.42
5	2	-7	3.16	3.60	10.07
5	2	-8	2.63	2.68	6.20
6	2	-7	2.62	2.01	7.15
6	2	-6	1.58*	1.73	0.40
6	2	-5	3.79	3.60	21.60
6	2	-4	1.40*	0.11	0.79
6	2	-3	4.89	5.45	28.20
6	2	-2	1.39*	1.15	0.52
6	2	-1	1.40*	2.36	0.51
6	2	0	2.82*	2.64	1.89
6	2	1	1.62*	3.46	0.38
6	2	2	1.41*	0.65	0.50
6	2	3	3.69	3.23	15.26
7	2	2	1.63*	1.05	0.38
7	2	1	1.73*	0.33	1.15
7	2	0	1.45*	0.87	0.48
7	2	-1	1.79*	1.15	0.14
7	2	-2	3.21	3.95	13.01
7	2	-3	3.32	3.40	17.22
7	2	-4	2.73*	2.52	1.30
7	2	-5	5.10	5.10	19.60
7	2	-6	2.54*	2.18	0.93
8	2	-4	1.05*	0.62	0.21
8	2	-3	5.08	4.88	18.97
8	2	-2	2.07*	1.16	0.75
8	2	-1	3.87	2.98	12.91
8	3	-1	2.67*	2.63	0.78
8	3	-2	2.07*	0.54	0.74
8	3	-3	1.80*	1.41	0.49
8	3	-4	1.58*	0.33	0.40
7	3	-6	1.64*	1.16	0.37
7	3	-5	2.99*	2.65	1.71
7	3	-4	2.74*	3.09	1.16
7	3	-3	1.98*	1.65	6.18
7	3	-2	2.89	2.33	11.21
7	3	-1	1.90*	1.70	0.68
7	3	0	1.54*	0.90	0.42
7	3	1	1.58*	1.21	0.68
7	3	2	1.75*	0.94	0.33
6	3	3	2.92	2.38	9.67
6	3	2	1.16*	0.97	0.47
6	3	1	3.30	3.07	19.73
6	3	0	6.44	6.96	35.92
6	3	-1	1.33*	0.01	0.56
6	3	-2	1.37*	1.33	0.54
6	3	-3	4.75	4.81	31.08
6	3	-4	3.07	3.03	16.92
6	3	-5	1.73*	1.14	0.57
6	3	-6	2.58*	1.63	1.73
6	3	-7	1.55*	2.58	0.42
5	3	-8	1.73*	0.89	0.33
5	3	-7	1.84*	1.85	0.60
5	3	-6	2.34*	0.02	1.56
5	3	-5	1.61*	0.95	0.73
5	3	-4	5.24	5.10	37.02
5	3	-3	5.28	5.55	40.68
5	3	-2	0.78*	0.06	1.61
5	3	-1	14.03	13.96	12.22
5	3	0	7.75	8.26	51.88
5	3	1	1.24*	1.86	3.50
5	3	2	3.65	3.88	22.25
5	3	3	1.45*	1.27	0.48
5	3	4	1.51*	0.30	0.44
5	3	5	1.66*	1.79	0.32
4	3	6	6.08	5.05	21.41
4	3	5	4.08	3.47	18.09
4	3	4	1.42*	1.85	0.70
4	3	3	1.76*	2.24	0.94
4	3	2	6.35	6.51	45.91
4	3	1	8.80	8.84	37.11
4	3	0	3.41	3.56	35.23
4	3	-1	2.64	3.11	25.76
4	3	-2	17.55	17.40	5.32
4	3	-3	13.37	13.31	13.84
4	3	-4	2.31*	1.00	2.34
4	3	-5	11.11	10.91	24.75
4	3	-6	8.94	8.68	42.77
4	3	-7	1.50*	2.05	0.44
4	3	-8	2.61*	3.34	0.74
3	3	-8	2.81	3.33	7.41
3	3	-7	4.85	4.30	27.52
3	3	-6	4.62	4.43	29.55
3	3	-5	3.91	3.59	27.73
3	3	-4	5.53	5.52	49.95
3	3	-3	12.50	11.96	12.14
3	3	-2	3.23	2.96	44.78
3	3	-1	4.89	4.97	76.65
3	3	0	3.00	3.16	48.63
3	3	1	11.47	11.33	22.97
3	3	2	1.18*	1.74	0.95
3	3	3	8.46	8.88	48.88
3	3	4	8.57	9.01	46.47
3	3	5	1.38*	0.08	0.53
3	3	6	1.48*	0.45	0.46
2	3	7	1.61*	0.96	0.39
2	3	6	1.61*	2.41	0.46
2	3	5	4.45	4.83	28.42
2	3	4	7.88	8.28	54.67
2	3	3	12.76	12.01	14.93
2	3	2	13.86	14.21	11.61
2	3	1	19.46	19.97	5.24
2	3	0	38.22	38.01	1.61
2	3	-1	17.55	17.52	6.33
2	3	-2	17.26	16.92	6.36
2	3	-3	1.66*	0.84	2.31
2	3	-4	7.18	7.13	56.46
2	3	-5	1.97*	2.20	1.04
2	3	-6	11.97	11.91	22.74
2	3	-7	2.67	2.37	11.65
2	3	-8	0.97*	1.25	0.82
1	3	-8	5.65	5.79	16.73
1	3	-7	0.65*	2.49	0.06
1	3	-6	3.53	3.08	19.63
1	3	-5	11.70	12.00	19.72
1	3	-4	1.24*	1.15	0.65
1	3	-3	7.33	7.03	48.37
1	3	-2	6.38	6.23	67.16
1	3	-1	54.05	55.75	0.83
1	3	0	54.28	56.64	0.05
1	3	1	15.79	16.44	7.78
1	3	2	20.82	20.69	4.72
1	3	3	22.47	21.09	3.94
1	3	4	13.11	13.62	10.55
1	3	5	9.77	9.43	29.48
1	3	6	1.35*	0.67	0.55
1	3	7	1.46*	1.58	0.47
0	3	8	2.19*	2.23	0.73
0	3	7	2.48*	1.65	1.86
0	3	6	5.38	5.45	35.52
0	3	5	6.41	6.46	50.59
0	3	4	8.89	8.99	46.01
0	3	3	3.47	3.44	55.15
0	3	2	36.56	36.02	1.76
0	3	1	2.25	1.91	53.15
0	4	0	76.26	87.38	0.02
0	4	1	20.40	20.46	5.24
0	4	2	31.78	31.71	2.28
0	4	3	19.26	18.32	5.10
0	4	4	14.84	14.51	9.74
0	4	5	7.77	7.69	54.35
0	4	6	1.59*	0.90	0.91
0	4	7	1.49*	1.88	0.50
0	4	8	1.60*	0.05	0.39
1	4	7	1.50*	1.50	0.44
1	4	6	8.88	9.32	35.15
1	4	5	3.14	3.47	18.99
1	4	4	10.66	10.98	26.67
1	4	3	1.96	1.94	18.11
1	4	2	1.00*	0.61	1.00
1	4	1	22.81	22.36	4.19
1	4	0	30.46	31.03	2.52
1	4	-1	39.00	39.14	1.57
1	4	-2	14.24	14.36	8.53
1	4	-3	36.14	35.50	1.75
1	4	-4	18.55	19.34	5.01
1	4	-5	1.67*	1.70	0.86
1	4	-6	4.22	4.59	22.35
1	4	-7	2.44*	2.43	1.07
1	4	-8	2.27*	3.10	0.77
2	4	-8	2.85	2.76	7.74
2	4	-7	6.21	6.19	28.31
2	4	-6	0.59*	1.30	0.15
2	4	-5	5.44	5.60	41.05
2	4	-4	1.26*	1.17	0.85
2	4	-3	5.66	5.97	77.94
2	4	-2	13.32	13.13	13.17
2	4	-1	29.60	29.15	2.59
2	4	0	5.09	4.87	110.65
2	4	1	11.26	11.11	20.84
2	4	2	18.89	18.15	5.11
2	4	3	2.06*	1.19	2.99
2	4	4	1.37*	0.77	0.54
2	4	5	5.37	5.32	38.14
2	4	6	4.38	3.48	21.58
2	4	7	1.25*	0.12	0.45
3	4	6	1.57*	1.56	0.57
3	4	5	5.91	5.60	30.56
3	4	4	11.49	11.09	24.17
3	4	3	9.60	9.71	32.74
3	4	2	6.31	6.53	62.18
3	4	1	1.98	2.38	19.79
3	4	0	1.03*	0.45	0.93
3	4	-1	23.57	23.18	3.71
3	4	-2	20.14	19.58	4.64
3	4	-3	5.74	5.61	68.97
3	4	-4	2.18*	2.39	1.74
3	4	-5	9.66	10.03	33.46
3	4	-6	5.60	5.90	31.51
3	4	-7	1.74*	1.29	0.63
3	4	-8	5.62	5.37	19.56
4	4	-8	2.19*	0.35	0.90
4	4	-7	1.49*	1.73	0.45
4	4	-6	4.01	4.33	21.40
4	4	-5	5.88	5.88	37.54
4	4	-4	9.62	9.35	39.52
4	4	-3	10.78	10.81	22.62
4	4	-2	5.06	4.65	88.48
4	4	-1	1.10*	0.37	0.82
4	4	0	8.18	7.98	44.89
4	4	1	6.21	6.35	55.83
4	4	2	3.50	3.16	26.05
4	4	3	7.75	7.99	46.28
4	4	4	4.29	4.25	24.30
4	4	5	5.27	5.04	25.26
4	4	6	2.24*	1.07	0.79
5	4	5	1.68*	0.91	0.35
5	4	4	2.68*	2.18	1.42
5	4	3	1.45*	2.06	0.61
5	4	2	5.52	6.55	34.88
5	4	1	7.17	7.21	46.04
5	4	0	9.82	3.45	29.45
5	4	-1	1.29*	0.66	0.60
5	4	-2	9.16	9.60	45.95
5	4	-3	8.63	8.54	51.90
5	4	-4	7.32	7.58	42.90
5	4	-5	1.32*	0.62	0.57
5	4	-6	2.69*	1.49	1.91
5	4	-7	2.62*	1.74	0.98
6	4	-7	1.47*	0.23	0.42
6	4	-6	2.19*	2.54	0.78

h	k	l	Fo	Fc	weight
6	4	-5	1.61*	1.74	0.58
6	4	-4	2.90*	3.37	1.62
6	4	-3	8.59	8.70	42.98
6	4	-2	9.20	9.08	44.84
6	4	-1	5.39	6.07	31.18
6	4	0	1.24*	1.80	1.03
6	4	1	3.40	3.40	17.05
6	4	2	4.49	4.30	20.68
6	4	3	5.85	5.45	23.62
7	4	2	1.82*	0.75	0.52
7	4	1	2.94*	2.34	1.18
7	4	0	1.54*	0.77	0.39
7	4	-1	1.54*	0.68	0.42
7	4	-2	3.08*	4.26	1.21
7	4	-3	2.53*	2.66	1.53
7	4	-4	5.60	4.91	23.55
7	4	-5	1.47*	0.70	0.46
7	4	-6	5.13	5.09	17.18
8	4	-4	2.37*	2.23	0.87
8	4	-3	2.56*	3.16	0.97
8	4	-2	1.72*	2.33	0.34
8	4	-1	1.87*	1.32	0.49
8	5	-2	2.57*	0.33	1.21
8	5	-3	3.57	3.20	10.80
7	5	-6	4.91	4.65	18.00
7	5	-5	1.97*	1.49	5.00
7	5	-4	1.53*	1.21	0.43
7	5	-3	1.18*	0.03	0.38
7	5	-2	5.48	5.62	26.70
7	5	-1	5.44	4.70	26.10
7	5	0	1.55*	1.62	0.41
7	5	1	2.38*	2.62	0.85
7	5	2	4.85	4.44	16.41
6	5	3	1.76*	0.56	0.60
6	5	2	2.04*	1.25	0.89
6	5	1	7.83	7.87	37.22
6	5	0	3.50	4.10	18.50
6	5	-1	1.38*	0.04	0.47
6	5	-2	7.45	7.11	41.65
6	5	-3	1.78*	0.30	1.04
6	5	-4	5.00	5.03	26.70
6	5	-5	1.99*	0.41	1.29
6	5	-6	2.43	1.76	7.95
6	5	-7	3.09	3.08	9.16
5	5	-7	1.57*	1.38	0.76
5	5	-6	6.63	6.71	30.33
5	5	-5	4.29	4.82	26.20
5	5	-4	1.42*	2.19	0.49
5	5	-3	5.66	5.50	42.77
5	5	-2	7.22	7.10	50.70
5	5	-1	2.31	2.61	13.38
5	5	0	11.78	11.53	18.70
5	5	1	6.02	5.89	41.36
5	5	2	1.38*	0.67	0.53
5	5	3	5.75	5.46	28.38
5	5	4	4.63	4.54	18.10
4	5	5	1.40*	0.47	0.51
4	5	4	5.54	5.75	28.73
4	5	3	7.04	7.34	42.37
4	5	2	1.26*	1.08	0.63
4	5	1	9.37	9.14	42.82
4	5	0	7.01	7.32	63.20
4	5	-1	8.83	9.09	49.04
4	5	-2	2.03*	1.34	1.80
4	5	-3	4.76	4.94	44.18
4	5	-4	3.91	4.03	29.61
4	5	-5	4.14	3.66	29.85
4	5	-6	1.41*	1.77	0.50
4	5	-7	1.80*	0.57	0.77
4	5	-8	0.73*	0.30	0.09
3	5	-8	3.14*	2.54	1.50
3	5	-7	4.45	3.94	22.07
3	5	-6	2.35*	3.78	1.11
3	5	-5	10.53	10.44	22.57
3	5	-4	1.25*	2.61	0.64
3	5	-3	2.09*	1.31	2.85
3	5	-2	17.25	16.91	5.71
3	5	-1	18.37	18.18	5.36
3	5	0	17.81	17.11	5.56
3	5	1	7.20	7.33	58.56
3	5	2	1.11*	0.03	0.72
3	5	3	17.75	17.98	6.91
3	5	4	6.04	6.87	39.77
3	5	5	2.59*	2.89	1.43
3	5	6	1.53*	1.56	0.43
2	5	7	1.93*	1.87	0.72
2	5	6	4.74	4.87	23.08
2	5	5	4.65	5.30	26.19
2	5	4	11.84	12.18	19.38
2	5	3	6.42	6.45	59.08
2	5	2	16.18	16.27	6.24
2	5	1	7.94	7.84	35.50
2	5	0	1.12*	0.13	1.47
2	5	-1	12.59	12.83	14.45
2	5	-2	5.72	5.73	87.02
2	5	-3	26.07	25.85	3.07
2	5	-4	9.19	8.83	39.35
2	5	-5	2.52*	1.88	1.65
2	5	-6	7.17	7.39	41.04
2	5	-7	2.54*	1.08	1.08
2	5	-8	2.49*	1.66	1.11
1	5	-8	2.51*	2.37	0.69
1	5	-7	1.86*	2.46	0.50
1	5	-6	1.58*	0.37	0.57
1	5	-5	3.67	4.28	21.29
1	5	-4	2.06*	3.63	1.54
1	5	-3	9.87	9.79	24.69
1	5	-2	1.37*	1.85	1.62
1	5	-1	25.89	24.74	3.34
1	5	0	6.39	6.15	65.85
1	5	1	2.31	2.06	46.63
1	5	2	7.42	7.64	50.55
1	5	3	19.73	19.08	4.70
1	5	4	15.00	14.18	12.07
1	5	5	3.62	3.23	23.56
1	5	6	3.32	2.96	18.07
1	5	7	2.70*	2.39	1.52
0	5	8	4.22	4.07	13.52
0	5	7	1.08*	1.32	1.77
0	5	6	0.86*	0.30	0.27
0	5	5	1.22*	0.83	0.51
0	5	4	5.81	5.74	61.38
0	5	3	19.81	19.52	4.79
0	5	2	30.87	30.17	2.38
0	5	1	41.94	43.05	1.36
0	6	0	7.13	7.03	55.81
0	6	1	19.22	19.40	5.50
0	6	2	13.55	12.81	13.06
0	6	3	0.99*	0.49	1.02
0	6	4	7.60	7.64	45.37
0	6	5	6.58	6.27	48.48
0	6	6	6.23	5.82	36.53
0	6	7	2.15*	1.62	0.99
0	6	8	5.22	5.28	16.76
1	6	7	1.35*	0.35	2.56
1	6	6	4.33	4.57	24.04
1	6	5	12.44	13.00	23.83
1	6	4	13.71	14.17	12.86
1	6	3	14.04	13.39	10.49
1	6	2	31.73	30.67	2.21
1	6	1	1.09*	0.48	1.58
1	6	0	31.74	31.60	2.28
1	6	-1	6.21	5.99	103.34
1	6	-2	1.02*	0.29	0.96
1	6	-3	7.31	7.16	77.88
1	6	-4	1.68*	1.13	1.35
1	6	-5	0.84*	0.15	0.29
1	6	-6	5.08	4.89	27.49
1	6	-7	1.63*	0.04	0.50
1	6	-8	1.69*	0.07	0.35
2	6	-8	1.77*	0.90	0.42
2	6	-7	4.94	4.70	20.92
2	6	-6	11.22	11.48	22.45
2	6	-5	7.56	7.26	90.03
2	6	-4	1.18*	1.67	0.72
2	6	-3	17.16	16.60	5.68
2	6	-2	29.43	29.05	2.53
2	6	-1	27.01	26.57	2.98
2	6	0	15.78	15.82	6.97
2	6	1	8.86	9.27	39.26
2	6	2	11.07	10.77	17.86
2	6	3	6.53	6.18	57.83
2	6	4	0.78*	1.55	0.17
2	6	5	1.44*	2.11	0.48
2	6	6	4.75	3.98	23.06
2	6	7	4.94	4.33	18.78
3	6	6	2.25*	2.02	0.96
3	6	5	2.07*	0.81	1.33
3	6	4	2.32*	1.33	1.68
3	6	3	9.62	9.75	33.50
3	6	2	19.12	19.59	4.55
3	6	1	2.12	1.79	19.78
3	6	0	6.04	5.52	72.30
3	6	-1	8.62	8.73	45.85
3	6	-2	31.90	31.89	2.15
3	6	-3	6.29	6.09	63.59
3	6	-4	5.13	5.26	46.43
3	6	-5	1.34*	0.56	0.55
3	6	-6	2.64	2.56	11.95
3	6	-7	1.49*	0.07	0.58
3	6	-8	1.66*	0.56	0.36
4	6	-8	5.38	5.12	17.79
4	6	-7	7.42	6.92	30.84
4	6	-6	3.30	3.38	17.24
4	6	-5	4.49	4.65	27.95
4	6	-4	8.14	8.48	41.07
4	6	-3	1.95*	1.05	2.24
4	6	-2	13.32	13.31	13.69
4	6	-1	1.12*	0.91	0.80
4	6	0	3.98	4.50	38.22
4	6	1	1.06*	0.38	0.51
4	6	2	1.78*	0.89	1.43
4	6	3	1.65*	1.40	6.17
4	6	4	2.90	3.62	11.44
4	6	5	1.55*	0.64	0.42
5	6	4	1.58*	0.21	0.56
5	6	3	1.48*	0.52	0.46
5	6	2	1.45*	1.47	0.48
5	6	1	1.35*	1.36	0.55
5	6	0	2.62	3.09	14.27
5	6	-1	2.30*	2.02	2.03
5	6	-2	5.17	5.29	37.43
5	6	-3	4.75	4.98	31.77
5	6	-4	5.76	5.71	37.93
5	6	-5	3.07*	3.50	1.56
6	6	-6	2.90*	2.05	1.66
6	6	-7	6.07	6.04	22.76
6	6	-7	1.55*	0.43	0.42
6	6	-6	3.26	2.63	11.87
6	6	-5	2.04*	1.65	6.75
6	6	-4	1.29*	0.12	0.41
6	6	-3	3.96	3.74	22.09
6	6	-2	4.78	4.83	28.13
6	6	-1	8.43	8.59	40.98
6	6	0	6.48	6.71	34.71
6	6	1	1.47*	1.16	0.46
6	6	2	4.08	3.90	17.01
6	6	3	1.70*	1.17	0.35
7	6	1	2.51*	2.28	0.90
7	6	0	2.28*	2.22	6.52
7	6	-1	1.61*	0.54	0.39
7	6	-2	1.38*	0.53	0.53
7	6	-3	3.75	4.35	14.75
7	6	-4	2.80*	0.36	1.85
7	6	-5	7.19	7.35	25.09
7	6	-6	1.06*	0.71	0.15
8	6	-3	1.63*	0.58	0.37
8	6	-2	1.60*	0.66	0.39
7	7	-5	1.58*	1.39	0.40
7	7	-4	2.55*	0.48	1.55
7	7	-3	2.30*	3.12	0.73
7	7	-2	1.95*	1.95	0.65

h	k	l	Fo	Fc	weight
7	7	-1	3.23	2.98	12.81
7	7	0	4.82	4.48	20.94
7	7	1	3.34*	2.89	1.22
6	7	3	3.35*	4.28	1.16
6	7	2	2.40*	2.31	1.51
6	7	1	1.57*	1.52	0.41
6	7	0	4.02	3.96	21.09
6	7	-1	4.39	4.50	27.63
6	7	-2	4.23	3.81	25.06
6	7	-3	1.37*	2.83	0.53
6	7	-4	1.40*	0.99	0.51
6	7	-5	1.40*	1.13	0.51
6	7	-6	1.51*	0.08	0.44
6	7	-7	2.39*	2.76	4.43
5	7	-7	2.27*	1.35	0.83
5	7	-6	2.60*	1.00	1.91
5	7	-5	6.45	6.08	35.56
5	7	-4	1.37*	0.54	0.53
5	7	-3	4.26	4.29	28.96
5	7	-2	11.58	11.21	21.74
5	7	-1	6.86	6.91	46.24
5	7	0	9.68	10.09	31.88
5	7	1	9.76	9.50	45.02
5	7	2	1.08*	0.36	0.32
5	7	3	8.37	8.10	33.67
5	7	4	1.55*	0.99	0.42
4	7	5	3.83	3.51	16.36
4	7	4	1.49*	0.44	0.45
4	7	3	15.12	15.56	12.04
4	7	2	1.34*	0.56	0.56
4	7	1	1.25*	0.70	0.64
4	7	0	2.62	2.71	21.70
4	7	-1	3.66	3.70	34.11
4	7	-2	2.11*	2.38	1.80
4	7	-3	3.43	3.59	25.03
4	7	-4	8.68	8.41	49.67
4	7	-5	3.64	3.83	19.09
4	7	-6	4.44	4.12	23.87
4	7	-7	1.20*	1.48	0.25
3	7	-8	3.11	2.92	8.13
3	7	-8	3.02*	2.36	1.63
3	7	-7	4.74	5.43	19.49
3	7	-6	2.68	2.45	11.71
3	7	-5	1.40*	0.56	0.77
3	7	-4	3.31	2.69	29.47
3	7	-3	2.98	2.45	27.67
3	7	-2	5.46	5.17	64.50
3	7	-1	20.06	19.71	4.54
3	7	0	10.23	10.25	22.63
3	7	1	17.47	17.04	5.29
3	7	2	2.60	2.15	20.13
3	7	3	1.85*	1.87	1.07
3	7	4	6.02	6.77	39.91
3	7	5	2.65*	3.69	1.03
3	7	6	1.24*	2.20	0.21
2	7	7	3.21	3.27	9.40
2	7	6	2.54*	1.41	1.41
2	7	5	7.51	7.42	43.46
2	7	4	14.22	13.42	11.14
2	7	3	4.38	4.55	46.69
2	7	2	8.92	8.70	37.43
2	7	1	3.79	3.53	61.31
2	7	0	4.36	3.89	75.48
2	7	-1	4.07	4.20	61.63
2	7	-2	3.50	3.17	53.31
2	7	-3	15.50	14.81	9.54
2	7	-4	14.78	14.88	9.07
2	7	-5	5.90	5.81	42.71
2	7	-6	2.20*	0.95	1.10
2	7	-7	2.99*	2.94	1.46
2	7	-8	1.69*	1.07	0.35
1	7	-8	6.96	6.66	21.19
1	7	-7	1.59*	0.49	0.39
1	7	-6	9.03	8.91	40.55
1	7	-5	3.39	3.47	19.36
1	7	-4	3.13	3.21	25.18
1	7	-3	15.23	14.96	9.75
1	7	-2	3.87	3.97	58.81
1	7	-1	6.62	6.76	103.05
1	7	0	7.72	7.87	40.70
1	7	1	29.45	30.28	2.55
1	7	2	15.76	14.93	9.84
1	7	3	18.17	18.14	5.10
1	7	4	7.25	7.07	53.41
1	7	5	8.63	9.30	44.59
1	7	6	3.58	3.89	17.57
1	7	7	2.93*	2.34	1.51
0	7	8	2.37*	1.88	0.75
0	7	7	4.21	3.62	18.15
0	7	6	9.01	9.23	41.45
0	7	5	2.46*	2.33	1.52
0	7	4	8.13	7.66	40.68
0	7	3	1.43*	2.23	1.38
0	7	2	12.54	12.42	13.45
0	7	1	28.10	28.40	2.81
0	8	0	61.84	63.51	0.63
0	8	1	16.01	15.83	6.83
0	8	2	24.43	25.39	3.46
0	8	3	1.09*	0.73	0.84
0	8	4	5.53	4.99	52.31
0	8	5	2.63*	1.87	2.28
0	8	6	4.09	4.28	21.64
0	8	7	2.86*	2.14	1.24
1	8	7	3.04*	2.67	1.29
1	8	6	6.57	6.73	35.22
1	8	5	3.94	4.14	23.85
1	8	4	8.22	8.79	48.95
1	8	3	12.04	11.92	19.25
1	8	2	4.48	4.39	64.06
1	8	1	17.15	16.90	6.05
1	8	0	29.88	30.35	2.48
1	8	-1	11.06	11.43	15.50
1	8	-2	15.84	15.33	6.60
1	8	-3	11.72	11.45	20.14
1	8	-4	6.64	6.38	54.92
1	8	-5	2.58*	1.85	2.25
1	8	-6	1.47*	2.06	0.46
1	8	-7	4.08	3.78	14.93
1	8	-8	1.49*	0.58	0.26
2	8	-8	1.47*	1.03	0.29
2	8	-7	1.62*	1.69	0.38
2	8	-6	4.78	4.44	28.36
2	8	-5	15.34	15.28	7.64
2	8	-4	13.24	13.23	16.08
2	8	-3	4.09	4.14	45.30
2	8	-2	7.20	7.16	69.39
2	8	-1	17.15	16.71	5.83
2	8	0	25.65	24.92	3.17
2	8	1	13.68	13.09	11.23
2	8	2	6.50	6.19	65.44
2	8	3	4.08	3.70	37.70
2	8	4	6.68	6.96	44.37
2	8	5	4.40	4.58	25.70
2	8	6	2.83*	2.45	1.15
2	8	7	2.70*	3.40	0.77
3	8	6	1.65*	0.75	0.37
3	8	5	1.16*	0.94	0.31
3	8	4	2.14*	2.09	1.00
3	8	3	1.36*	0.28	0.54
3	8	2	8.01	8.30	55.80
3	8	1	12.74	12.01	14.55
3	8	0	10.99	10.62	21.20
3	8	-1	2.29*	3.43	2.43
3	8	-2	11.88	11.26	16.05
3	8	-3	6.38	6.27	53.89
3	8	-4	8.76	8.80	46.59
3	8	-5	2.85	3.59	15.05
3	8	-6	3.59	3.60	17.94
3	8	-7	2.58	2.39	7.39
3	8	-8	3.65	3.30	9.93
4	8	-7	2.10*	1.15	1.16
4	8	-6	6.76	6.92	32.64
4	8	-5	9.92	10.25	34.02
4	8	-4	3.99	4.03	25.32
4	8	-3	2.78	2.74	19.59
4	8	-2	8.24	8.18	50.82
4	8	-1	10.21	10.21	33.51
4	8	0	4.54	4.30	42.16
4	8	1	2.20*	0.26	2.56
4	8	2	1.43*	0.66	0.74
4	8	3	2.26	2.56	9.44
4	8	4	8.25	8.19	33.12
4	8	5	1.45*	0.83	0.48
5	8	4	1.62*	1.13	0.38
5	8	3	1.15*	1.58	2.11
5	8	2	3.81	3.82	23.47
5	8	1	1.34*	0.06	0.56
5	8	0	9.92	9.71	30.32
5	8	-1	2.42	2.52	13.48
5	8	-2	6.83	6.90	44.91
5	8	-3	13.92	14.12	13.33
5	8	-4	1.37*	0.11	0.56
5	8	-5	4.45	4.63	23.04
5	8	-6	4.31	4.07	19.33
5	8	-7	1.78*	0.87	0.51
6	8	-6	1.48*	0.45	0.46
6	8	-5	5.50	5.60	23.09
6	8	-4	1.87*	1.94	0.57
6	8	-3	3.22*	3.74	1.53
6	8	-2	7.13	7.24	36.99
6	8	-1	1.69*	2.25	0.57
6	8	0	5.32	5.44	27.12
6	8	1	2.69*	1.80	1.41
6	8	2	2.86	3.00	10.47
6	8	3	8.12	7.99	24.98
7	8	1	3.16	2.73	8.97
7	8	0	1.24*	0.20	0.27
7	8	-1	0.70*	1.44	0.08
7	8	-2	4.26	3.96	16.92
7	8	-3	5.00	4.69	20.56
7	8	-4	2.15*	2.41	5.06
7	8	-5	1.27*	0.76	0.25
7	9	-5	1.49*	0.81	0.45
7	9	-4	1.62*	0.45	0.38
7	9	-3	6.00	5.97	22.74
7	9	-2	4.09	4.20	16.23
7	9	-1	0.71*	0.88	0.69
7	9	0	1.62*	1.08	0.46
7	9	1	1.83*	0.19	0.72
6	9	3	2.69*	0.53	2.16
6	9	2	4.17	3.57	14.15
6	9	1	2.69	2.42	8.90
6	9	0	5.41	5.46	24.53
6	9	-1	8.34	8.05	38.05
6	9	-2	1.29*	0.27	0.47
6	9	-3	1.73*	1.80	0.52
6	9	-4	4.33	5.14	19.11
6	9	-5	1.84*	1.19	0.56
6	9	-6	1.78*	2.25	0.54
5	9	-7	1.51*	1.10	0.44
5	9	-6	0.91*	1.16	1.21
5	9	-5	1.46*	0.94	0.47
5	9	-4	4.45	4.25	26.08
5	9	-3	2.88*	2.24	1.77
5	9	-2	2.60*	0.22	2.29
5	9	-1	3.17	3.15	20.28
5	9	0	7.90	7.95	45.62
5	9	1	5.12	4.85	31.70
5	9	2	6.03	5.47	34.21
5	9	3	1.45*	0.58	0.47
5	9	4	1.46*	2.66	0.32
4	9	5	1.85*	0.56	0.42
4	9	4	2.14*	2.33	5.77
4	9	3	0.65*	1.15	0.94
4	9	2	15.02	15.00	9.96
4	9	1	15.67	15.93	7.79
4	9	0	5.96	5.48	47.49
4	9	-1	1.59*	1.47	7.36
4	9	-2	5.10	5.26	39.24
4	9	-3	2.47	2.63	13.75
4	9	-4	6.83	7.27	41.98
4	9	-5	4.18	4.08	24.32

h	k	l	Fo	Fc	weight
4	9	-6	5.52	5.05	27.31
4	9	-7	1.00*	0.56	0.16
3	9	-8	1.65*	1.05	0.37
3	9	-7	1.83*	0.60	0.64
3	9	-6	10.87	11.25	32.58
3	9	-5	1.18*	0.80	0.37
3	9	-4	6.70	6.64	46.61
3	9	-3	3.76	4.15	31.00
3	9	-2	8.82	8.51	50.00
3	9	-1	10.82	10.84	25.46
3	9	0	13.44	13.38	13.91
3	9	1	6.30	6.61	55.09
3	9	2	8.19	8.76	51.88
3	9	3	9.84	10.10	40.52
3	9	4	4.94	5.11	28.75
3	9	5	1.48*	0.31	0.45
3	9	6	4.39	3.67	15.30
2	9	6	4.25	4.51	15.40
2	9	5	3.91	3.77	20.15
2	9	4	4.23	3.71	27.97
2	9	3	8.45	8.32	47.08
2	9	2	6.68	6.40	67.40
2	9	1	15.26	14.96	9.74
2	9	0	15.08	15.35	10.19
2	9	-1	19.16	19.00	4.93
2	9	-2	13.89	13.37	10.59
2	9	-3	2.29*	2.14	2.58
2	9	-4	1.98*	1.75	1.81
2	9	-5	1.33*	0.54	0.56
2	9	-6	1.49*	2.91	0.45
2	9	-7	2.57*	0.30	1.60
2	9	-8	1.04*	1.08	0.93
1	9	-8	2.91*	2.57	0.86
1	9	-7	5.21	4.49	22.10
1	9	-6	6.98	6.57	37.29
1	9	-5	15.92	15.43	7.35
1	9	-4	2.03*	1.16	1.87
1	9	-3	13.58	13.77	10.38
1	9	-2	0.65*	0.59	2.37
1	9	-1	13.73	13.01	11.90
1	9	0	5.03	5.01	73.19
1	9	1	14.34	14.24	11.10
1	9	2	19.77	18.90	4.60
1	9	3	8.70	8.56	59.88
1	9	4	2.21*	1.30	1.97
1	9	5	1.61*	0.51	0.89
1	9	6	2.49*	2.32	1.27
1	9	7	2.29*	1.75	1.31
0	9	7	1.72*	0.52	0.62
0	9	6	1.29*	2.27	0.28
0	9	5	16.37	17.23	7.26
0	9	4	0.78*	0.51	1.80
0	9	3	8.70	8.07	49.96
0	9	2	5.75	5.69	81.83
0	9	1	21.35	21.83	4.33
0	10	0	10.12	10.24	25.53
0	10	1	29.86	29.59	2.42
0	10	2	1.09*	0.66	0.84
0	10	3	0.86*	1.01	0.38
0	10	4	5.81	5.86	46.06
0	10	5	1.41*	0.92	0.51
0	10	6	1.40*	0.84	0.51
0	10	7	0.71*	0.18	0.07
1	10	7	1.82*	1.89	3.82
1	10	6	3.63	2.94	17.95
1	10	5	12.92	12.85	18.19
1	10	4	10.40	10.78	25.12
1	10	3	5.86	6.15	52.70
1	10	2	1.43*	1.90	1.60
1	10	1	8.70	9.28	35.47
1	10	0	27.03	26.23	2.88
1	10	-1	19.04	18.86	5.02
1	10	-2	11.38	11.41	21.35
1	10	-3	7.53	7.56	63.50
1	10	-4	2.57	3.01	14.78
1	10	-5	1.41*	1.01	0.51
1	10	-6	6.88	6.59	33.98
1	10	-7	2.00*	1.36	4.61
2	10	-7	0.70*	0.15	0.11
2	10	-6	6.69	7.33	31.20
2	10	-5	1.30*	0.87	0.59
2	10	-4	4.42	4.19	36.13
2	10	-3	14.40	14.45	12.33
2	10	-2	2.58	2.91	25.85
2	10	-1	12.54	12.12	15.49
2	10	0	4.69	5.04	56.80
2	10	1	6.35	6.37	68.80
2	10	2	11.32	11.34	26.22
2	10	3	4.64	4.76	34.45
2	10	4	2.45	2.87	12.02
2	10	5	3.05*	3.38	1.46
2	10	6	1.47*	0.98	0.46
3	10	6	1.66*	1.05	0.77
3	10	5	1.19*	0.94	0.40
3	10	4	1.35*	1.62	0.55
3	10	3	12.91	12.68	19.65
3	10	2	6.00	5.96	43.73
3	10	1	7.60	7.87	52.83
3	10	0	9.40	9.57	27.22
3	10	-1	4.27	4.58	42.57
3	10	-2	0.51*	0.60	0.12
3	10	-3	7.87	7.85	46.64
3	10	-4	1.30*	0.45	0.59
3	10	-5	6.26	7.04	36.97
3	10	-6	2.44*	1.73	1.20
3	10	-7	3.35	2.96	12.56
4	10	-7	1.61*	2.08	0.43
4	10	-6	9.45	3.52	11.54
4	10	-5	2.18*	2.72	0.92
4	10	-4	9.63	9.65	29.57
4	10	-3	10.27	10.12	25.83
4	10	-2	6.97	7.07	48.85
4	10	-1	6.87	7.02	49.44
4	10	0	4.78	5.13	36.63
4	10	1	1.41*	1.75	0.86
4	10	2	1.37*	0.82	0.53
4	10	3	5.63	5.99	30.43
4	10	4	2.57*	3.63	1.21
4	10	5	2.44*	2.20	0.91
5	10	4	1.60*	0.46	0.39
5	10	3	1.21*	0.11	0.27
5	10	2	1.45*	0.30	0.47
5	10	1	1.45*	1.90	0.47
5	10	0	3.12	3.95	17.64
5	10	-1	3.03	3.15	19.05
5	10	-2	8.22	8.37	43.12
5	10	-3	4.37	4.03	26.89
5	10	-4	9.11	9.26	38.50
5	10	-5	2.48*	2.88	1.58
5	10	-6	1.21*	1.21	0.33
5	10	-7	3.85	3.95	12.05
6	10	-6	1.47*	0.05	0.31
6	10	-5	1.52*	0.35	0.43
6	10	-4	1.52*	2.16	0.52
6	10	-3	0.66*	1.61	0.11
6	10	-2	3.96	3.52	19.19
6	10	-1	1.32*	0.60	0.48
6	10	0	3.25	3.72	13.53
6	10	1	1.83*	2.91	0.69
6	10	2	6.60	6.08	22.58
7	10	0	1.50*	0.45	0.45
7	10	-1	1.56*	0.89	0.41
7	10	-2	1.76*	0.52	0.60
7	10	-3	1.55*	1.12	0.42
7	10	-4	1.77*	1.28	0.32
7	10	-5	1.03*	1.98	1.07
7	11	-4	3.06*	2.87	1.29
7	11	-3	2.31*	1.60	0.67
7	11	-2	5.68	5.41	20.60
7	11	-1	1.56*	0.77	0.41
7	11	0	1.05*	1.01	0.21
6	11	2	1.57*	1.00	0.40
6	11	1	1.45*	1.04	0.48
6	11	0	4.11	4.53	15.26
6	11	-1	2.01*	2.47	1.07
6	11	-2	1.58*	2.33	0.40
6	11	-3	1.51*	0.81	0.57
6	11	-4	1.48*	0.64	0.46
6	11	-5	1.60*	0.12	0.47
6	11	-6	2.59*	1.54	1.02
5	11	-7	3.10*	0.04	1.55
5	11	-6	2.28*	1.75	6.77
5	11	-5	1.65*	0.99	0.80
5	11	-4	3.13	3.29	14.90
5	11	-3	6.15	5.99	36.16
5	11	-2	5.07	4.98	31.72
5	11	-1	3.80	3.93	21.13
5	11	0	5.99	5.72	37.24
5	11	1	4.73	4.70	24.77
5	11	2	2.85	2.77	12.45
5	11	3	4.33	5.08	16.34
5	11	4	1.30*	0.62	0.25
4	11	5	1.53*	0.49	0.43
4	11	4	1.61*	2.13	0.38
4	11	3	4.63	4.66	24.67
4	11	2	2.14*	1.35	1.16
4	11	1	5.23	5.21	37.59
4	11	0	1.80*	1.71	0.95
4	11	-1	7.49	7.62	48.77
4	11	-2	5.82	6.02	42.94
4	11	-3	9.38	9.31	42.51
4	11	-4	2.35*	1.93	1.87
4	11	-5	8.36	7.99	38.83
4	11	-6	1.81*	2.63	0.50
4	11	-7	2.90	1.93	8.78
3	11	-7	1.55*	0.51	0.41
3	11	-6	3.21	3.02	11.75
3	11	-5	9.00	8.96	43.21
3	11	-4	6.96	6.69	44.90
3	11	-3	2.67*	2.65	1.98
3	11	-2	4.86	4.69	42.28
3	11	-1	6.24	6.21	52.53
3	11	0	3.19	2.76	27.16
3	11	1	1.21*	0.98	0.72
3	11	2	1.39*	1.37	0.51
3	11	3	3.59	4.00	21.92
3	11	4	2.25	2.11	8.09
3	11	5	1.47*	2.04	0.46
2	11	6	2.68*	2.19	1.18
2	11	5	2.09*	1.96	1.04
2	11	4	1.39*	0.68	0.52
2	11	3	6.85	6.98	45.42
2	11	2	8.52	8.44	46.16
2	11	1	15.06	15.36	9.03
2	11	0	2.57	2.40	23.81
2	11	-1	15.97	16.16	8.98
2	11	-2	16.91	17.43	8.08
2	11	-3	1.41*	2.15	0.51
2	11	-4	4.95	4.54	34.55
2	11	-5	2.63	2.72	12.10
2	11	-6	2.69*	4.30	0.92
2	11	-7	1.61*	0.59	0.38
1	11	-7	1.96*	1.96	3.91
1	11	-6	1.48*	1.06	0.46
1	11	-5	1.20*	0.51	0.42
1	11	-4	2.35	1.97	12.94
1	11	-3	5.75	5.60	49.91
1	11	-2	13.03	12.73	10.77
1	11	-1	3.68	3.31	47.01
1	11	0	8.41	8.25	54.78
1	11	1	2.38*	2.01	2.70
1	11	2	9.10	9.21	29.85
1	11	3	8.58	8.72	41.26
1	11	4	1.30*	0.89	0.56
1	11	5	6.04	6.39	36.70
2	11	6	2.28*	2.96	1.05
1	11	7	1.65*	1.01	0.37
0	11	7	2.61*	2.83	1.48
0	11	6	7.08	7.70	30.20
0	11	5	2.28*	2.67	1.12
0	11	4	0.79*	2.19	0.28
0	11	3	12.50	12.60	17.23

h	k	l	Fo	Fc	weight
0	11	2	8.89	9.12	36.81
0	11	1	8.07	8.15	43.51
0	12	0	18.59	17.21	4.99
0	12	1	8.75	9.29	44.84
0	12	2	1.22*	2.21	0.85
0	12	3	1.18*	0.28	0.71
0	12	4	8.39	8.29	48.93
0	12	5	1.41*	1.67	0.51
0	12	6	1.66*	2.28	0.44
0	12	7	1.67*	0.05	0.36
1	12	6	1.21*	1.26	2.02
1	12	5	5.08	4.64	27.72
1	12	4	2.22*	1.22	1.72
1	12	3	3.14	3.39	19.32
1	12	2	2.80	3.17	22.17
1	12	1	6.18	5.86	63.25
1	12	0	23.10	23.22	3.57
1	12	-1	9.58	8.84	35.37
1	12	-2	12.08	11.92	18.14
1	12	-3	17.13	17.88	7.33
1	12	-4	3.00	3.89	15.25
1	12	-5	6.34	6.09	37.01
1	12	-6	2.83*	4.05	1.22
1	12	-7	1.59*	1.36	0.40
2	12	-7	1.44*	0.94	0.44
2	12	-6	1.55*	1.25	0.41
2	12	-5	10.16	10.08	33.10
2	12	-4	1.40*	1.38	0.61
2	12	-3	9.15	8.87	50.20
2	12	-2	12.96	12.95	13.82
2	12	-1	9.95	9.67	24.29
2	12	0	1.26*	0.99	0.63
2	12	1	2.36*	3.42	2.06
2	12	2	12.94	12.91	15.65
2	12	3	1.00*	1.91	0.28
2	12	4	2.07*	3.25	1.00
2	12	5	2.43*	1.66	1.05
2	12	6	1.78*	1.76	0.50
3	12	5	2.19*	2.09	5.56
3	12	4	1.57*	1.29	3.84
3	12	3	4.37	3.95	26.78
3	12	2	7.32	7.16	45.34
3	12	1	1.25*	1.16	0.64
3	12	0	2.66	2.95	17.19
3	12	-1	14.34	14.56	11.60
3	12	-2	2.60	2.44	16.32
3	12	-3	1.33*	0.38	0.57
3	12	-4	12.08	12.45	19.89
3	12	-5	5.26	4.87	30.71
3	12	-6	1.79*	1.15	0.78
4	12	-7	1.66*	2.08	0.36
4	12	-7	1.81*	0.88	0.49
4	12	-6	1.48*	0.34	0.45
4	12	-5	1.73*	1.40	0.67
4	12	-4	5.38	5.47	31.31
4	12	-3	6.64	6.86	39.18
4	12	-2	1.30*	2.05	0.38
4	12	-1	5.57	5.28	38.44
4	12	0	11.84	12.23	20.18
4	12	1	1.36*	0.64	0.54
4	12	2	1.40*	0.91	0.51
4	12	3	2.11*	2.54	0.95
4	12	4	1.50*	0.51	0.45
5	12	3	5.10	5.38	20.76
5	12	2	2.71	2.09	8.99
5	12	1	6.41	6.42	34.41
5	12	0	5.50	5.27	30.23
5	12	-1	2.35	2.21	10.67
5	12	-2	5.37	5.33	31.53
5	12	-3	6.18	6.59	34.02
5	12	-4	1.43*	0.22	0.49
5	12	-5	2.04*	1.58	6.22
5	12	-6	2.29*	2.83	0.62
6	12	-6	1.59*	1.74	0.39
6	12	-4	1.00*	0.84	0.16
6	12	-3	2.28*	2.34	1.04
6	12	-2	3.62	3.93	12.40
6	12	-1	1.93*	0.12	1.37
6	12	0	2.78*	1.72	1.40
6	12	1	2.02*	1.06	0.92
6	12	2	4.30	3.32	15.03
7	12	-1	3.23	2.92	9.55
7	12	-2	1.96*	1.69	0.60
7	12	-3	0.74*	0.88	0.10
7	12	-4	2.61*	0.64	1.00
7	13	-3	5.78	5.47	18.13
7	13	-2	0.75*	0.00	0.09
7	13	-1	3.79	3.39	12.43
6	13	2	2.92*	0.76	1.67
6	13	1	1.60*	2.51	0.39
6	13	0	3.64	3.45	14.24
6	13	-1	3.54	3.39	14.12
6	13	-2	1.60*	0.15	0.39
6	13	-3	1.57*	1.11	0.40
6	13	-4	1.46*	0.59	0.47
6	13	-5	2.45*	0.22	1.04
5	13	-6	5.57	5.50	18.76
5	13	-5	1.40*	0.72	0.31
5	13	-4	2.12*	1.08	1.52
5	13	-3	1.84*	1.25	0.87
5	13	-2	7.31	6.86	38.21
5	13	-1	2.40*	1.30	1.47
5	13	0	2.64*	2.47	1.55
5	13	1	1.34*	1.66	0.43
5	13	2	2.61*	2.13	1.55
5	13	3	5.08	4.36	19.64
4	13	4	2.67	3.12	7.03
4	13	3	5.18	4.79	22.61
4	13	2	6.41	5.97	35.52
4	13	1	2.62*	2.42	1.65
4	13	0	1.80*	1.83	1.15
4	13	-1	3.86	3.69	26.05
4	13	-2	10.55	10.85	26.13
4	13	-3	1.39*	0.67	0.52
4	13	-4	1.74*	2.05	5.54
4	13	-5	1.55*	1.96	0.42
4	13	-6	1.41*	2.94	0.26
4	13	-7	1.30*	1.36	0.20
3	13	-7	0.74*	1.94	0.09
3	13	-6	4.83	4.82	20.66
3	13	-5	2.75	2.85	12.08
3	13	-4	4.16	4.01	25.24
3	13	-3	1.40*	1.80	0.51
3	13	-2	3.15	2.76	20.98
3	13	-1	9.39	9.05	42.97
3	13	0	19.04	19.10	6.32
3	13	1	13.83	13.76	11.28
3	13	2	7.76	7.42	44.78
3	13	3	1.36*	0.15	0.54
3	13	4	7.03	6.99	28.57
3	13	5	1.78*	0.32	0.54
2	13	6	2.56*	0.08	1.12
2	13	5	0.97*	1.90	0.21
2	13	4	1.92*	3.09	0.75
2	13	3	6.38	6.74	39.61
2	13	2	2.10*	1.05	1.71
2	13	1	5.78	6.33	46.46
2	13	0	6.43	6.81	53.90
2	13	-1	8.01	8.65	52.36
2	13	-2	0.77*	0.35	1.68
2	13	-3	20.27	20.86	3.87
2	13	-4	14.30	14.13	12.98
2	13	-5	3.95	4.08	19.08
2	13	-6	1.54*	0.17	0.42
1	13	-7	1.94*	0.83	0.57
1	13	-7	1.80*	0.65	0.46
1	13	-6	0.36*	0.56	0.17
1	13	-5	3.93	4.33	20.83
1	13	-4	6.19	6.72	42.16
1	13	-3	7.46	7.65	47.61
1	13	-2	3.80	3.79	29.55
1	13	-1	8.27	8.09	44.85
1	13	0	1.22*	2.23	0.67
1	13	1	1.52*	1.64	1.13
1	13	2	7.63	7.42	55.23
1	13	3	10.54	10.89	28.49
1	13	4	1.34*	0.04	0.56
1	13	5	3.13	3.17	15.69
1	13	6	2.85*	2.59	1.12
0	13	7	4.66	3.67	17.11
0	13	6	2.19*	1.05	1.10
0	13	5	10.25	10.27	35.40
0	13	4	1.18*	2.22	0.39
0	13	3	17.50	17.96	6.93
0	13	2	0.90*	1.01	0.38
0	13	1	4.12	3.95	44.02
0	14	0	1.28*	1.54	0.61
0	14	1	5.46	5.70	49.35
0	14	2	4.96	5.07	37.64
0	14	3	1.46*	2.03	0.47
0	14	4	3.83	3.75	24.33
0	14	5	2.61*	2.19	1.41
0	14	6	1.99*	1.56	0.70
1	14	6	2.63	1.41	8.64
1	14	5	0.67*	0.08	0.11
1	14	4	0.63*	2.02	0.12
1	14	3	5.45	5.27	37.62
1	14	2	22.76	22.82	3.36
1	14	1	2.24*	0.45	2.37
1	14	0	3.00	3.23	25.14
1	14	-1	4.96	4.80	44.60
1	14	-2	12.21	12.79	16.45
1	14	-3	7.31	7.71	44.18
1	14	-4	2.89	3.24	15.86
1	14	-5	1.12*	1.39	0.33
1	14	-6	1.52*	0.12	0.43
1	14	-7	3.34	2.55	10.15
2	14	-7	1.72*	2.39	0.34
2	14	-6	1.56*	1.34	0.41
2	14	-5	5.33	5.33	25.63
2	14	-4	1.05*	1.89	0.28
2	14	-3	14.91	15.27	12.89
2	14	-2	4.08	3.98	29.30
2	14	-1	4.74	4.65	38.81
2	14	0	0.54*	0.18	0.11
2	14	1	10.59	10.57	32.93
2	14	2	2.52*	1.74	2.33
2	14	3	1.50*	1.77	0.71
2	14	4	1.47*	0.11	0.46
2	14	5	6.08	5.86	23.81
2	14	6	3.20*	2.20	1.50
3	14	5	2.66*	1.31	1.94
3	14	4	2.02*	1.96	5.27
3	14	3	2.52*	1.95	1.63
3	14	2	5.53	5.34	33.83
3	14	1	3.67	3.65	22.31
3	14	0	8.59	8.46	41.86
3	14	-1	3.88	3.64	27.01
3	14	-2	17.96	17.89	6.47
3	14	-3	6.00	5.81	38.93
3	14	-4	5.65	5.20	33.65
3	14	-5	1.35*	1.53	0.55
3	14	-6	3.26	3.09	11.80
3	14	-7	1.06*	1.77	0.13
4	14	-6	2.16*	2.39	0.80
4	14	-5	4.17	4.35	15.84
4	14	-4	2.16*	0.46	1.76
4	14	-3	2.94*	4.23	1.39
4	14	-2	4.18	4.41	23.02
4	14	-1	6.84	6.89	38.47
4	14	0	5.77	5.19	36.23
4	14	1	1.55*	1.61	0.83
4	14	2	1.87*	4.03	0.60
4	14	3	3.70	3.81	13.11
4	14	4	0.74*	0.24	0.12
5	14	3	1.61*	0.72	0.38
5	14	2	1.61*	1.58	0.39
5	14	1	1.42*	1.36	0.50
5	14	0	2.11*	1.58	0.96
5	14	-1	5.01	5.57	24.91
5	14	-2	2.08*	1.28	1.32
5	14	-3	1.36*	0.80	0.54

h	k	l	Fo	Fc	weight
5	14	-4	1.62*	2.12	0.38
5	14	-5	1.64*	0.60	0.37
5	14	-6	1.50*	0.14	0.45
6	14	-5	1.68*	1.74	0.37
6	14	-4	2.19*	1.61	0.83
6	14	-3	3.70	3.12	13.89
6	14	-2	1.49*	1.17	0.45
6	14	-1	7.51	7.25	27.87
6	14	0	2.25*	1.84	5.72
6	14	1	1.51*	1.03	0.44
6	15	1	1.51*	1.67	0.28
6	15	0	4.35	4.21	16.26
6	15	-1	1.25*	1.74	0.26
6	15	-2	1.52*	0.37	0.43
6	15	-3	0.73*	1.06	0.12
6	15	-4	1.66*	0.65	0.51
6	15	-5	4.10	4.08	13.69
5	15	-4	2.53*	1.50	1.57
5	15	-3	1.54*	0.37	0.42
5	15	-2	1.78*	1.62	4.62
5	15	-1	4.47	4.17	20.81
5	15	0	1.53*	1.27	0.43
5	15	1	4.77	4.88	18.91
5	15	2	1.55*	0.20	0.41
4	15	4	0.75*	1.39	0.07
4	15	3	3.50	3.50	14.35
4	15	2	1.51*	0.97	0.44
4	15	1	2.25*	0.53	1.57
4	15	0	0.63*	2.52	0.10
4	15	-1	7.47	7.49	42.38
4	15	-2	1.54*	2.11	0.42
4	15	-3	3.36	3.37	17.23
4	15	-4	3.44	4.04	14.30
4	15	-5	1.28*	0.42	2.45
4	15	-6	6.12	6.08	19.88
3	15	-6	1.01*	0.53	0.16
3	15	-5	5.06	4.90	20.17
3	15	-4	1.94*	1.81	6.60
3	15	-3	8.83	8.91	42.35
3	15	-2	6.61	6.78	43.18
3	15	-1	9.70	9.62	32.33
3	15	0	9.12	9.12	47.13
3	15	1	10.64	10.64	32.67
3	15	2	3.64	3.59	20.05
3	15	3	1.88*	2.36	0.59
3	15	4	3.00*	2.17	1.71
3	15	5	1.56*	0.16	0.41
2	15	6	1.89*	1.60	0.89
2	15	4	6.73	6.08	29.34
2	15	3	2.60*	1.72	1.69
2	15	2	1.58*	0.82	0.99
2	15	1	0.57*	1.77	0.12
2	15	0	6.31	6.25	42.95
2	15	-1	8.82	8.85	48.97
2	15	-2	14.91	15.79	10.35
2	15	-3	9.68	9.92	31.33
2	15	-4	5.08	5.48	27.16
2	15	-5	5.65	5.03	28.44
2	15	-6	1.31*	0.88	2.15
1	15	-6	2.92*	2.56	1.33
1	15	-5	1.44*	0.08	0.48
1	15	-4	1.34*	0.35	0.55
1	15	-3	9.77	9.95	30.02
1	15	-2	7.80	8.02	48.00
1	15	-1	7.93	8.10	51.05
1	15	0	1.28*	0.21	0.61
1	15	1	1.65*	1.34	0.97
1	15	2	2.74*	3.65	1.88
1	15	3	13.48	13.82	13.06
1	15	4	5.16	5.28	28.13
1	15	5	1.41*	0.56	0.50
1	15	6	2.45*	1.36	1.13
0	15	6	2.69*	1.68	1.58
0	15	5	1.77*	1.17	0.73
0	15	4	3.72	3.41	22.11
0	15	3	2.20*	2.42	1.40
0	15	2	4.61	4.30	36.02
0	15	1	1.08*	1.37	0.39
0	16	0	3.88	4.05	27.82
0	16	1	1.59*	2.23	0.70
0	16	2	8.93	8.73	48.50
0	16	3	2.78*	3.06	1.76
0	16	4	2.87*	2.45	1.85
0	16	5	4.56	4.35	21.76
0	16	6	1.57*	0.47	0.41
1	16	6	3.01*	2.66	1.48
1	16	5	1.99*	2.83	0.70
1	16	4	1.98*	2.20	0.74
1	16	3	6.15	6.04	36.82
1	16	2	7.10	6.81	42.60
1	16	1	10.64	10.18	29.20
1	16	0	1.35*	0.48	0.55
1	16	-1	0.86*	0.31	0.10
1	16	-2	7.54	7.59	47.68
1	16	-3	11.22	11.64	31.69
1	16	-4	8.90	8.95	37.42
1	16	-5	0.96*	0.50	0.20
1	16	-6	1.57*	0.97	0.40
2	16	-6	2.71*	2.15	1.33
2	16	-5	2.54*	0.53	1.95
2	16	-4	2.22*	2.36	1.21
2	16	-3	9.10	9.44	29.86
2	16	-2	7.28	7.51	44.03
2	16	-1	8.16	8.28	47.54
2	16	0	6.53	6.33	41.70
2	16	1	1.45*	1.08	0.54
2	16	2	11.21	11.20	28.31
2	16	3	1.71*	0.38	0.73
2	16	4	4.64	5.22	21.81
2	16	5	3.35*	3.12	1.27
3	16	4	1.54*	0.05	0.42
3	16	3	0.86*	0.26	0.23
3	16	2	1.13*	1.33	0.41
3	16	1	3.23	2.74	18.00
3	16	0	5.16	4.69	28.63
3	16	-1	12.33	12.17	22.23
3	16	-2	2.79	2.54	15.60
3	16	-3	2.00*	1.94	0.95
3	16	-4	3.00	3.25	12.55
3	16	-5	4.80	4.89	17.08
3	16	-6	1.70*	2.11	0.35
4	16	-6	3.52*	3.70	1.20
4	16	-5	2.67*	4.26	0.75
4	16	-4	2.05*	0.72	0.89
4	16	-3	0.93*	0.37	0.30
4	16	-2	2.59*	3.45	1.85
4	16	-1	1.37*	0.93	0.54
4	16	0	3.72	4.22	19.79
4	16	1	4.97	4.64	23.56
4	16	2	1.55*	0.25	0.59
4	16	3	2.90*	3.24	1.29
5	16	2	3.66	2.83	11.96
5	16	1	5.37	5.23	20.80
5	16	0	3.68	3.24	14.16
5	16	-1	2.29*	2.51	1.42
5	16	-2	2.07*	2.16	0.93
5	16	-3	2.10*	0.17	1.17
5	16	-4	3.12*	1.96	1.43
5	16	-5	1.49*	0.00	0.50
6	16	-3	2.78*	2.28	0.97
6	16	-2	6.76	6.41	22.77
6	16	-1	1.81*	0.04	0.66
6	16	0	1.64*	2.08	0.37
6	17	-1	1.85*	0.63	0.54
6	17	-2	1.69*	2.09	0.35
5	17	-5	1.67*	2.44	0.36
5	17	-4	1.53*	0.99	0.42
5	17	-3	2.14*	1.27	0.94
5	17	-2	1.00*	1.79	0.17
5	17	-1	5.97	5.52	22.14
5	17	0	3.41	3.28	12.35
5	17	1	4.64	4.76	15.78
5	17	2	4.01	3.83	13.38
4	17	3	1.65*	2.23	0.44
4	17	2	1.47*	0.11	0.46
4	17	1	1.19*	1.60	0.32
4	17	0	1.48*	0.73	0.46
4	17	-1	4.68	5.04	21.85
4	17	-2	5.01	4.97	26.09
4	17	-3	1.49*	0.34	0.45
4	17	-4	2.32*	0.88	1.38
4	17	-5	5.27	4.81	19.01
3	17	-6	2.89*	0.58	1.43
3	17	-5	2.24*	2.16	0.80
3	17	-4	6.99	6.39	26.69
3	17	-3	1.49*	0.56	0.45
3	17	-2	1.78*	1.85	0.77
3	17	-1	4.35	4.32	24.11
3	17	0	6.52	7.21	36.51
3	17	1	1.93*	2.04	0.70
3	17	2	1.49*	2.06	0.40
3	17	3	2.80*	2.99	1.59
3	17	4	2.33*	3.24	0.74
2	17	5	1.58*	0.81	0.40
2	17	4	2.22*	1.32	1.26
2	17	3	1.33*	0.29	0.36
2	17	2	1.44*	1.66	0.48
2	17	1	10.62	10.83	28.11
2	17	0	5.14	4.93	35.14
2	17	-1	7.28	7.76	41.16
2	17	-2	4.48	4.96	27.19
2	17	-3	7.19	7.77	36.65
2	17	-4	6.82	6.74	34.70
2	17	-5	2.70*	2.12	1.78
1	17	-6	1.62*	1.55	0.38
1	17	-6	2.67*	2.20	0.82
1	17	-5	2.50	1.71	9.02
1	17	-4	2.36*	2.39	1.25
1	17	-3	1.87*	0.85	1.24
1	17	-2	4.43	4.37	27.45
1	17	-1	9.01	9.33	38.60
1	17	0	1.89*	1.73	9.74
1	17	1	1.43*	0.26	0.49
1	17	2	4.21	5.05	23.87
1	17	3	1.28*	0.99	0.39
1	17	4	2.25*	0.91	1.24
1	17	5	1.56*	1.08	0.41
0	17	6	1.30*	1.04	0.31
0	17	5	1.47*	0.93	0.46
0	17	4	2.19*	2.18	1.55
0	17	3	9.69	9.91	37.72
0	17	2	3.33	3.77	18.71
0	17	1	1.16*	1.54	0.40
0	18	0	1.80*	0.72	1.59
0	18	1	1.36*	0.08	0.54
0	18	2	2.40*	2.81	1.33
0	18	3	1.29*	0.25	0.66
0	18	4	1.43*	1.10	0.49
0	18	5	1.52*	1.70	0.43
1	18	5	2.76*	2.84	1.28
1	18	4	1.20*	2.04	0.29
1	18	3	1.48*	1.95	0.46
1	18	2	2.89*	4.63	1.88
1	18	1	1.35*	0.78	0.55
1	18	0	1.78*	0.94	7.35
1	18	-1	1.38*	0.34	0.52
1	18	-2	5.92	6.13	34.22
1	18	-3	2.23*	2.28	0.82
1	18	-4	1.35*	1.22	0.35
1	18	-5	1.74*	0.15	0.56
1	18	-6	1.65*	1.61	0.37
2	18	-6	2.72*	2.74	0.75
2	18	-5	1.55*	0.73	0.42
2	18	-4	1.36*	0.81	0.46
2	18	-3	2.06*	2.98	0.70
2	18	-2	2.09*	2.66	1.09
2	18	-1	1.35*	0.72	0.55
2	18	0	1.87*	2.88	0.72
2	18	1	7.70	7.89	37.35
2	18	2	1.85*	1.68	1.01
2	18	3	3.88	4.16	15.03
2	18	4	1.50*	0.43	0.44

h	k	l	Fo	Fc	weight
3	18	4	1.64*	1.61	0.37
3	18	3	3.37	3.08	12.07
3	18	2	1.94*	0.09	0.85
3	18	1	6.42	6.25	30.58
3	18	0	1.59*	1.59	0.95
3	18	-1	5.17	4.80	28.64
3	18	-2	3.77	4.26	19.06
3	18	-3	1.45*	2.47	2.96
3	18	-4	3.10*	1.55	1.59
3	18	-5	1.62*	1.83	2.78
4	18	-5	1.28*	0.01	0.23
4	18	-4	4.81	4.71	19.27
4	18	-3	1.58*	2.01	0.40
4	18	-2	1.81*	1.50	0.98
4	18	-1	1.50*	0.24	0.44
4	18	0	3.34	3.74	12.03
4	18	1	2.43*	2.62	1.08
4	18	2	2.90*	2.82	1.29
4	18	3	2.27*	0.74	0.63
5	18	1	1.62*	0.02	0.38
5	18	0	2.79	2.47	8.45
5	18	-1	2.47*	3.30	5.86
5	18	-2	1.57*	0.94	0.41
6	18	-3	3.75	3.91	12.51
6	18	-4	2.48*	1.40	1.10
5	19	-3	2.70*	0.50	1.26
5	19	-2	2.92	2.61	8.09
5	19	-1	1.55*	0.37	0.42
5	19	0	2.38*	1.84	5.74
4	19	2	0.96*	1.22	1.09
4	19	1	3.38*	4.34	1.36
4	19	0	1.53*	0.68	0.43
4	19	-1	1.50*	1.28	0.44
4	19	-2	1.56*	0.83	0.41
4	19	-3	2.37*	2.33	1.04
4	19	-4	2.20*	1.44	0.97
3	19	-5	1.96*	0.33	0.70
3	19	-4	1.65*	2.32	0.37
3	19	-3	4.93	5.04	22.47
3	19	-2	1.56*	1.23	0.41
3	19	-1	3.27	3.38	12.16
3	19	0	2.01*	0.85	1.07
3	18	1	2.80*	2.42	1.35
3	19	2	2.23*	1.74	1.06
3	19	3	1.68*	1.81	0.35
2	19	4	3.30*	2.98	1.40
2	19	3	0.70*	0.66	0.10
2	19	2	1.65*	1.26	0.63
2	19	1	4.92	4.65	25.12
2	19	0	3.34	3.19	17.79
2	19	-1	1.93*	1.43	1.26
2	19	-2	1.43*	1.29	3.78
2	19	-3	1.32*	0.74	2.66
2	19	-4	5.76	5.20	25.51
2	19	-5	2.83*	2.37	1.49
1	19	-5	1.26*	2.49	0.20
1	19	-4	1.47*	0.12	0.46
1	19	-3	1.46*	1.27	0.47
1	19	-2	1.39*	0.66	0.52
1	19	-1	1.47*	0.06	0.46
1	19	0	2.43*	2.70	1.45
1	19	1	1.10*	2.38	0.32
1	19	2	2.44*	1.28	1.64
1	19	3	1.45*	0.93	0.48
1	19	4	1.43*	1.12	0.41
0	19	5	1.62*	0.19	0.38
0	19	5	1.64*	1.19	0.37
0	19	4	2.68	2.50	9.80
0	19	3	7.43	6.83	31.61
0	19	2	1.70*	0.60	0.80
0	19	1	1.41*	0.47	0.50
0	20	0	8.88	9.50	39.54
0	20	1	2.34*	0.92	1.45
0	20	2	1.50*	0.87	0.44
0	20	3	4.36	3.43	21.05
0	20	4	0.72*	0.84	0.09
0	20	5	2.39*	1.20	1.09
1	20	4	2.09*	1.92	5.47
1	20	3	2.32*	2.07	1.01
1	20	2	1.51*	0.77	0.53
1	20	1	3.85	2.82	25.47
1	20	0	1.48*	1.70	0.45
1	20	-1	1.43*	1.35	0.49
1	20	-2	1.51*	0.13	0.44
1	20	-3	1.81*	1.01	0.62
1	20	-4	5.23	5.89	18.41
1	20	-5	2.12*	2.53	0.47
2	20	-5	2.60*	1.00	1.18
2	20	-4	3.20*	3.52	1.41
2	20	-3	2.83	3.19	9.53
2	20	-2	1.43*	0.46	0.49
2	20	-1	1.49*	2.34	0.45
2	20	0	1.40*	0.33	0.51
2	20	1	1.52*	2.05	0.43
2	20	2	1.55*	1.63	0.42
2	20	3	0.72*	2.15	0.10
2	20	4	2.32*	1.97	4.81
3	20	3	1.99*	0.86	0.74
3	20	2	3.13	3.06	9.37
3	20	1	1.51*	0.86	0.44
3	20	0	1.59*	2.38	0.39
3	20	-1	1.54*	1.14	0.42
3	20	-2	2.50*	2.19	1.11
3	20	-3	2.61	2.43	8.04
3	20	-4	1.51*	1.53	0.44
4	20	-4	1.51*	1.80	0.28
4	20	-3	1.61*	0.13	0.39
4	20	-2	1.41*	0.64	0.50
4	20	-1	1.02*	0.80	0.19
4	20	0	5.75	4.93	21.25
4	20	1	2.09*	2.61	0.53
5	20	-1	1.58*	0.06	0.40
5	20	-2	1.70*	2.16	0.42
4	21	1	4.48	5.03	12.84
4	21	0	2.68*	1.57	1.03
4	21	-1	1.81*	1.24	0.56
4	21	-2	1.71*	1.35	0.34
4	21	-3	1.68*	2.33	0.35
3	21	-4	1.62*	0.87	0.38
3	21	-3	0.73*	1.60	0.09
3	21	-2	2.36*	3.04	1.22
3	21	-1	2.55*	2.23	1.07
3	21	0	5.04	4.63	20.13
3	21	1	4.66	4.69	16.58
2	21	2	1.59*	2.69	0.40
2	21	3	3.91	3.33	11.52
2	21	2	2.58	2.71	6.85
2	21	1	1.84*	0.75	0.86
2	21	0	1.38*	0.64	0.52
2	21	-1	6.01	5.86	25.37
2	21	-2	2.94*	1.91	1.77
2	21	-3	6.63	6.06	26.79
2	21	-4	0.74*	1.05	0.08
1	21	-4	5.97	5.90	22.65
1	21	-3	1.55*	0.43	0.42
1	21	-2	2.56*	1.35	1.15
1	21	-1	2.77*	1.61	1.80
1	21	0	2.84*	3.26	1.48
1	21	1	1.62*	2.59	0.38
1	21	2	1.53*	0.04	0.43
1	21	3	2.16*	1.39	0.75
0	21	4	1.62*	1.36	0.38
0	21	4	2.55*	2.54	0.92
0	21	3	3.30	3.01	11.31
0	21	2	1.67*	2.12	0.36
0	21	1	1.36*	0.16	0.54
0	22	0	0.69*	1.08	0.11
0	22	1	2.08*	3.13	0.81
0	22	2	4.48	4.38	16.56
0	22	3	1.45*	2.06	0.37
0	22	4	1.31*	1.75	0.30
1	22	3	2.86*	0.40	1.35
1	22	2	5.93	5.90	23.67
1	22	1	1.54*	0.54	0.42
1	22	0	2.40*	1.61	1.38
1	22	-1	1.45*	0.91	0.48
1	22	-2	4.52	4.15	17.71
1	22	-3	5.40	5.02	20.60
1	22	-4	1.84*	1.17	0.42
2	22	-4	1.85*	0.99	0.44
2	22	-3	1.20*	0.21	1.86
2	22	-2	2.86*	2.08	1.78
2	22	-1	2.66	3.09	7.18
2	22	0	2.00*	0.45	0.80
2	22	1	4.07	3.76	13.99
2	22	2	3.83	3.93	12.34
3	22	1	1.64*	2.60	0.37
3	22	0	1.46*	1.77	0.30
3	22	-1	2.11*	1.93	4.77
3	22	-2	1.71*	1.63	3.25
3	22	-3	2.36*	2.64	0.58
4	22	-1	2.94	3.81	6.72
3	23	-2	1.07*	0.01	0.21
3	23	-1	4.36	4.96	13.08
3	23	0	5.80	5.22	20.44
2	23	2	1.69*	0.86	0.35
2	23	1	2.83	2.69	7.08
2	23	0	4.25	4.42	13.76
2	23	-1	2.18*	0.33	1.08
2	23	-2	4.24	4.24	14.09
2	23	-3	4.24	3.78	12.34
1	23	-3	8.28	7.90	24.28
1	23	-2	2.49	2.19	5.94
1	23	-1	2.77*	2.51	1.69
1	23	0	1.51*	1.49	0.44
1	23	1	2.28*	1.15	1.10
1	23	2	1.47*	1.59	0.42
0	23	3	2.48*	2.99	5.22
0	23	2	1.92*	1.15	0.87
0	23	1	1.60*	2.04	0.44
0	24	0	2.20*	1.25	0.83
0	24	1	1.28*	0.56	0.27
0	24	2	2.12*	1.10	0.84
1	24	2	2.73*	1.88	1.23
1	24	1	3.07*	1.87	1.59
1	24	0	0.74*	0.38	0.08
1	24	-1	3.86	3.75	12.54
1	24	-2	1.75*	1.67	0.33
2	24	-2	3.11	2.72	8.95
2	24	-1	2.70*	2.49	0.95
2	24	0	1.84*	1.98	0.51
2	24	1	1.68*	0.90	0.35
1	25	0	2.01*	1.30	0.90
0	25	1	3.29	2.21	9.76

1828 reflections

5-(2,3-dimethylphenyl)-γ-butyrolactone

h	k	l	Fo	Fc	weight
0	0	2	48.50	52.46	0.02
0	0	4	57.35	63.49	0.02
0	0	6	3.02	3.06	0.49
0	0	8	17.26	16.33	0.21
0	0	10	1.90*	3.16	0.42
0	0	12	2.28*	4.74	0.44
0	0	14	1.80*	1.89	0.41
0	1	14	2.20*	2.27	0.44
0	1	13	1.89*	0.04	0.42
0	1	12	2.93*	0.01	0.49
0	1	11	0.77*	0.15	0.35
0	1	10	4.61	4.09	0.60
0	1	9	6.97	7.69	0.69
0	1	8	1.70*	0.18	0.40
0	1	7	1.78*	2.24	0.41
0	1	6	18.23	18.18	0.19
0	1	5	20.07	21.02	0.15
0	1	4	50.67	53.52	0.02
0	1	3	53.19	56.94	0.02
0	1	2	36.54	38.65	0.04
0	1	1	57.43	58.11	0.02
0	2	0	16.53	17.18	0.24
0	2	1	12.97	13.79	0.39
0	2	2	2.29*	0.48	0.44
0	2	3	1.35*	1.03	0.38
0	2	4	33.76	33.10	0.05
0	2	5	7.06	7.02	0.69
0	2	6	2.74	2.62	0.47
0	2	7	13.88	14.53	0.34
0	2	8	1.80*	1.35	0.42
0	2	9	5.20	5.20	0.64
0	2	10	1.76*	0.78	0.41
0	2	11	5.37	5.21	0.64
0	2	12	2.63*	0.34	0.47
0	2	13	1.98*	1.26	0.42
0	2	14	2.59*	0.90	0.46
0	3	13	2.01*	2.69	0.42
0	3	12	3.86*	4.32	0.55
0	3	11	3.07	2.52	0.50
0	3	10	3.50	2.88	0.53
0	3	9	6.17	5.40	0.68
0	3	8	3.28*	3.75	0.51
0	3	7	1.73*	1.20	0.41
0	3	6	2.83*	3.75	0.48
0	3	5	15.78	16.30	0.26
0	3	4	6.53	7.69	0.69
0	3	3	28.26	27.00	0.07
0	3	2	1.50*	0.62	0.39
0	3	1	11.10	11.34	0.51
0	4	0	5.68	5.91	0.66
0	4	1	12.12	13.30	0.44
0	4	2	16.61	15.70	0.23
0	4	3	12.72	12.98	0.41
0	4	4	10.22	10.77	0.57
0	4	5	2.18*	0.93	0.44
0	4	6	6.24	6.04	0.68
0	4	7	5.32	4.94	0.64
0	4	8	3.08*	3.48	0.50
0	4	9	2.41*	0.88	0.45
0	4	10	4.59	4.32	0.60
0	4	11	1.74*	2.83	0.41
0	4	12	3.27*	2.13	0.51
0	5	10	2.19*	3.57	0.44
0	5	9	1.93*	1.36	0.42
0	5	8	3.49	3.36	0.53
0	5	7	0.81*	0.79	0.35
0	5	6	1.90*	1.82	0.42
0	5	5	3.33*	1.94	0.51
0	5	4	1.95*	0.32	0.42
0	5	3	1.63*	1.07	0.40
0	5	2	2.04*	4.89	0.43
0	5	1	8.44	9.16	0.67
0	6	0	1.59*	0.73	0.40
0	6	1	9.01	9.51	0.64
0	6	2	2.41*	1.37	0.45
0	6	3	10.55	11.52	0.55
0	6	4	7.05	7.26	0.69
0	6	5	5.73	5.76	0.68
0	6	6	6.30	6.27	0.68
0	6	7	1.97*	2.89	0.42
0	6	8	2.99*	1.70	0.49
0	7	5	3.79*	1.03	0.55
0	7	4	2.14*	2.60	0.43
0	7	3	5.79	5.81	0.66
0	7	2	4.40	5.59	0.59
0	7	1	0.88*	0.67	0.36
1	7	-5	4.10	3.63	0.57
1	7	-4	9.72	9.90	0.60
1	7	-3	3.58*	2.60	0.53
1	7	-2	3.44*	2.31	0.52
1	7	-1	3.06*	1.35	0.50
1	7	0	7.57	7.88	0.69
1	7	1	2.26*	1.67	0.44
1	7	2	3.98*	3.73	0.56
1	7	3	0.90*	0.39	0.36
1	7	4	2.15*	0.02	0.43
1	6	8	1.28*	1.24	0.38
1	6	7	2.50*	1.94	0.46
1	6	6	1.96*	2.17	0.42
1	6	5	1.89*	1.63	0.42
1	6	4	7.15	7.31	0.69
1	6	3	3.65*	4.40	0.54
1	6	2	9.43	9.74	0.62
1	6	1	2.07*	2.69	0.43
1	6	0	4.96	5.07	0.62
1	6	-1	9.22	10.03	0.63
1	6	-2	12.24	11.26	0.44
1	6	-3	12.74	12.24	0.41
1	6	-4	2.48*	0.17	0.46
1	6	-5	3.36*	0.81	0.52
1	6	-6	6.33	7.16	0.68
1	6	-7	2.16*	0.71	0.43
1	6	-8	2.11*	0.02	0.43
1	5	-10	2.08*	1.52	0.43
1	5	-9	7.23	7.56	0.69
1	5	-8	3.49	3.78	0.53
1	5	-7	15.04	15.43	0.29
1	5	-6	3.51*	4.17	0.53
1	5	-5	3.89*	2.53	0.55
1	5	-4	12.83	12.28	0.40
1	5	-3	1.90*	1.02	0.42
1	5	-2	8.96	8.36	0.64
1	5	-1	11.42	12.18	0.49
1	5	0	7.94	7.72	0.68
1	5	1	12.80	13.53	0.40
1	5	2	1.89*	1.56	0.42
1	5	3	1.89*	1.91	0.42
1	5	4	1.87*	1.26	0.42
1	5	5	1.85*	0.20	0.41
1	5	6	2.62*	1.44	0.46
1	5	7	4.89	4.87	0.62
1	5	8	1.19*	1.49	0.37
1	5	9	7.06	7.08	0.69
1	5	10	3.11*	2.82	0.50
1	4	12	2.89*	2.37	0.48
1	4	11	2.03*	1.10	0.43
1	4	10	1.82*	0.74	0.41
1	4	9	2.43*	1.86	0.45
1	4	8	8.49	8.24	0.66
1	4	7	1.94*	2.72	0.42
1	4	6	1.44*	0.98	0.39
1	4	5	2.69*	4.16	0.47
1	4	4	4.88	3.71	0.62
1	4	3	11.26	11.25	0.50
1	4	2	1.69*	1.22	0.40
1	4	1	9.06	8.76	0.64
1	4	0	23.96	25.54	0.10
1	4	-1	1.69*	1.60	0.40
1	4	-2	14.92	14.48	0.30
1	4	-3	8.58	8.53	0.66
1	4	-4	4.32	3.79	0.58
1	4	-5	8.48	8.55	0.67
1	4	-6	12.71	12.09	0.41
1	4	-7	5.73	6.18	0.66
1	4	-8	1.72*	0.53	0.41
1	4	-9	3.00*	0.23	0.49
1	4	-10	7.39	8.20	0.69
1	4	-11	1.98*	1.51	0.42
1	4	-12	1.28*	2.14	0.38
1	3	-13	2.01*	2.63	0.42
1	3	-12	3.46	3.00	0.52
1	3	-11	1.93*	0.86	0.42
1	3	-10	5.81	5.90	0.66
1	3	-9	3.58	3.70	0.53
1	3	-8	2.06*	2.79	0.43
1	3	-7	4.25	4.03	0.58
1	3	-6	13.85	13.72	0.35
1	3	-5	9.73	9.60	0.60
1	3	-4	22.20	20.19	0.12
1	3	-3	34.38	29.15	0.04
1	3	-2	18.79	17.07	0.18
1	3	-1	21.10	19.30	0.13
1	3	0	4.70	5.61	0.61
1	3	1	1.50*	0.94	0.39
1	3	2	6.10	6.37	0.67
1	3	3	3.01	2.82	0.49
1	3	4	13.41	13.10	0.37
1	3	5	7.45	7.15	0.69
1	3	6	1.57*	2.58	0.40
1	3	7	12.30	11.84	0.43
1	3	8	1.25*	1.87	0.38
1	3	9	1.86*	0.15	0.41
1	3	10	8.40	8.36	0.67
1	3	11	1.91*	2.13	0.42
1	3	12	1.74*	0.76	0.41
1	3	13	1.58*	1.08	0.40
1	2	13	2.92*	0.45	0.49
1	2	12	1.68*	0.43	0.40
1	2	11	2.56*	2.60	0.46
1	2	10	6.17	6.16	0.68
1	2	9	3.38	3.81	0.52
1	2	8	4.89	5.32	0.62
1	2	7	9.67	9.71	0.60
1	2	6	38.10	37.18	0.04
1	2	5	18.59	18.28	0.18
1	2	4	18.65	18.69	0.18
1	2	3	6.32	6.36	0.68
1	2	2	25.32	24.93	0.09
1	2	1	12.65	13.61	0.41
1	2	0	12.91	13.01	0.40
1	2	-1	35.41	31.66	0.04
1	2	-2	7.84	7.27	0.68
1	2	-3	32.55	30.46	0.05
1	2	-4	37.02	38.93	0.04
1	2	-5	13.66	14.11	0.36
1	2	-6	9.74	9.17	0.60
1	2	-7	25.68	27.25	0.08
1	2	-8	2.01*	1.02	0.42
1	2	-9	5.36	6.14	0.64
1	2	-10	1.65*	1.32	0.40
1	2	-11	3.44*	1.32	0.52
1	2	-12	3.21*	1.73	0.51
1	2	-13	3.26*	1.88	0.51
1	2	-14	1.99*	1.71	0.42
1	1	-14	1.95*	0.73	0.42
1	1	-13	4.08*	4.29	0.57
1	1	-12	2.06*	2.52	0.43
1	1	-11	5.49	5.95	0.65
1	1	-10	3.40*	3.49	0.52
1	1	-9	1.55*	0.78	0.40
1	1	-8	13.98	14.79	0.34
1	1	-7	4.35	4.06	0.58
1	1	-6	2.72*	4.60	0.47
1	1	-5	17.51	19.50	0.21
1	1	-4	0.80*	0.87	0.35
1	1	-3	2.30	2.88	0.44
1	1	-2	12.31	12.87	0.43
1	1	-1	46.48	42.21	0.02
1	1	0	37.21	37.50	0.04
1	1	1	49.32	50.59	0.02
1	1	2	46.17	44.87	0.02
1	1	3	96.66	97.18	0.01

h	k	l	Fo	Fc	weight
1	1	4	20.60	20.44	0.14
1	1	5	20.38	21.10	0.15
1	1	6	9.10	9.30	0.64
1	1	7	5.11	5.64	0.63
1	1	8	1.50*	0.71	0.39
1	1	9	7.10	8.18	0.69
1	1	10	9.75	9.88	0.60
1	1	11	4.33	3.89	0.58
1	1	12	1.81*	2.11	0.41
1	1	13	1.86*	2.31	0.41
1	1	14	1.98*	1.17	0.42
1	0	13	5.79	4.97	0.66
1	0	11	1.88*	3.31	0.42
1	0	9	15.97	16.83	0.25
1	0	7	21.11	20.25	0.13
1	0	5	16.72	17.93	0.23
1	0	3	34.97	39.30	0.04
1	0	1	11.91	13.31	0.46
1	0	-1	9.37	9.25	0.62
1	0	-3	32.35	35.71	0.05
1	0	-5	24.44	26.06	0.09
1	0	-7	1.44*	1.59	0.39
1	0	-9	6.56	6.05	0.68
1	0	-11	5.01	5.75	0.62
1	0	-13	3.05*	3.83	0.49
2	0	-14	2.95*	0.84	0.49
2	0	-12	1.87*	1.71	0.42
2	0	-10	7.19	8.31	0.69
2	0	-8	15.89	15.87	0.26
2	0	-6	4.49	4.60	0.59
2	0	-4	22.88	23.47	0.11
2	0	-2	43.81	45.38	0.03
2	0	0	41.39	45.10	0.03
2	0	2	113.25	131.03	0.01
2	0	4	1.28*	0.75	0.38
2	0	6	3.89	3.82	0.55
2	0	8	6.96	7.00	0.69
2	0	10	2.67*	1.98	0.47
2	0	12	7.25	7.45	0.69
2	0	14	2.04*	1.80	0.43
2	1	14	0.95*	0.72	0.36
2	1	13	2.00*	2.15	0.42
2	1	12	1.94*	2.34	0.42
2	1	11	4.23	3.72	0.58
2	1	10	2.61*	2.48	0.46
2	1	9	1.56*	0.45	0.40
2	1	8	13.14	12.80	0.38
2	1	7	12.85	12.79	0.40
2	1	6	37.47	39.67	0.04
2	1	5	27.18	25.60	0.07
2	1	4	9.66	9.22	0.61
2	1	3	21.84	21.34	0.12
2	1	2	46.92	46.07	0.02
2	1	1	33.22	30.87	0.05
2	1	0	46.07	47.93	0.02
2	1	-1	19.82	19.94	0.15
2	1	-2	31.82	30.95	0.05
2	1	-3	7.85	7.35	0.68
2	1	-4	24.28	25.49	0.10
2	1	-5	1.37*	1.84	0.38
2	1	-6	3.23	2.56	0.51
2	1	-7	3.48	4.37	0.52
2	1	-8	8.32	8.12	0.67
2	1	-9	2.64	3.48	0.47
2	1	-10	10.01	9.87	0.58
2	1	-11	2.44*	2.76	0.45
2	1	-12	8.78	8.88	0.65
2	1	-13	3.08*	3.66	0.50
2	1	-14	0.90*	0.04	0.36
2	2	-14	1.87*	0.70	0.42
2	2	-13	7.22	7.21	0.69
2	2	-12	4.69	4.39	0.61
2	2	-11	2.10*	3.01	0.43
2	2	-10	3.11*	2.30	0.50
2	2	-9	9.86	9.17	0.59
2	2	-8	1.52*	3.45	0.39
2	2	-7	2.48*	1.05	0.46
2	2	-6	4.08	2.85	0.57
2	2	-5	4.29	4.81	0.58
2	2	-4	7.84	6.92	0.68
2	2	-3	11.51	11.09	0.48
2	2	-2	15.02	13.27	0.29
2	2	-1	8.57	9.71	0.61
2	2	0	4.10	4.11	0.57
2	2	1	1.39*	1.45	0.39
2	2	2	31.47	29.89	0.05
2	2	3	2.66*	0.36	0.47
2	2	4	8.76	9.32	0.65
2	2	5	16.10	15.84	0.25
2	2	6	41.63	40.03	0.03
2	2	7	5.30	5.04	0.64
2	2	8	3.11*	4.99	0.50
2	2	9	12.13	12.41	0.44
2	2	10	6.93	6.72	0.69
2	2	11	1.94*	2.51	0.42
2	2	12	1.80*	0.71	0.41
2	2	13	3.22*	1.53	0.51
2	3	12	1.86*	2.24	0.42
2	3	11	3.58*	4.74	0.53
2	3	10	5.10	4.80	0.63
2	3	9	5.88	5.33	0.67
2	3	8	3.54*	6.18	0.53
2	3	7	6.72	6.34	0.69
2	3	6	6.78	6.27	0.69
2	3	5	1.45*	0.36	0.39
2	3	4	4.90	4.67	0.62
2	3	3	20.12	21.16	0.15
2	3	2	21.88	20.65	0.12
2	3	1	7.66	7.30	0.69
2	3	0	22.18	22.23	0.12
2	3	-1	14.27	13.86	0.32
2	3	-2	7.63	7.17	0.69
2	3	-3	14.97	13.39	0.29
2	3	-4	11.04	10.39	0.52
2	3	-5	5.92	5.33	0.67
2	3	-6	5.25	5.16	0.64
2	3	-7	3.16*	0.91	0.50
2	3	-8	5.12	4.99	0.63
2	3	-9	1.83*	0.16	0.41
2	3	-10	5.96	6.56	0.67
2	3	-11	4.97	5.23	0.62
2	3	-12	3.12*	3.24	0.50
2	3	-13	2.05*	0.67	0.43
2	4	-12	2.05*	0.37	0.43
2	4	-11	1.95*	1.24	0.42
2	4	-10	2.22*	1.75	0.44
2	4	-9	5.20	4.91	0.63
2	4	-8	3.20*	0.73	0.50
2	4	-7	3.26*	4.01	0.51
2	4	-6	6.23	5.77	0.68
2	4	-5	3.81	3.15	0.55
2	4	-4	12.65	11.38	0.41
2	4	-3	2.89*	1.39	0.48
2	4	-2	1.30*	2.67	0.38
2	4	-1	21.04	20.00	0.13
2	4	0	12.34	11.66	0.43
2	4	1	2.76	3.23	0.47
2	4	2	13.15	11.82	0.38
2	4	3	9.59	9.18	0.61
2	4	4	1.94*	0.47	0.42
2	4	5	1.80*	0.63	0.41
2	4	6	3.36*	5.16	0.52
2	4	7	6.56	6.12	0.69
2	4	8	1.93*	1.01	0.42
2	4	9	1.96*	2.79	0.42
2	4	10	1.90*	1.02	0.42
2	4	11	1.54*	1.12	0.39
2	5	10	2.40*	1.41	0.45
2	5	9	2.15*	0.15	0.43
2	5	8	3.96	3.47	0.56
2	5	7	2.61*	0.49	0.46
2	5	6	2.03*	2.04	0.43
2	5	5	5.00	5.28	0.62
2	5	4	3.40*	1.48	0.52
2	5	3	24.66	25.92	0.09
2	5	2	10.80	10.92	0.53
2	5	1	4.46	4.54	0.59
2	5	0	19.70	20.80	0.16
2	5	-1	8.50	8.27	0.66
2	5	-2	6.34	6.46	0.68
2	5	-3	1.96*	4.10	0.42
2	5	-4	2.51*	2.04	0.46
2	5	-5	4.31	4.54	0.58
2	5	-6	7.91	8.04	0.68
2	5	-7	1.41*	0.37	0.39
2	5	-8	3.35*	1.66	0.52
2	5	-9	2.16*	1.96	0.43
2	5	-10	1.93*	0.26	0.42
2	6	-8	1.33*	0.11	0.38
2	6	-7	1.77*	0.34	0.41
2	6	-6	2.73*	3.16	0.47
2	6	-5	2.22*	1.74	0.44
2	6	-4	9.74	9.65	0.60
2	6	-3	11.94	11.20	0.46
2	6	-2	1.41*	1.27	0.39
2	6	-1	16.75	16.44	0.23
2	6	0	8.90	9.15	0.65
2	6	1	10.91	10.59	0.52
2	6	2	0.82*	2.12	0.35
2	6	3	8.29	8.48	0.67
2	6	4	5.55	5.09	0.65
2	6	5	1.89*	2.44	0.42
2	6	6	1.95*	3.25	0.42
2	6	7	1.99*	0.12	0.42
2	6	8	3.43*	0.22	0.52
2	7	4	2.14*	2.07	0.43
2	7	3	1.57*	1.52	0.40
2	7	2	2.10*	0.55	0.43
2	7	1	2.05*	2.48	0.43
2	7	0	2.52*	0.94	0.46
2	7	-1	4.27*	5.06	0.58
2	7	-2	2.97*	3.60	0.49
2	7	-3	4.23*	4.72	0.58
2	7	-4	6.07	6.53	0.67
2	7	-5	2.89*	1.59	0.48
2	7	-6	5.54	6.21	0.65
2	7	-7	2.19*	1.14	0.44
2	7	0	3.13*	2.60	0.50
2	7	1	2.40*	3.44	0.45
2	7	2	1.29*	1.81	0.38
2	7	3	3.05*	4.04	0.49
2	6	7	2.23*	2.30	0.44
2	6	6	4.97	4.93	0.62
2	6	5	2.07*	1.56	0.43
2	6	4	5.90	6.33	0.67
2	6	3	1.97*	1.00	0.42
2	6	2	6.75	7.22	0.69
2	6	1	8.57	9.26	0.66
2	6	0	5.84	5.82	0.67
2	6	-1	11.80	12.26	0.47
2	6	-2	2.15*	3.28	0.43
2	6	-3	3.91*	3.20	0.55
2	6	-4	9.09	9.05	0.64
2	6	-5	2.06*	0.92	0.43
2	6	-6	1.64*	1.92	0.40
2	6	-7	2.00*	1.51	0.42
2	6	-8	1.29*	0.53	0.38
3	5	-10	2.02*	0.41	0.43
3	5	-9	2.62*	3.69	0.47
3	5	-8	2.81*	2.30	0.48
3	5	-7	3.22	3.74	0.51
3	5	-6	2.89*	0.37	0.48
3	5	-5	6.26	6.51	0.68
3	5	-4	2.77*	0.16	0.48
3	5	-3	2.83*	3.74	0.48
3	5	-2	3.59	3.54	0.53
3	5	-1	1.81*	0.79	0.41
3	5	0	2.10*	0.33	0.43
3	5	1	2.53*	2.77	0.46
3	5	2	14.29	14.24	0.32
3	5	3	1.89*	2.24	0.42
3	5	4	1.97*	1.64	0.42

h	k	l	Fo	Fc	weight
3	5	5	5.21	5.03	0.64
3	5	6	10.60	9.88	0.55
3	5	7	1.16*	1.21	0.37
3	5	8	2.31*	3.26	0.44
3	5	9	1.55*	0.55	0.40
3	4	11	2.86*	3.33	0.48
3	4	10	1.51*	0.07	0.39
3	4	9	3.56*	2.80	0.53
3	4	8	8.25	7.51	0.67
3	4	7	3.12*	2.95	0.50
3	4	6	8.97	8.98	0.64
3	4	5	15.05	14.47	0.29
3	4	4	2.74*	1.43	0.47
3	4	3	20.18	19.91	0.15
3	4	2	12.57	12.30	0.42
3	4	1	1.16*	0.58	0.37
3	4	0	15.13	14.46	0.29
3	4	-1	5.13	5.59	0.63
3	4	-2	3.07*	1.45	0.50
3	4	-3	20.34	18.07	0.15
3	4	-4	6.45	5.76	0.68
3	4	-5	2.76*	4.35	0.47
3	4	-6	2.23*	2.04	0.44
3	4	-7	0.76*	0.31	0.35
3	4	-8	9.41	9.38	0.62
3	4	-9	5.60	6.18	0.66
3	4-10		3.60*	3.67	0.53
3	4-11		3.52*	3.48	0.53
3	4-12		2.11*	2.45	0.43
3	3-13		3.28*	0.51	0.51
3	3-12		5.38	4.80	0.64
3	3-11		2.77*	2.47	0.48
3	3-10		2.78*	2.34	0.48
3	3	-9	2.87*	3.16	0.48
3	3	-8	6.38	7.16	0.68
3	3	-7	0.70*	0.86	0.35
3	3	-6	1.62*	1.94	0.40
3	3	-5	17.72	17.78	0.20
3	3	-4	32.02	29.77	0.05
3	3	-3	3.84	3.46	0.55
3	3	-2	4.57	3.94	0.60
3	3	-1	33.22	29.27	0.05
3	3	0	4.77	4.08	0.61
3	3	1	1.45*	1.22	0.39
3	3	2	1.91*	0.56	0.42
3	3	3	3.73	4.23	0.54
3	3	4	8.78	8.21	0.65
3	3	5	12.43	12.28	0.43
3	3	6	2.60*	3.33	0.46
3	3	7	1.78*	1.49	0.41
3	3	8	12.67	11.90	0.41
3	3	9	15.82	15.46	0.26
3	3	10	1.78*	0.57	0.41
3	3	11	2.11*	2.54	0.43
3	3	12	4.86	4.48	0.62
3	2	13	3.40*	0.62	0.52
3	2	12	1.36*	2.61	0.38
3	2	11	2.68*	1.71	0.47
3	2	10	6.46	6.25	0.68
3	2	9	8.00	8.09	0.68
3	2	8	12.09	12.03	0.45
3	2	7	2.15*	2.89	0.43
3	2	6	6.34	6.06	0.68
3	2	5	9.90	10.16	0.59
3	2	4	18.64	19.06	0.16
3	2	3	1.11*	1.67	0.37
3	2	2	6.95	7.23	0.69
3	2	1	9.04	8.75	0.64
3	2	0	12.85	13.27	0.40
3	2	-1	22.87	19.65	0.11
3	2	-2	15.72	14.54	0.26
3	2	-3	9.86	9.49	0.58
3	2	-4	15.88	16.32	0.25
3	2	-5	18.31	18.05	0.19
3	2	-6	3.85	3.42	0.55
3	2	-7	2.71*	3.34	0.47
3	2	-8	1.83*	1.04	0.41
3	2	-9	2.63*	3.97	0.47
3	2-10		3.95	4.46	0.56
3	2-11		1.88*	0.61	0.42
3	2-12		1.46*	0.79	0.39
3	2-13		2.16*	1.53	0.43
3	1-13		3.62*	2.57	0.53
3	1-13		4.75	4.33	0.61
3	1-12		3.18*	0.25	0.50
3	1-11		4.92	5.17	0.62
3	1-10		8.74	8.87	0.65
3	1	-9	3.06*	0.66	0.50
3	1	-8	10.04	10.56	0.58
3	1	-7	7.40	8.01	0.69
3	1	-6	19.55	18.66	0.16
3	1	-5	10.18	10.45	0.57
3	1	-4	12.91	12.67	0.40
3	1	-3	20.91	21.68	0.14
3	1	-2	23.43	23.29	0.10
3	1	-1	25.30	26.27	0.09
3	1	0	21.15	21.13	0.13
3	1	1	5.67	6.10	0.66
3	1	2	9.21	8.79	0.63
3	1	3	7.84	7.13	0.68
3	1	4	3.95	4.54	0.56
3	1	5	12.52	11.76	0.42
3	1	6	1.44*	1.04	0.39
3	1	7	1.86*	2.17	0.42
3	1	8	1.60*	0.71	0.40
3	1	9	2.53*	0.98	0.46
3	1	10	1.88*	0.41	0.42
3	1	11	1.81*	3.30	0.41
3	1	12	2.69*	5.04	0.47
3	1	13	0.70*	0.02	0.35
3	0	13	2.50*	1.20	0.46
3	0	11	9.27	9.82	0.63
3	0	9	10.20	9.99	0.57
3	0	7	7.66	7.43	0.69
3	0	5	7.49	7.65	0.69
3	0	3	1.27*	0.93	0.38
3	0	1	60.92	68.93	0.01
3	0	-1	91.56	102.07	0.01
3	0	-3	47.04	50.78	0.02
3	0	-5	2.41	2.05	0.45
3	0	-7	35.37	35.18	0.04
3	0	-9	15.43	16.08	0.27
3	0-11		3.38*	5.52	0.52
3	0-13		6.08	6.16	0.67
3	0-14		1.82*	0.78	0.41
3	0-12		2.62*	2.63	0.47
3	0-10		2.71*	1.31	0.47
3	0	-8	4.18	3.79	0.57
3	0	-6	8.77	8.10	0.65
3	0	-4	31.06	33.01	0.06
3	0	-2	38.49	42.26	0.03
3	0	0	28.45	30.31	0.07
3	0	2	6.27	6.85	0.68
3	0	4	2.56*	2.76	0.46
3	0	6	15.10*	15.65	0.29
3	0	8	1.01*	1.33	0.36
3	0	10	2.08*	0.34	0.43
3	0	12	1.89*	1.68	0.42
3	1	13	2.04*	0.48	0.43
3	1	12	0.97*	1.40	0.36
3	1	11	1.71*	0.32	0.41
3	1	10	1.74*	0.91	0.41
3	1	9	5.41	5.22	0.65
3	1	8	2.16*	0.57	0.43
3	1	7	1.53*	2.28	0.39
3	1	6	2.25*	0.72	0.44
3	1	5	9.97	9.02	0.59
3	1	4	1.55*	0.65	0.40
3	1	3	4.38	3.81	0.59
3	1	2	30.07	32.81	0.06
3	1	1	12.04	11.63	0.45
3	1	0	4.53	4.66	0.60
3	1	-1	14.50	14.03	0.31
3	1	-2	11.23	11.33	0.50
3	1	-3	9.35	9.89	0.62
3	1	-4	13.61	11.84	0.36
3	1	-5	7.56	7.77	0.69
3	1	-6	12.46	12.69	0.42
3	1	-7	2.16*	2.99	0.43
3	1	-8	10.65	9.74	0.54
3	1	-9	4.01	3.37	0.56
3	1-10		7.64	8.16	0.69
3	1-11		2.76*	6.28	0.47
3	1-12		1.18*	2.11	0.37
3	1-13		1.99*	3.01	0.42
3	1-14		2.57*	2.61	0.46
3	2-13		2.65*	3.33	0.47
3	2-12		2.04*	1.37	0.43
3	2-11		10.65	10.99	0.54
3	2-10		7.67	7.74	0.69
3	2	-9	2.24*	1.59	0.44
3	2	-8	3.27*	2.95	0.51
3	2	-7	4.44	4.48	0.59
3	2	-6	12.30	12.34	0.43
4	2	-5	6.39	6.67	0.68
4	2	-4	3.93	3.99	0.56
4	2	-3	1.00*	1.12	0.36
4	2	-2	22.13	21.31	0.12
4	2	-1	14.31	12.49	0.32
4	2	0	10.69	10.56	0.54
4	2	1	15.47	15.50	0.27
4	2	2	25.25	24.18	0.09
4	2	3	2.74*	2.32	0.47
4	2	4	14.31	13.89	0.32
4	2	5	8.19	7.82	0.68
4	2	6	2.80*	3.71	0.48
4	2	7	7.71	8.11	0.69
4	2	8	7.83	7.40	0.68
4	2	9	0.78*	1.44	0.35
4	2	10	2.45*	0.12	0.45
4	2	11	3.26	3.44	0.51
4	2	12	1.99*	0.49	0.42
4	3	11	0.88*	2.56	0.36
4	3	10	1.20*	1.65	0.37
4	3	9	5.12	4.22	0.63
4	3	8	13.64	13.31	0.36
4	3	7	2.91*	2.22	0.48
4	3	6	3.39*	1.53	0.52
4	3	5	1.70*	2.04	0.41
4	3	4	2.85*	2.31	0.48
4	3	3	10.96	10.77	0.52
4	3	2	6.63	6.36	0.69
4	3	1	2.34*	1.72	0.45
4	3	0	7.01	6.40	0.69
4	3	-1	1.86*	2.81	0.42
4	3	-2	3.67	3.77	0.54
4	3	-3	10.05	10.12	0.58
4	3	-4	4.84	4.96	0.61
4	3	-5	1.61*	0.10	0.40
4	3	-6	9.34	8.26	0.62
4	3	-7	14.29	13.58	0.32
4	3	-8	6.51	6.55	0.69
4	3	-9	5.73	5.84	0.66
4	3-10		10.10	10.33	0.58
4	3-11		5.59	5.01	0.65
4	3-12		1.54*	1.27	0.39
4	4-11		2.13*	1.89	0.43
4	4-10		2.59*	3.27	0.46
4	4	-9	0.83*	3.90	0.35
4	4	-8	3.22*	2.85	0.51
4	4	-7	3.39	2.98	0.52
4	4	-6	5.44	5.18	0.65
4	4	-5	5.85	5.66	0.67
4	4	-4	7.08	6.19	0.69
4	4	-3	3.74	3.67	0.54
4	4	-2	2.30*	2.41	0.44
4	4	-1	8.34	7.56	0.67
4	4	0	3.45*	3.34	0.52
4	4	1	4.40	4.45	0.59
4	4	2	8.16	8.27	0.68
4	4	3	1.60*	0.66	0.40
4	4	4	6.69	5.77	0.69
4	4	5	11.57	12.02	0.48
4	4	6	11.04	11.17	0.52
4	4	7	1.78*	0.74	0.41
4	4	8	6.85	6.31	0.69
4	4	9	7.03	7.49	0.69
4	4	10	2.52*	2.44	0.46
4	5	9	1.94*	0.38	0.42
4	5	8	1.54*	0.71	0.39
4	5	7	1.72*	1.04	0.41
4	5	6	1.89*	0.43	0.42
4	5	5	14.48	14.44	0.32
4	5	4	4.02	3.68	0.56
4	5	3	5.92	5.63	0.67
4	5	2	12.87	13.32	0.40
4	5	1	10.67	11.22	0.54
4	5	0	9.19	9.05	0.63
4	5	-1	2.86*	2.32	0.48
4	5	-2	3.35*	3.71	0.52
4	5	-3	3.22	3.77	0.51
4	5	-4	2.08*	0.01	0.43
4	5	-5	6.86	6.97	0.69
4	5	-6	6.52	6.01	0.69
4	5	-7	2.03*	1.97	0.43
4	5	-8	6.23	6.09	0.68
4	5	-9	1.97*	1.21	0.42
4	5-10		2.09*	0.88	0.43
4	6	-7	4.14	3.78	0.57
4	6	-6	2.10*	0.12	0.43
4	6	-5	5.15	5.14	0.63
4	6	-4	3.55*	0.99	0.53
4	6	-3	3.56	3.26	0.53
4	6	-2	1.89*	0.39	0.42
4	6	-1	7.52	7.22	0.69
4	6	0	1.46*	3.40	0.39
4	6	1	3.77*	2.39	0.54
4	6	2	4.66	4.73	0.60
4	6	3	7.24	6.95	0.69
4	6	4	3.70*	4.96	0.54
4	6	5	1.78*	0.84	0.41
4	6	6	1.97*	0.42	0.42
4	7	0	3.44*	1.60	0.52
4	7	-1	2.43*	1.25	0.45
5	6	5	1.58*	0.13	0.40
5	6	4	2.83*	0.34	0.48
5	6	3	3.06*	3.21	0.50
5	6	2	4.60	4.38	0.60
5	6	1	2.01*	0.75	0.42
5	6	0	0.86*	2.99	0.36
5	6	-1	2.99*	0.09	0.49
5	6	-2	9.04	7.83	0.64
5	6	-3	1.28*	1.80	0.38
5	6	-4	2.06*	0.77	0.43
5	6	-5	3.79*	0.63	0.55
5	6	-6	2.27*	1.21	0.44
5	5	-9	2.11*	2.65	0.43
5	5	-8	2.65*	1.74	0.47
5	5	-7	3.95*	4.58	0.56
5	5	-6	1.46*	4.43	0.39
5	5	-5	2.06*	0.30	0.43
5	5	-4	10.28	10.14	0.57
5	5	-3	1.79*	0.29	0.41
5	5	-2	2.00*	1.17	0.42
5	5	-1	6.83	7.29	0.69
5	5	0	3.68	3.60	0.54
5	5	1	5.67	5.13	0.66
5	5	2	3.00	3.07	0.49
5	5	3	1.82*	0.49	0.41
5	5	4	3.20*	3.50	0.51
5	5	5	1.46*	0.63	0.39
5	5	6	1.97*	1.36	0.42
5	5	7	3.20*	3.19	0.50
5	5	8	3.50	3.19	0.53
5	4	10	4.00*	4.19	0.56
5	4	9	3.20*	2.88	0.50
5	4	8	6.01	5.80	0.67
5	4	7	2.75*	3.84	0.47
5	4	6	1.84*	0.82	0.41
5	4	5	7.37	7.06	0.69
5	4	4	1.92*	2.28	0.42
5	4	3	2.44*	1.70	0.45
5	4	2	1.73*	0.39	0.41
5	4	1	1.03*	0.76	0.36
5	4	0	3.23*	0.68	0.51
5	4	-1	2.04*	0.53	0.43
5	4	-2	1.03*	0.62	0.36
5	4	-3	3.59*	4.06	0.53
5	4	-4	8.93	8.36	0.65
5	4	-5	4.14	4.07	0.57
5	4	-6	1.74*	0.07	0.41
5	4	-7	3.00*	3.67	0.49
5	4	-8	6.33	6.09	0.68
5	4	-9	1.79*	1.58	0.41
5	4-10		5.13	6.26	0.63
5	4-11		3.76*	4.34	0.54
5	3-12		3.73*	3.44	0.54
5	3-11		2.46*	1.49	0.45
5	3-10		1.98*	1.96	0.42
5	3	-9	2.81*	2.03	0.48
5	3	-8	1.90*	2.24	0.42
5	3	-7	5.22	5.52	0.64
5	3	-6	3.08*	1.64	0.50
5	3	-5	5.52	6.18	0.65
5	3	-4	6.73	6.73	0.69
5	3	-3	7.31	6.81	0.69
5	3	-2	14.32	13.77	0.32
5	3	-1	1.68*	1.55	0.40
5	3	0	0.93*	1.70	0.36
5	3	1	1.64*	1.40	0.40
5	3	2	3.31	2.52	0.51
5	3	3	1.69*	0.81	0.40
5	3	4	4.99	6.43	0.62
5	3	5	7.22	7.29	0.69
5	3	6	1.72*	1.64	0.41
5	3	7	6.79	6.13	0.69
5	3	8	6.63	7.02	0.69
5	3	9	4.47	3.78	0.59
5	3	10	3.28*	2.97	0.51
5	3	11	7.25	7.32	0.69
5	2	12	5.38	5.38	0.64
5	2	11	3.83*	2.83	0.55
5	2	10	1.83*	1.28	0.41
5	2	9	3.53*	1.77	0.53
5	2	8	4.68	4.70	0.61
5	2	7	2.78*	2.25	0.48
5	2	6	1.68*	0.67	0.40
5	2	5	0.98*	2.86	0.36
5	2	4	3.05	2.53	0.49
5	2	3	16.98	15.85	0.22
5	2	2	0.88*	1.25	0.36
5	2	1	13.87	13.02	0.34
5	2	0	7.35	8.03	0.69
5	2	-1	19.33	18.07	0.16
5	2	-2	5.14	4.67	0.63
5	2	-3	3.40	3.29	0.52
5	2	-4	9.92	9.32	0.59
5	2	-5	1.58*	0.94	0.40
5	2	-6	2.05*	3.17	0.43
5	2	-7	1.62*	0.27	0.40
5	2	-8	4.26	4.08	0.58
5	2	-9	1.87*	2.97	0.42
5	2-10		3.31*	1.63	0.51
5	2-11		3.56*	3.53	0.53
5	2-12		3.27*	0.87	0.51
5	2-13		2.23*	0.26	0.44
5	1-13		3.46*	3.59	0.52
5	1-12		1.88*	0.58	0.42
5	1-11		2.17*	1.22	0.43
5	1-10		1.99*	2.27	0.42
5	1	-9	2.95	2.80	0.49
5	1	-8	9.61	9.82	0.61
5	1	-7	1.54*	0.33	0.39
5	1	-6	3.00*	2.92	0.48
5	1	-5	1.09*	0.52	0.37
5	1	-4	16.94	15.64	0.22
5	1	-3	10.56	11.10	0.55
5	1	-2	12.55	12.09	0.42
5	1	-1	35.21	36.27	0.04
5	1	0	12.57	12.08	0.42
5	1	1	1.41*	1.14	0.39
5	1	2	19.18	19.56	0.17
5	1	3	1.82*	0.03	0.41
5	1	4	1.47*	1.32	0.39
5	1	5	14.54	15.17	0.31
5	1	6	5.63	5.96	0.66
5	1	7	4.62	4.71	0.60
5	1	8	1.73*	1.71	0.41
5	1	9	2.07*	1.28	0.43
5	1	10	1.84*	3.20	0.41
5	1	11	1.01*	2.12	0.36
5	1	12	0.90*	0.24	0.36
5	0	11	1.21*	2.58	0.37
5	0	9	3.82	4.46	0.55
5	0	7	2.56*	0.95	0.46
5	0	5	10.11	10.57	0.58
5	0	3	9.45	10.59	0.62
5	0	1	21.14	22.77	0.13
5	0	-1	14.29	13.67	0.32
5	0	-3	14.22	14.72	0.33
5	0	-5	22.81	20.21	0.11
5	0	-7	14.16	13.58	0.33
5	0	-9	3.74	3.21	0.54
5	0-11		1.73*	2.01	0.41
5	0-13		1.98*	1.19	0.42
6	0-12		1.19*	2.75	0.37
6	0-10		4.34	4.71	0.58
6	0	-8	8.86	8.94	0.65
6	0	-6	4.80	5.35	0.61
6	0	-4	11.87	12.53	0.46
6	0	-2	11.33	11.82	0.50
6	0	0	27.82	28.77	0.07
6	0	2	12.94	13.56	0.39
6	0	4	12.35	12.62	0.43
6	0	6	2.12*	1.59	0.43
6	0	8	10.54	11.03	0.55
6	0	10	3.07*	1.64	0.50
6	1	11	2.00*	1.93	0.42
6	1	10	3.09*	0.16	0.50
6	1	9	3.19*	1.25	0.50
6	1	8	1.77*	1.51	0.41
6	1	7	7.67	7.89	0.69
6	1	6	1.67*	2.51	0.40
6	1	5	7.31	7.01	0.69
6	1	4	5.85	6.66	0.67
6	1	3	7.77	8.19	0.69
6	1	2	1.43*	0.79	0.39
6	1	1	9.70	9.82	0.60
6	1	0	3.82	2.41	0.55
6	1	-1	7.14	7.82	0.69
6	1	-2	1.56*	1.76	0.40
6	1	-3	5.85	5.79	0.67
6	1	-4	2.06*	3.09	0.43
6	1	-5	3.89	3.77	0.55
6	1	-6	1.55*	2.07	0.40
6	1	-7	1.44*	1.79	0.39
6	1	-8	2.36*	1.12	0.45
6	1	-9	5.41	5.87	0.65
6	1-10		1.83*	1.45	0.41
6	1-11		5.25	5.13	0.64
6	1-12		1.85*	0.85	0.41
6	1-13		0.92*	0.66	0.36
6	2-12		1.96*	1.44	0.42
6	2-11		2.86*	3.26	0.48
6	2-10		1.66*	2.56	0.40
6	2	-9	5.64	5.95	0.66
6	2	-8	1.09*	0.54	0.37
6	2	-7	8.33	8.54	0.67
6	2	-6	2.03*	1.79	0.43
6	2	-5	4.20	3.70	0.57
6	2	-4	1.92*	2.07	0.42
6	2	-3	6.49	6.39	0.68
6	2	-2	2.18*	1.70	0.44
6	2	-1	1.58*	0.67	0.40

h	k	l	Fo	Fc	weight
6	2	0	3.20*	3.84	0.51
6	2	1	1.53*	0.78	0.39
6	2	2	8.82	8.73	0.65
6	2	3	7.02	7.08	0.69
6	2	4	5.88	4.62	0.67
6	2	5	1.75*	1.61	0.41
6	2	6	1.65*	0.00	0.40
6	2	7	1.76*	0.58	0.41
6	2	8	2.43*	2.48	0.45
6	2	9	1.85*	1.57	0.41
6	2	10	1.24*	3.10	0.38
6	2	11	4.37	4.03	0.59
6	3	10	2.04*	4.20	0.43
6	3	9	2.62*	0.82	0.47
6	3	8	1.97*	3.32	0.42
6	3	7	6.47	5.57	0.68
6	3	6	1.85*	3.36	0.41
6	3	5	4.72	4.59	0.61
6	3	4	2.48*	2.49	0.46
6	3	3	2.92*	1.26	0.49
6	3	2	6.64	6.10	0.69
6	3	1	3.16*	3.60	0.50
6	3	0	1.57*	0.68	0.40
6	3	-1	2.71*	0.75	0.47
6	3	-2	2.22*	1.09	0.44
6	3	-3	5.54	5.40	0.65
6	3	-4	12.03	12.05	0.45
6	3	-5	10.12	10.16	0.58
6	3	-6	1.70*	0.37	0.40
6	3	-7	6.73	6.69	0.69
6	3	-8	15.34	15.40	0.28
6	3	-9	0.83*	4.32	0.35
6	3	-10	4.59	4.56	0.60
6	3	-11	4.00*	4.86	0.56
6	4	-10	5.21	5.30	0.64
6	4	-9	2.14*	0.00	0.43
6	4	-8	4.66	4.60	0.60
6	4	-7	4.67	5.39	0.60
6	4	-6	5.10	4.62	0.63
6	4	-5	6.38	7.19	0.68
6	4	-4	8.93	8.08	0.65
6	4	-3	2.77*	0.13	0.47
6	4	-2	10.73	10.61	0.54
6	4	-1	1.84*	1.72	0.41
6	4	0	1.72*	0.55	0.41
6	4	1	6.89	6.39	0.69
6	4	2	1.78*	0.25	0.41
6	4	3	1.92*	2.83	0.42
6	4	4	2.11*	0.11	0.43
6	4	5	2.95*	1.76	0.49
6	4	6	2.65*	2.57	0.47
6	4	7	2.72*	3.22	0.47
6	4	8	1.78*	2.93	0.41
6	4	9	2.75*	0.54	0.47
6	5	7	2.05*	0.39	0.43
6	5	6	1.95*	0.59	0.42
6	5	5	1.24*	0.11	0.38
6	5	4	1.47*	1.33	0.39
6	5	3	2.06*	1.30	0.43
6	5	2	1.95*	1.11	0.42
6	5	1	1.88*	2.27	0.42
6	5	0	3.29*	3.38	0.51
6	5	-1	6.29	6.85	0.68
6	5	-2	2.00*	2.68	0.42
6	5	-3	2.49*	3.22	0.46
6	5	-4	1.94*	0.15	0.42
6	5	-5	4.24	4.37	0.58
6	5	-6	2.13*	3.33	0.43
6	5	-7	3.43*	0.13	0.52
6	5	-8	2.09*	0.98	0.43
6	6	-5	6.49	6.15	0.68
6	6	-4	2.40*	1.67	0.45
6	6	-3	3.97	3.34	0.56
6	6	-2	2.36*	1.09	0.45
6	6	-1	0.89*	1.15	0.36
6	6	0	3.99*	3.41	0.56
6	6	1	3.58*	1.32	0.53
6	6	2	2.62*	3.55	0.47
6	6	3	1.98*	0.02	0.42
7	5	-7	4.22	4.06	0.58
7	5	-6	0.70*	0.33	0.35
7	5	-5	2.16*	2.36	0.43
7	5	-4	5.07	5.55	0.63
7	5	-3	1.22*	3.55	0.38
7	5	-2	8.85	9.01	0.65
7	5	-1	2.26*	1.21	0.44
7	5	0	2.02*	2.69	0.42
7	5	1	4.87	5.31	0.62
7	5	2	4.94	4.26	0.62
7	5	3	1.99*	0.95	0.42
7	5	4	3.68*	2.00	0.54
7	5	5	2.87*	0.85	0.48
7	4	7	1.94*	2.24	0.42
7	4	6	1.92*	0.89	0.42
7	4	5	1.75*	1.45	0.41
7	4	4	1.18*	1.71	0.37
7	4	3	3.58*	3.10	0.53
7	4	2	5.20	5.62	0.64
7	4	1	3.76*	3.08	0.54
7	4	0	1.98*	1.88	0.42
7	4	-1	8.44	8.43	0.67
7	4	-2	3.03	2.53	0.49
7	4	-3	2.41*	0.27	0.45
7	4	-4	1.87*	0.66	0.42
7	4	-5	2.02*	2.42	0.43
7	4	-6	2.38*	3.22	0.45
7	4	-7	1.72*	0.66	0.41
7	4	-8	2.16*	2.81	0.43
7	4	-9	2.03*	3.05	0.43
7	3	-10	4.28	3.80	0.58
7	3	-9	1.50*	1.91	0.39
7	3	-8	5.30	5.28	0.64
7	3	-7	1.15*	0.62	0.37
7	3	-6	4.78	4.50	0.61
7	3	-5	6.63	6.45	0.69
7	3	-4	1.80*	1.33	0.41
7	3	-3	1.68*	0.70	0.40
7	3	-2	0.75*	2.92	0.35
7	3	-1	1.79*	1.39	0.41
7	3	0	1.76*	0.84	0.41
7	3	1	4.66	5.42	0.60
7	3	2	2.01*	2.09	0.42
7	3	3	2.56*	2.78	0.46
7	3	4	2.95*	1.41	0.49
7	3	5	4.51	4.75	0.59
7	3	6	2.75*	1.45	0.47
7	3	7	2.70*	2.23	0.47
7	3	8	2.49*	0.25	0.46
7	3	9	0.91*	0.15	0.36
7	2	10	4.09	4.40	0.57
7	2	9	0.88*	0.17	0.36
7	2	8	2.25*	3.18	0.44
7	2	7	1.84*	0.03	0.41
7	2	6	1.81*	0.46	0.41
7	2	5	4.19	4.38	0.57
7	2	4	4.95	4.51	0.62
7	2	3	2.54*	0.16	0.46
7	2	2	1.82*	0.72	0.41
7	2	1	4.53	5.10	0.60
7	2	0	5.89	6.00	0.67
7	2	-1	5.18	5.61	0.63
7	2	-2	2.00*	0.09	0.42
7	2	-3	1.01*	1.01	0.36
7	2	-4	2.90*	3.97	0.48
7	2	-5	11.43	11.21	0.49
7	2	-6	3.31*	2.67	0.51
7	2	-7	3.58	4.04	0.53
7	2	-8	3.71	3.66	0.54
7	2	-9	0.83*	1.14	0.35
7	2	-10	0.86*	2.29	0.36
7	2	-11	1.97*	0.44	0.42
7	1	-12	1.88*	1.10	0.42
7	1	-11	3.32	3.04	0.51
7	1	-10	2.79*	2.11	0.48
7	1	-9	3.54*	3.04	0.53
7	1	-8	1.85*	2.20	0.41
7	1	-7	4.65	4.52	0.60
7	1	-6	3.45*	3.86	0.52
7	1	-5	4.33	3.86	0.58
7	1	-4	6.93	7.48	0.69
7	1	-3	2.82	2.21	0.48
7	1	-2	8.44	8.17	0.67
7	1	-1	3.28	3.25	0.51
7	1	0	0.68*	1.64	0.34
7	1	1	6.66	6.83	0.69
7	1	2	4.35	4.76	0.58
7	1	3	2.35*	1.24	0.45
7	1	4	3.25*	3.35	0.51
7	1	5	3.18*	2.42	0.50
7	1	6	1.83*	0.09	0.41
7	1	7	2.12*	0.00	0.43
7	1	8	1.17*	2.57	0.37
7	1	9	2.19*	1.31	0.44
7	1	10	1.94*	0.19	0.42
7	0	9	1.87*	0.29	0.42
7	0	7	5.92	7.44	0.67
7	0	5	2.87*	0.96	0.48
7	0	3	1.21*	0.68	0.38
7	0	1	3.58	4.52	0.53
7	0	-1	16.02	16.13	0.25
7	0	-3	1.79*	5.29	0.41
7	0	-5	2.55*	0.94	0.46
7	0	-7	1.72*	0.61	0.41
7	0	-9	2.90*	1.63	0.48
7	0	-11	3.25*	2.80	0.51
8	0	-10	1.51*	1.02	0.39
8	0	-8	4.98	5.45	0.62
8	0	-6	6.60	6.58	0.69
8	0	-4	2.34*	1.41	0.45
8	0	-2	3.73	2.64	0.54
8	0	0	1.66*	0.81	0.40
8	0	2	2.66*	1.69	0.47
8	0	4	1.70*	0.12	0.40
8	0	6	1.84*	0.53	0.41
8	0	8	1.80*	1.46	0.41
8	1	9	3.38*	2.76	0.52
8	1	8	2.14*	0.08	0.43
8	1	7	1.46*	1.48	0.39
8	1	6	2.84*	1.80	0.48
8	1	5	2.76*	1.32	0.47
8	1	4	1.33*	0.29	0.38
8	1	3	2.28*	0.30	0.44
8	1	2	2.89*	2.50	0.48
8	1	1	1.47*	1.16	0.39
8	1	0	3.35*	4.53	0.52
8	1	-1	1.03*	2.51	0.36
8	1	-2	12.54	13.48	0.42
8	1	-3	1.71*	0.47	0.41
8	1	-4	1.77*	1.59	0.41
8	1	-5	2.85*	0.83	0.49
8	1	-6	2.70*	3.06	0.47
8	1	-7	2.26*	0.19	0.44
8	1	-8	1.78*	0.59	0.41
8	1	-9	3.80*	3.81	0.55
8	1	-10	1.81*	1.81	0.42
8	1	-11	1.87*	2.10	0.42
8	2	-10	0.80*	0.78	0.36
8	2	-9	3.01*	3.49	0.49
8	2	-8	2.67*	1.59	0.47
8	2	-7	1.89*	1.04	0.42
8	2	-6	5.18	4.97	0.63
8	2	-5	11.65	11.14	0.48
8	2	-4	2.98*	2.49	0.49
8	2	-3	6.08	5.53	0.67
8	2	-2	5.66	5.01	0.66
8	2	-1	4.26	4.53	0.58
8	2	0	2.82*	1.76	0.48
8	2	1	0.76*	1.73	0.35
8	2	2	1.54*	1.07	0.39
8	2	3	1.82*	1.15	0.42
8	2	4	1.71*	1.89	0.41
8	2	5	2.45*	1.14	0.45
8	2	6	2.06*	0.19	0.43
8	2	7	1.50*	0.21	0.39
8	2	8	1.54*	0.97	0.40
8	2	9	2.14*	0.91	0.43
8	3	7	1.79*	2.33	0.41
8	3	6	1.91*	0.61	0.42
8	3	5	0.85*	1.35	0.35
8	3	4	3.74	4.13	0.54
8	3	3	1.80*	3.48	0.41
8	3	2	3.64	3.18	0.54
8	3	1	1.78*	0.09	0.41
8	3	0	1.78*	0.97	0.41
8	3	-1	1.12*	0.84	0.37
8	3	-2	1.97*	2.26	0.42
8	3	-3	1.04*	1.90	0.37
8	3	-4	1.80*	1.88	0.41
8	3	-5	3.28*	3.46	0.51
8	3	-6	6.82	6.82	0.69
8	3	-7	3.19*	1.40	0.50
8	3	-8	3.46	3.15	0.52
8	3	-9	2.97*	4.24	0.49
8	4	-8	2.00*	2.42	0.42
8	4	-7	3.80*	0.45	0.55
8	4	-6	3.04*	1.17	0.49
8	4	-5	0.86*	0.30	0.36
8	4	-4	1.88*	1.98	0.42
8	4	-3	1.98*	1.05	0.42
8	4	-2	3.79	4.42	0.55
8	4	-1	1.95*	0.36	0.42
8	4	0	1.87*	2.84	0.42
8	4	1	2.92*	1.44	0.49
8	4	2	1.92*	1.48	0.42
8	4	3	3.56*	1.46	0.53
8	4	4	1.95*	0.33	0.42
8	4	5	1.95*	0.37	0.42
8	4	6	2.89*	0.45	0.48
8	5	3	2.43*	1.11	0.45
8	5	2	3.14*	2.75	0.50
8	5	1	2.54*	4.02	0.46
8	5	0	1.55*	2.48	0.40
8	5	-1	2.19*	1.56	0.44
8	5	-2	1.98*	1.00	0.42
8	5	-3	2.70*	2.79	0.47
8	5	-4	1.91*	0.81	0.42
8	5	-5	1.08*	1.60	0.37
9	4	4	1.80*	2.68	0.41
9	4	3	1.28*	0.64	0.38
9	4	2	2.83*	0.93	0.48
9	4	1	2.35*	3.03	0.45
9	4	0	1.25*	1.30	0.38
9	4	-1	2.16*	1.28	0.43
9	4	-2	1.92*	1.31	0.42
9	4	-3	3.07*	0.35	0.50
9	4	-4	1.55*	0.09	0.40
9	4	-5	2.22*	1.42	0.44
9	4	-6	0.92*	1.26	0.36
9	3	-8	3.03*	2.84	0.49
9	3	-7	1.26*	0.44	0.38
9	3	-6	2.32*	1.85	0.44
9	3	-5	1.93*	0.71	0.42
9	3	-4	1.94*	3.40	0.42
9	3	-3	1.19*	0.34	0.37
9	3	-2	2.65*	2.15	0.47
9	3	-1	1.91*	0.15	0.42
9	3	0	1.79*	2.29	0.41
9	3	1	1.89*	1.40	0.42
9	3	2	1.68*	0.48	0.40
9	3	3	2.28*	1.90	0.44
9	3	4	2.91*	3.49	0.49
9	3	5	1.55*	0.02	0.40
9	3	6	1.92*	0.07	0.42
9	2	7	1.24*	0.29	0.38
9	2	6	2.67*	1.58	0.47
9	2	5	3.00*	1.21	0.49
9	2	4	1.89*	2.18	0.42
9	2	3	2.63*	0.95	0.47
9	2	2	1.76*	1.76	0.41
9	2	1	1.83*	0.62	0.41
9	2	0	2.67*	0.32	0.47
9	2	-1	1.74*	1.08	0.41
9	2	-2	3.29	3.24	0.51
9	2	-3	5.79	5.71	0.66
9	2	-4	2.45*	0.53	0.45
9	2	-5	2.20*	0.72	0.44
9	2	-6	2.80*	2.05	0.48
9	2	-7	2.73*	1.89	0.47
9	2	-8	1.84*	0.65	0.41
9	2	-9	2.06*	0.10	0.43
9	1	-10	3.30*	0.48	0.51
9	1	-8	0.89*	0.63	0.36
9	1	-8	1.91*	1.83	0.42
9	1	-7	1.98*	0.38	0.42
9	1	-6	1.93*	2.30	0.42
9	1	-5	3.45	3.54	0.52
9	1	-4	1.13*	2.15	0.37
9	1	-3	3.43	3.67	0.52
9	1	-2	8.31	8.46	0.67
9	1	-1	4.26	3.65	0.58
9	1	0	5.00	5.06	0.62
9	1	1	4.22	3.72	0.58
9	1	2	6.32	6.07	0.68
9	1	3	1.81*	1.06	0.41
9	1	4	3.31*	3.61	0.51
9	1	5	1.89*	1.09	0.42
9	1	6	3.36*	2.68	0.52
9	1	7	1.54*	0.56	0.40
9	1	8	1.25*	1.24	0.38
9	0	7	1.77*	0.66	0.41
9	0	5	4.72	3.58	0.61
9	0	3	3.41*	2.30	0.52
9	0	1	14.17	15.16	0.33
9	0	-1	4.25	4.23	0.58
9	0	-3	7.32	7.45	0.69
9	0	-5	0.80*	0.83	0.35
9	0	-7	4.55	3.95	0.60
9	0	-9	1.89*	1.06	0.42
10	0	-8	0.90*	0.63	0.36
10	0	-6	3.36*	2.71	0.52
10	0	-4	1.97*	0.08	0.42
10	0	-2	1.82*	0.83	0.41
10	0	0	1.44*	4.77	0.39
10	0	2	1.91*	1.66	0.42
10	0	4	6.76	6.64	0.69
10	0	6	1.82*	0.72	0.41
10	1	6	2.08*	1.24	0.43
10	1	5	2.83*	0.50	0.48
10	1	4	1.90*	2.21	0.42
10	1	3	3.66*	3.41	0.54
10	1	2	2.69*	0.57	0.47
10	1	1	1.87*	2.65	0.42
10	1	0	1.87*	3.55	0.42
10	1	-1	2.77*	3.47	0.48
10	1	-2	0.84*	0.74	0.35
10	1	-3	1.79*	1.01	0.41
10	1	-4	3.29*	2.73	0.51
10	1	-5	1.91*	2.37	0.42
10	1	-6	2.06*	1.35	0.43
10	1	-7	2.95*	1.70	0.49
10	1	-8	1.95*	1.02	0.42
10	2	-7	2.07*	2.23	0.43
10	2	-6	2.36*	1.47	0.45
10	2	-5	1.94*	0.04	0.42
10	2	-4	1.65*	0.34	0.40
10	2	-3	2.27*	3.96	0.44
10	2	-2	1.87*	0.19	0.42
10	2	-1	2.09*	1.86	0.43
10	2	0	1.96*	0.01	0.42
10	2	1	1.87*	0.14	0.42
10	2	2	2.89*	1.04	0.48
10	2	3	1.88*	0.64	0.42
10	2	4	2.54*	0.75	0.46
10	2	5	2.74*	1.10	0.47
10	3	3	1.94*	0.02	0.42
10	3	2	1.86*	0.05	0.42
10	3	1	1.86*	0.93	0.42
10	3	0	3.32*	0.48	0.51
10	3	-1	1.53*	0.71	0.39
10	3	-2	1.81*	0.28	0.41
10	3	-3	1.78*	0.19	0.41
10	3	-4	2.02*	1.17	0.43
10	3	-5	3.52*	0.33	0.53
11	2	1	2.10*	1.44	0.43
11	2	0	3.15*	0.17	0.50
11	2	-1	1.89*	1.44	0.42
11	2	-2	1.87*	0.93	0.42
11	2	-3	1.82*	1.84	0.41
11	2	-4	1.84*	0.82	0.41
11	1	-5	2.02*	1.24	0.43
11	1	-4	2.01*	0.04	0.42
11	1	-3	1.77*	0.71	0.41
11	1	-2	0.89*	0.16	0.36
11	1	-1	2.04*	0.75	0.43
11	1	0	2.68*	2.77	0.47
11	1	1	1.91*	0.79	0.42
11	1	2	1.94*	1.26	0.42
11	1	3	1.30*	1.43	0.38
11	0	3	5.15	5.75	0.63
11	0	1	2.00*	0.70	0.42
11	0	-1	3.30*	4.95	0.51
11	0	-3	2.17*	1.95	0.44
11	0	-5	2.21*	1.15	0.44

1341 reflections

1,3,4,5,6,9-hexamethyl-8-exo-methylenetricyclo[4.4.0.$0^{3,9}$]dec-4-ene-2-one

h	k	l	Fo	Fc	weight
0	0	1	31.49	33.12	0.92
0	0	2	130.81	131.12	0.05
0	0	3	23.99	24.57	1.52
0	0	4	100.41	97.98	0.09
0	0	5	75.70	73.26	0.16
0	0	6	40.40	40.26	0.54
0	0	7	36.03	34.96	0.67
0	0	8	11.61	11.40	3.60
0	0	9	5.21	5.44	2.77
0	0	10	9.68	9.81	3.25
0	0	11	10.92	10.53	2.81
0	0	12	6.64	6.03	2.37
0	0	13	3.42*	2.88	0.86
0	0	14	5.13	4.71	1.42
0	0	15	2.42*	4.17	0.20
0	0	16	2.33*	1.79	0.18
0	0	17	2.24*	0.80	0.22
2	0	-17	8.71	7.97	1.58
2	0	-16	3.40*	1.86	0.68
2	0	-15	3.82*	3.08	0.95
2	0	-14	6.32	6.11	1.91
2	0	-13	8.42	8.27	2.40
2	0	-12	9.24	9.10	2.54
2	0	-11	7.80	8.34	2.96
2	0	-10	9.91	10.02	3.22
2	0	-9	4.15	3.29	1.93
2	0	-8	2.91*	3.82	1.43
2	0	-7	5.50	4.66	3.88
2	0	-6	9.37	9.87	4.90
2	0	-5	21.06	21.14	1.84
2	0	-4	85.09	82.66	0.13
2	0	-3	12.76	12.70	4.28
2	0	-2	68.61	71.19	0.20
2	0	-1	101.91	103.18	0.09
2	0	0	44.31	45.55	0.47
2	0	1	76.80	80.49	0.16
2	0	2	16.30	16.48	2.96
2	0	3	50.87	53.26	0.35
2	0	4	6.76	6.46	5.77
2	0	5	48.78	46.69	0.38
2	0	6	2.47*	3.14	1.30
2	0	7	42.77	41.64	0.48
2	0	8	9.83	9.99	3.64
2	0	9	4.93	4.86	2.40
2	0	10	1.82*	1.09	0.30
2	0	11	1.10*	1.73	0.14
2	0	12	5.08	4.63	1.60
2	0	13	7.76	7.76	2.07
2	0	14	6.10	5.79	1.46
2	0	15	2.50*	2.76	0.51
2	0	16	3.30	3.29	0.47
4	0	-17	9.17	7.57	1.62
4	0	-16	7.40	7.84	1.57
4	0	-15	3.24*	3.15	0.62
4	0	-14	4.11*	5.15	0.80
4	0	-13	8.91	9.37	2.26
4	0	-12	16.35	16.68	2.03
4	0	-11	1.81*	1.63	0.37
4	0	-10	3.42	3.79	1.20
4	0	-9	15.18	15.26	2.54
4	0	-8	42.58	43.05	0.48
4	0	-7	24.37	24.07	1.35
4	0	-6	1.23*	0.46	0.30
4	0	-5	9.43	9.12	4.69
4	0	-4	27.64	28.58	1.12
4	0	-3	65.71	67.38	0.21
4	0	-2	5.88	5.90	4.64
4	0	-1	68.95	70.75	0.19
4	0	0	30.76	31.00	0.93
4	0	1	33.34	33.34	0.78
4	0	2	21.33	20.74	1.78
4	0	3	19.25	20.14	2.07
4	0	4	1.44*	0.17	0.48
4	0	5	4.06	4.40	2.51
4	0	6	19.60	19.98	1.86
4	0	7	5.16	5.97	2.62
4	0	8	3.19	3.80	1.85
4	0	9	12.17	11.92	2.67
4	0	10	11.01	11.09	2.59
4	0	11	3.08*	2.88	0.75
4	0	12	5.34	5.47	1.50
4	0	13	1.95*	0.23	0.26
4	0	14	6.40	6.89	1.32
4	0	15	4.33	4.23	0.73
6	0	-17	2.12*	2.19	0.22
6	0	-16	8.82	8.28	1.76
6	0	-15	1.99*	2.64	0.25
6	0	-14	5.81	6.10	1.51
6	0	-13	1.67*	2.92	0.21
6	0	-12	1.13*	0.43	0.10
6	0	-11	2.41*	2.84	0.41
6	0	-10	21.55	21.40	1.50
6	0	-9	2.51*	1.85	0.54
6	0	-8	12.68	12.78	2.90
6	0	-7	15.33	15.81	2.51
6	0	-6	4.63	5.37	2.38
6	0	-5	25.80	26.02	1.22
6	0	-4	18.41	19.06	2.14
6	0	-3	15.48	15.38	2.70
6	0	-2	2.20*	0.22	0.70
6	0	-1	16.84	15.77	2.45
6	0	0	14.90	15.94	2.89
6	0	1	14.86	14.36	2.86
6	0	2	3.96	4.69	2.30
6	0	3	26.15	25.72	1.17
6	0	4	22.95	23.05	1.45
6	0	5	0.67*	1.36	0.07
6	0	6	7.69	7.83	2.99
6	0	7	3.15	4.18	0.91
6	0	8	16.84	16.74	1.95
6	0	9	10.15	10.01	2.54
6	0	10	1.85*	0.57	0.29
6	0	11	6.53	6.27	1.69
6	0	12	3.58	3.77	0.63
6	0	13	2.22*	1.36	0.20
6	0	14	3.83	3.17	0.55
8	0	-17	3.79*	3.45	0.49
8	0	-16	3.51*	4.85	0.36
8	0	-15	11.15	10.89	1.91
8	0	-14	1.28*	1.28	0.11
8	0	-13	2.23*	2.55	0.20
8	0	-12	3.54*	0.85	0.90
8	0	-11	27.52	27.47	0.98
8	0	-10	8.91	9.17	2.28
8	0	-9	34.62	35.31	0.68
8	0	-8	4.30	4.69	1.10
8	0	-7	3.23	3.97	0.73
8	0	-6	22.48	22.57	1.46
8	0	-5	5.03	4.82	1.68
8	0	-4	16.89	16.69	2.21
8	0	-3	1.94*	0.34	0.27
8	0	-2	2.14*	4.12	0.33
8	0	-1	23.85	24.23	1.35
8	0	0	7.97	7.52	3.08
8	0	1	10.59	9.98	3.09
8	0	2	11.94	11.42	2.81
8	0	3	6.39	6.08	2.38
8	0	4	7.00	6.88	2.43
8	0	5	15.11	15.39	2.17
8	0	6	1.92*	4.23	0.23
8	0	7	18.42	18.70	1.71
8	0	8	11.52	11.92	2.24
8	0	9	1.96*	0.20	0.31
8	0	10	3.42*	1.96	0.78
8	0	11	9.48	9.48	1.73
8	0	12	7.42	6.95	1.27
10	0	-16	2.32*	0.29	0.19
10	0	-15	0.98*	2.17	0.04
10	0	-14	2.29*	1.27	0.19
10	0	-13	1.29*	2.59	0.07
10	0	-12	2.19*	0.85	0.21
10	0	-11	2.97*	0.68	0.49
10	0	-10	12.14	12.00	2.17
10	0	-9	5.06	5.11	1.08
10	0	-8	3.79*	4.92	0.70
10	0	-7	6.53	6.92	1.61
10	0	-6	15.93	16.09	1.97
10	0	-5	10.89	10.40	2.41
10	0	-4	20.18	20.58	1.57
10	0	-3	10.17	9.55	2.32
10	0	-2	6.77	6.72	1.82
10	0	-1	8.76	9.19	2.37
10	0	0	3.76*	4.37	0.66
10	0	1	21.27	22.41	1.48
10	0	2	13.24	13.40	2.26
10	0	3	19.56	19.84	1.60
10	0	4	17.36	17.61	1.79
10	0	5	3.86*	4.67	0.83
10	0	6	2.88*	0.23	0.52
10	0	7	6.41	5.98	1.42
10	0	8	8.82	7.94	1.82
10	0	9	3.71*	3.80	0.46
10	0	10	10.27	9.74	1.49
12	0	-14	3.31*	0.99	0.41
12	0	-13	2.40*	0.32	0.17
12	0	-12	6.96	7.04	1.20
12	0	-11	2.37*	4.70	0.18
12	0	-10	9.07	9.00	1.63
12	0	-9	8.34	8.25	1.55
12	0	-8	6.81	6.64	1.34
12	0	-7	5.35	6.00	0.91
12	0	-6	2.79*	2.18	0.36
12	0	-5	11.45	10.86	2.01
12	0	-4	10.57	10.19	1.99
12	0	-3	3.87	4.08	0.54
12	0	-2	6.37	6.31	1.44
12	0	-1	12.93	12.99	2.04
12	0	0	13.79	14.63	1.92
12	0	1	2.84	2.51	0.41
12	0	2	1.23*	0.65	0.08
12	0	3	4.36*	4.83	0.69
12	0	4	3.53*	5.30	0.47
12	0	5	2.18*	0.92	0.21
12	0	6	4.13	3.84	0.64
12	0	7	3.26*	1.72	0.45
12	0	8	4.29*	2.97	0.68
14	0	-12	6.45	6.14	0.86
14	0	-11	6.15	5.81	0.78
14	0	-10	5.49	5.28	0.70
14	0	-9	2.31*	3.57	0.13
14	0	-8	2.12*	1.23	0.14
14	0	-7	3.75*	3.27	0.49
14	0	-6	2.26*	0.01	0.20
14	0	-5	6.80	6.52	1.18
14	0	-4	2.35*	2.96	0.18
14	0	-3	3.81*	2.84	0.49
14	0	-2	8.31	7.38	1.33
14	0	-1	3.96*	0.62	0.91
14	0	0	5.50	5.28	0.84
14	0	1	2.33*	2.21	0.18
14	0	2	3.99*	4.40	0.45
14	0	3	3.55*	1.93	0.44
14	0	4	3.48*	4.43	0.36
16	0	-5	2.67*	1.76	0.14
16	0	-4	7.57	6.79	0.94
15	1	-9	2.50*	0.59	0.16
15	1	-8	4.22*	1.50	0.50
15	1	-7	2.58*	2.39	0.15
15	1	-6	3.81*	0.78	0.40
15	1	-5	2.25*	1.74	0.20
15	1	-4	1.95*	3.81	0.11
15	1	-3	6.74	6.52	0.96
15	1	-2	7.02	6.92	0.97
15	1	-1	5.41	5.15	0.69
15	1	0	2.95*	3.75	0.22
15	1	1	3.48*	2.82	0.34
14	1	4	4.03*	3.26	0.48
14	1	3	3.13*	1.46	0.33
14	1	2	2.75*	2.57	0.33
14	1	1	1.92*	1.94	0.15
14	1	0	3.54*	0.35	0.60
14	1	-1	2.35*	0.11	0.18

h	k	l	Fo	Fc	weight
14	1	-2	2.79*	0.37	0.31
14	1	-3	4.35*	2.77	0.55
14	1	-4	2.27*	2.19	0.20
14	1	-5	3.22*	2.13	0.36
14	1	-6	2.70*	2.43	0.25
14	1	-7	4.10*	2.34	0.52
14	1	-8	3.54	2.50	0.42
14	1	-9	2.38*	1.28	0.18
14	1	-10	2.39*	1.50	0.18
14	1	-11	3.99*	3.21	0.37
14	1	-12	4.66*	3.72	0.51
13	1	-13	5.86	5.48	0.84
13	1	-12	2.36*	0.48	0.18
13	1	-11	9.10	8.91	1.47
13	1	-10	2.35*	0.66	0.18
13	1	-9	8.40	8.47	1.49
13	1	-8	2.37*	1.06	0.18
13	1	-7	2.32*	1.85	0.19
13	1	-6	3.81	4.17	0.55
13	1	-5	1.53*	4.07	0.07
13	1	-4	4.31*	5.37	0.59
13	1	-3	2.21*	1.74	0.21
13	1	-2	3.53*	2.41	0.58
13	1	-1	2.35*	0.23	0.25
13	1	0	1.80*	0.52	0.17
13	1	1	4.27*	4.98	0.61
13	1	2	2.28*	0.64	0.19
13	1	3	7.00	6.44	1.35
13	1	4	2.29*	0.75	0.19
13	1	5	3.80*	2.90	0.48
13	1	6	2.06*	1.46	0.16
12	1	8	2.36*	1.67	0.18
12	1	7	2.26*	1.33	0.20
12	1	6	2.21*	0.06	0.21
12	1	5	2.27*	2.57	0.19
12	1	4	2.13*	1.84	0.22
12	1	3	4.38*	3.17	0.79
12	1	2	3.28*	3.58	0.50
12	1	1	5.15	5.55	1.04
12	1	0	7.02	7.25	1.50
12	1	-1	6.10	6.34	1.42
12	1	-2	8.87	9.43	1.93
12	1	-3	8.68	8.23	1.83
12	1	-4	3.01*	3.39	0.38
12	1	-5	2.81*	2.59	0.38
12	1	-6	12.21	12.63	2.00
12	1	-7	9.95	9.33	1.96
12	1	-8	4.26*	1.81	0.81
12	1	-9	3.43*	3.64	0.46
12	1	-10	6.29	6.62	1.11
12	1	-11	2.22*	1.29	0.20
12	1	-12	3.29*	0.48	0.42
12	1	-13	2.76*	1.19	0.34
12	1	-14	4.01*	2.48	0.47
11	1	-15	1.74*	0.11	0.09
11	1	-14	2.19*	0.85	0.21
11	1	-13	5.64	5.04	1.07
11	1	-12	2.22*	1.51	0.20
11	1	-11	6.52	6.19	1.34
11	1	-10	6.04	5.96	1.23
11	1	-9	0.85*	0.06	0.04
11	1	-8	6.79	7.04	1.47
11	1	-7	3.37*	0.27	0.61
11	1	-6	0.80*	1.88	0.03
11	1	-5	3.65*	3.07	0.56
11	1	-4	7.15	7.04	1.72
11	1	-3	2.03*	0.47	0.24
11	1	-2	5.69	5.90	1.46
11	1	-1	2.17*	1.61	0.21
11	1	0	13.63	13.33	2.19
11	1	1	10.06	10.62	2.24
11	1	2	4.08	3.72	0.88
11	1	3	7.43	7.81	1.82
11	1	4	3.36*	2.70	0.50
11	1	5	3.64	3.44	0.63
11	1	6	2.11*	0.44	0.22
11	1	7	7.05	6.52	1.48
11	1	8	2.14*	0.95	0.22
11	1	9	5.61	5.28	0.89
10	1	10	2.98*	0.89	0.53
10	1	9	3.96*	2.07	0.88
10	1	8	2.08*	1.06	0.28
10	1	7	2.21*	0.08	0.33
10	1	6	2.07*	1.13	0.23
10	1	5	2.06*	1.09	0.24
10	1	4	3.95*	3.10	0.84
10	1	3	3.35	3.18	0.74
10	1	2	7.67	8.23	2.16
10	1	1	4.66	4.50	1.24
10	1	0	12.24	12.50	2.38
10	1	-1	3.59*	3.78	0.67
10	1	-2	1.97*	1.64	0.26
10	1	-3	13.65	13.44	2.36
10	1	-4	9.80	10.04	2.34
10	1	-5	11.60	12.00	2.39
10	1	-6	7.33	7.61	1.99
10	1	-7	7.30	7.83	1.83
10	1	-8	5.31	5.21	1.21
10	1	-9	6.53	6.86	1.59
10	1	-10	2.12*	1.35	0.22
10	1	-11	8.74	8.86	1.85
10	1	-12	3.45*	2.53	0.59
10	1	-13	3.68*	1.78	0.71
10	1	-14	2.33*	2.31	0.18
10	1	-15	2.29*	1.98	0.19
10	1	-16	2.44*	1.33	0.17
9	1	-16	1.97*	2.21	0.14
9	1	-15	3.72*	2.49	0.65
9	1	-14	2.31*	1.35	0.19
9	1	-13	2.19*	2.26	0.21
9	1	-12	4.43	4.66	1.00
9	1	-11	3.92*	4.21	0.81
9	1	-10	11.71	11.87	2.31
9	1	-9	1.11*	2.22	0.08
9	1	-8	13.37	13.49	2.34
9	1	-7	6.67	6.05	1.98
9	1	-6	2.06*	2.80	0.24
9	1	-5	3.34*	4.36	0.73
9	1	-4	10.63	10.36	2.70
9	1	-3	3.28*	0.21	1.12
9	1	-2	7.83	8.02	2.55
9	1	-1	3.14*	1.87	0.81
9	1	0	1.92*	3.08	0.27
9	1	1	2.60*	0.70	0.57
9	1	2	10.94	11.39	2.59
9	1	3	3.85	4.27	0.96
9	1	4	11.90	12.33	2.38
9	1	5	8.34	9.45	2.51
9	1	6	0.83*	0.23	0.04
9	1	7	3.99	5.17	0.78
9	1	8	5.70	5.54	1.39
9	1	9	2.61*	1.79	0.41
9	1	10	3.43	3.80	0.49
9	1	11	3.96*	3.67	0.61
8	1	12	3.57*	3.97	0.55
8	1	11	4.27*	5.40	0.62
8	1	10	10.19	9.44	2.11
8	1	9	1.89*	0.17	0.28
8	1	8	7.67	7.83	2.11
8	1	7	3.66*	2.11	1.02
8	1	6	18.07	18.90	1.78
8	1	5	11.42	11.51	2.59
8	1	4	8.78	8.60	2.77
8	1	3	3.78	4.15	1.12
8	1	2	3.98	4.67	1.40
8	1	1	20.23	19.72	1.71
8	1	0	9.48	9.90	3.17
8	1	-1	2.27*	2.00	0.67
8	1	-2	13.13	13.42	2.88
8	1	-3	4.87	4.53	1.95
8	1	-4	16.53	16.75	2.31
8	1	-5	17.35	17.19	2.10
8	1	-6	8.65	8.74	2.78
8	1	-7	10.20	10.44	2.82
8	1	-8	1.93*	1.86	0.27
8	1	-9	5.13	5.37	1.49
8	1	-10	10.15	10.53	2.34
8	1	-11	8.00	8.07	2.12
8	1	-12	3.15*	3.22	0.52
8	1	-13	2.03*	1.64	0.24
8	1	-14	0.91*	1.99	0.05
8	1	-15	3.53*	2.13	0.73
8	1	-16	2.19*	3.64	0.15
8	1	-17	2.36*	1.81	0.18
7	1	-17	3.99	4.37	0.48
7	1	-16	3.21*	4.39	0.33
7	1	-15	7.69	7.99	1.49
7	1	-14	8.96	8.57	1.80
7	1	-13	2.15*	1.45	0.30
7	1	-12	2.72*	2.48	0.41
7	1	-11	9.69	9.91	2.50
7	1	-10	17.03	18.24	1.91
7	1	-9	12.25	12.81	2.68
7	1	-8	15.13	15.03	2.40
7	1	-7	8.83	9.13	3.08
7	1	-6	6.93	6.09	2.87
7	1	-5	2.30	3.05	0.65
7	1	-4	13.76	13.41	2.87
7	1	-3	17.20	15.70	2.29
7	1	-2	1.71*	2.10	0.41
7	1	-1	22.23	20.55	1.55
7	1	0	13.56	13.61	2.97
7	1	1	4.46	4.36	2.22
7	1	2	1.12*	0.44	0.21
7	1	3	10.84	10.84	3.23
7	1	4	12.03	12.18	2.83
7	1	5	10.90	11.47	2.86
7	1	6	2.12*	0.27	0.43
7	1	7	7.98	8.12	2.60
7	1	8	11.47	11.37	2.31
7	1	9	5.52	5.77	1.47
7	1	10	6.94	6.67	1.81
7	1	11	3.19*	2.41	0.63
7	1	12	1.92*	0.91	0.27
7	1	13	2.16*	0.93	0.21
6	1	14	2.31*	2.98	0.19
6	1	13	4.10*	2.71	0.61
6	1	12	1.61*	2.42	0.14
6	1	11	3.44*	3.06	0.77
6	1	10	1.90*	0.64	0.28
6	1	9	5.89	5.85	1.85
6	1	8	10.11	10.25	2.67
6	1	7	9.45	9.77	2.83
6	1	6	9.70	9.99	3.15
6	1	5	1.68*	0.87	0.35
6	1	4	15.50	15.00	2.51
6	1	3	4.18	4.41	2.27
6	1	2	14.82	15.17	2.79
6	1	1	23.32	23.19	1.46
6	1	0	27.57	27.32	1.10
6	1	-1	20.14	19.59	1.86
6	1	-2	12.20	12.02	3.50
6	1	-3	2.99*	3.28	1.28
6	1	-4	15.40	15.19	2.67
6	1	-5	7.92	8.29	3.85
6	1	-6	3.24	2.50	1.35
6	1	-7	1.29*	0.92	0.25
6	1	-8	4.82	5.41	2.08
6	1	-9	13.07	12.61	2.68
6	1	-10	4.33	4.50	1.28
6	1	-11	2.44*	3.45	0.58
6	1	-12	5.43	5.29	1.54
6	1	-13	2.53*	2.96	0.40
6	1	-14	2.78*	2.41	0.81
6	1	-15	2.05*	2.41	0.25
6	1	-16	1.13*	0.36	0.06
6	1	-17	2.31*	0.52	0.19
5	1	-17	6.41	6.93	1.06
5	1	-16	2.33*	1.29	0.28
5	1	-15	6.45	5.36	1.58
5	1	-14	1.98*	1.74	0.25
5	1	-13	3.22*	3.62	0.65

h	k	l	Fo	Fc	weight
5	1	-12	6.81	6.41	2.43
5	1	-11	2.00*	2.46	0.39
5	1	-10	15.77	16.01	2.26
5	1	-9	8.85	8.81	3.11
5	1	-8	18.84	18.59	1.94
5	1	-7	5.78	6.40	2.99
5	1	-6	9.79	9.87	4.00
5	1	-5	10.48	10.45	4.13
5	1	-4	58.75	58.54	0.25
5	1	-3	8.12	7.88	4.64
5	1	-2	52.07	50.82	0.33
5	1	-1	24.09	23.14	1.42
5	1	0	16.76	16.45	2.58
5	1	1	16.99	17.83	2.46
5	1	2	6.31	6.03	4.10
5	1	3	24.41	24.53	1.35
5	1	4	6.00	6.11	3.73
5	1	5	13.85	13.45	2.91
5	1	6	6.30	5.88	3.06
5	1	7	5.73	6.19	2.44
5	1	8	2.68*	4.51	0.56
5	1	9	1.75*	0.79	0.37
5	1	10	2.46*	1.89	0.58
5	1	11	5.00	4.67	1.43
5	1	12	8.56	7.63	2.06
5	1	13	3.87*	3.17	0.62
5	1	14	7.19	6.61	1.39
5	1	15	2.89*	0.59	0.50
4	1	15	1.72*	1.35	0.14
4	1	14	2.13*	0.20	0.22
4	1	13	6.35	6.59	1.48
4	1	12	1.81*	0.61	0.31
4	1	11	1.66*	1.26	0.23
4	1	10	1.77*	1.68	0.30
4	1	9	8.41	8.26	2.74
4	1	8	7.65	8.08	2.83
4	1	7	11.15	11.45	3.30
4	1	6	5.95	6.87	3.22
4	1	5	12.15	11.34	3.55
4	1	4	29.13	29.42	0.99
4	1	3	3.51	3.09	2.54
4	1	2	1.42*	1.27	0.49
4	1	1	31.48	31.35	0.88
4	1	0	38.66	37.72	0.60
4	1	-1	17.28	17.70	2.57
4	1	-2	2.59	1.77	1.62
4	1	-3	30.72	32.03	0.92
4	1	-4	1.93	1.53	0.88
4	1	-5	5.36	5.01	4.15
4	1	-6	3.88	3.94	2.37
4	1	-7	20.30	19.24	1.83
4	1	-8	10.09	9.99	3.73
4	1	-9	2.84*	1.74	0.96
4	1	-10	2.43	2.15	0.66
4	1	-11	19.70	19.95	1.66
4	1	-12	3.42*	3.71	0.85
4	1	-13	8.10	7.86	2.17
4	1	-14	7.47	6.90	2.08
4	1	-15	1.83*	0.64	0.30
4	1	-16	2.09*	0.42	0.23
4	1	-17	1.40*	3.77	0.06
3	1	-17	2.08*	0.95	0.23
3	1	-16	2.51*	2.71	0.31
3	1	-15	3.00*	1.27	0.54
3	1	-14	6.80	7.29	1.78
3	1	-13	3.08*	0.56	0.80
3	1	-12	13.23	13.71	2.35
3	1	-11	3.23*	0.19	1.27
3	1	-10	2.53*	1.72	0.77
3	1	-9	12.04	12.98	3.12
3	1	-8	6.42	6.75	3.65
3	1	-7	47.19	45.01	0.40
3	1	-6	18.16	18.98	2.25
3	1	-5	41.29	41.79	0.52
3	1	-4	3.28	3.53	2.57
3	1	-3	16.82	16.14	2.72
3	1	-2	108.04	105.33	0.08
3	1	-1	30.43	29.77	0.96
3	1	0	47.20	47.89	0.41
3	1	1	29.02	29.10	1.04
3	1	2	51.19	50.05	0.35
3	1	3	36.47	35.82	0.66
3	1	4	12.96	12.79	3.69
3	1	5	13.70	13.08	3.30
3	1	6	19.63	19.52	1.92
3	1	7	6.65	6.95	3.42
3	1	8	2.74*	3.41	0.77
3	1	9	1.80*	3.77	0.31
3	1	10	1.72*	1.50	0.34
3	1	11	5.67	5.69	1.78
3	1	12	10.74	10.79	2.40
3	1	13	3.73	4.17	0.81
3	1	14	2.01*	2.31	0.25
3	1	15	3.65*	3.84	0.57
3	1	16	5.97	5.85	0.91
2	1	16	2.26*	2.59	0.20
2	1	15	2.09*	1.06	0.23
2	1	14	1.95*	0.67	0.26
2	1	13	1.23*	1.03	0.15
2	1	12	0.83*	2.98	0.06
2	1	11	1.92*	0.32	0.44
2	1	10	5.43	5.94	2.04
2	1	9	11.35	11.51	3.07
2	1	8	14.41	14.61	2.74
2	1	7	2.15*	3.08	0.88
2	1	6	18.53	17.44	2.14
2	1	5	14.30	14.26	3.21
2	1	4	20.98	20.76	1.84
2	1	3	15.20	14.77	3.18
2	1	2	46.08	47.47	0.43
2	1	1	46.37	47.14	0.42
2	1	0	63.77	65.73	0.23
2	1	-1	28.58	29.96	1.09
2	1	-2	38.98	39.70	0.60
2	1	-3	44.69	45.56	0.45
2	1	-4	1.34*	2.10	0.62
2	1	-5	2.13*	2.18	1.29
2	1	-6	19.44	18.75	2.05
2	1	-7	21.19	20.77	1.72
2	1	-8	2.73	1.74	1.34
2	1	-9	1.57*	1.30	0.40
2	1	-10	25.46	26.16	1.18
2	1	-11	4.80	5.53	1.63
2	1	-12	10.68	10.91	2.65
2	1	-13	3.08*	2.06	0.80
2	1	-14	2.04*	1.54	0.24
2	1	-15	2.10*	0.49	0.23
2	1	-16	6.58	6.26	1.47
2	1	-17	3.45*	2.54	0.48
1	1	-17	1.00*	1.74	0.04
1	1	-16	3.83*	2.66	0.66
1	1	-15	3.66*	3.68	0.68
1	1	-14	6.56	5.93	1.85
1	1	-13	2.20*	3.12	0.36
1	1	-12	2.61*	0.88	0.71
1	1	-11	1.87*	1.10	0.29
1	1	-10	1.75*	0.39	0.33
1	1	-9	1.49*	1.47	0.37
1	1	-8	1.75*	1.14	0.69
1	1	-7	7.00	7.23	4.43
1	1	-6	21.38	20.57	1.74
1	1	-5	1.32*	1.02	0.58
1	1	-4	39.67	40.91	0.57
1	1	-3	37.56	39.24	0.64
1	1	-2	1.78*	0.34	1.59
1	1	-1	85.06	85.60	0.13
1	1	0	55.24	56.07	0.30
1	1	1	66.32	67.99	0.21
1	1	2	25.21	26.67	1.38
1	1	3	26.35	27.41	1.25
1	1	4	11.07	11.09	4.80
1	1	5	44.84	44.49	0.45
1	1	6	11.27	11.00	4.10
1	1	7	20.05	19.11	1.86
1	1	8	1.53*	0.64	0.43
1	1	9	1.93*	1.02	0.57
1	1	10	1.59*	1.57	0.40
1	1	11	2.30*	1.81	0.48
1	1	12	5.85	6.64	1.98
1	1	13	2.83*	3.26	0.64
1	1	14	3.90*	4.24	0.92
1	1	15	1.63*	0.77	0.20
1	1	16	2.78*	0.48	0.45
0	1	17	6.85	6.11	1.25
0	1	16	3.36*	2.41	0.86
0	1	15	1.97*	2.12	0.26
0	1	14	2.33*	3.96	0.27
0	1	13	2.37*	0.89	0.50
0	1	12	7.89	7.84	2.56
0	1	11	2.00*	1.32	0.46
0	1	10	2.85*	1.05	1.35
0	1	9	1.57*	1.44	0.40
0	1	8	1.40*	0.23	0.51
0	1	7	1.44*	1.31	0.48
0	1	6	58.47	56.29	0.26
0	1	5	5.47	5.27	5.39
0	1	4	32.86	33.10	0.82
0	1	3	20.70	20.57	1.96
0	1	2	4.20	4.44	6.13
0	1	1	104.09	102.22	0.09
0	2	0	3.36	3.08	3.78
0	2	1	6.59	6.47	7.19
0	2	2	36.64	37.32	0.67
0	2	3	31.11	31.83	0.91
0	2	4	7.65	7.71	5.90
0	2	5	15.97	15.38	2.80
0	2	6	3.92	4.32	3.12
0	2	7	20.62	20.13	1.78
0	2	8	8.79	8.64	3.92
0	2	9	1.61*	0.16	0.39
0	2	10	16.09	16.75	2.22
0	2	11	2.65	4.02	0.62
0	2	12	2.56*	2.37	0.81
0	2	13	1.93*	1.71	0.27
0	2	14	2.53*	3.91	0.35
0	2	15	3.97*	4.26	0.76
0	2	16	4.91	4.64	0.87
0	2	17	2.29*	2.25	0.19
1	2	16	2.16*	0.53	0.21
1	2	15	2.32*	0.92	0.35
1	2	14	3.01*	1.66	0.70
1	2	13	1.80*	0.19	0.31
1	2	12	2.97*	1.75	0.80
1	2	11	1.89*	2.56	0.28
1	2	10	9.81	9.72	2.98
1	2	9	1.65*	4.08	0.37
1	2	8	9.75	10.96	3.54
1	2	7	2.23*	1.63	1.19
1	2	6	9.98	10.59	4.24
1	2	5	11.05	10.26	4.35
1	2	4	26.53	26.23	1.21
1	2	3	11.77	12.31	4.49
1	2	2	4.41	4.66	4.83
1	2	1	10.80	10.75	5.23
1	2	0	21.36	21.18	1.86
1	2	-1	13.75	13.89	3.87
1	2	-2	13.47	13.79	3.94
1	2	-3	2.33	1.83	1.95
1	2	-4	2.29*	3.04	1.48
1	2	-5	17.61	17.29	2.41
1	2	-6	23.95	23.61	1.41
1	2	-7	3.86	2.88	2.56
1	2	-8	5.59	5.57	3.45
1	2	-9	5.43	5.25	2.56
1	2	-10	16.69	16.71	2.13
1	2	-11	4.36	4.58	1.47
1	2	-12	3.09	2.68	0.71
1	2	-13	3.97	3.41	1.01
1	2	-14	3.06*	3.38	0.74
1	2	-15	0.93*	0.89	0.04
1	2	-16	1.68*	2.53	0.14
1	2	-17	3.14*	3.12	0.35

h	k	l	Fo	Fc	weight
2	2	-17	6.17	5.61	1.10
2	2	-16	1.36*	1.76	0.11
2	2	-15	4.12*	4.47	0.65
2	2	-14	4.82	4.97	1.16
2	2	-13	1.95*	2.07	0.26
2	2	-12	13.37	13.65	2.39
2	2	-11	15.09	15.30	2.24
2	2	-10	5.30	5.75	1.94
2	2	-9	16.33	15.88	2.29
2	2	-8	0.90*	1.13	0.16
2	2	-7	2.74*	3.62	1.49
2	2	-6	9.21	8.78	4.42
2	2	-5	8.37	8.45	5.14
2	2	-4	10.65	11.18	4.84
2	2	-3	1.29*	1.54	0.60
2	2	-2	14.96	14.78	3.32
2	2	-1	16.39	16.76	2.89
2	2	0	8.62	9.44	6.03
2	2	1	19.97	20.53	2.07
2	2	2	1.32*	0.49	0.58
2	2	3	27.34	27.52	1.15
2	2	4	16.94	16.64	2.58
2	2	5	6.39	6.17	4.51
2	2	6	13.42	12.83	3.23
2	2	7	6.05	5.99	3.37
2	2	8	10.98	11.20	3.37
2	2	9	19.74	19.71	1.74
2	2	10	6.51	6.98	2.31
2	2	11	20.02	20.57	1.58
2	2	12	2.22*	2.66	0.47
2	2	13	3.63*	2.76	1.14
2	2	14	1.96*	1.08	0.26
2	2	15	4.99	4.40	0.99
2	2	16	2.02*	0.37	0.28
3	2	15	5.05	4.18	0.98
3	2	14	8.04	7.71	1.74
3	2	13	3.93*	2.71	0.91
3	2	12	1.98*	0.93	0.26
3	2	11	2.89	2.75	0.63
3	2	10	13.33	13.59	2.43
3	2	9	11.39	11.38	2.75
3	2	8	1.67*	1.47	0.36
3	2	7	1.68*	0.63	0.35
3	2	6	1.43*	1.24	0.49
3	2	5	20.13	20.00	1.85
3	2	4	24.71	24.97	1.34
3	2	3	3.39	3.44	2.61
3	2	2	1.85*	2.13	0.94
3	2	1	14.79	14.41	3.28
3	2	0	27.89	28.63	1.10
3	2	-1	17.85	18.52	2.44
3	2	-2	24.43	25.25	1.42
3	2	-3	14.46	14.33	3.33
3	2	-4	14.65	14.35	3.22
3	2	-5	12.64	11.32	3.76
3	2	-6	40.73	39.24	0.53
3	2	-7	21.82	21.83	1.60
3	2	-8	19.97	19.68	1.81
3	2	-9	1.74*	0.89	0.33
3	2	-10	7.17	7.86	2.67
3	2	-11	15.38	15.24	2.16
3	2	-12	2.52*	3.71	0.54
3	2	-13	8.48	8.30	2.25
3	2	-14	3.04*	3.33	0.59
3	2	-15	2.05*	0.71	0.34
3	2	-16	0.96*	1.45	0.05
3	2	-17	2.20*	1.80	0.21
4	2	-17	2.29*	1.11	0.19
4	2	-16	2.72*	2.89	0.28
4	2	-15	3.31*	1.86	0.73
4	2	-14	3.73*	4.53	0.75
4	2	-13	3.14*	3.05	0.87
4	2	-12	13.07	12.90	2.36
4	2	-11	12.09	12.56	2.55
4	2	-10	18.45	18.64	1.89
4	2	-9	1.95*	1.45	0.42
4	2	-8	3.89	3.50	1.86
4	2	-7	9.39	8.85	3.91
4	2	-6	0.83*	0.76	0.18
4	2	-5	30.68	30.08	0.91
4	2	-4	3.34	3.03	2.09
4	2	-3	9.59	9.59	4.75
4	2	-2	7.99	7.51	5.30
4	2	-1	4.47	4.31	3.82
4	2	0	2.56	2.64	1.72
4	2	1	26.64	26.69	1.19
4	2	2	9.67	9.66	4.66
4	2	3	13.98	13.98	3.27
4	2	4	5.28	4.46	3.93
4	2	5	4.69	4.84	2.62
4	2	6	11.31	11.70	3.40
4	2	7	17.22	17.21	2.12
4	2	8	1.93*	2.30	0.40
4	2	9	13.23	13.96	2.45
4	2	10	8.15	7.45	2.50
4	2	11	3.05*	5.70	0.47
4	2	12	0.88*	1.48	0.08
4	2	13	3.58*	4.16	0.60
4	2	14	2.90*	2.64	0.45
5	2	15	3.02*	4.68	0.27
5	2	14	2.30*	0.90	0.19
5	2	13	3.56*	3.88	0.73
5	2	12	7.22	6.37	1.83
5	2	11	1.23*	0.52	0.13
5	2	10	2.21*	1.64	0.36
5	2	9	2.98*	0.64	1.11
5	2	8	11.42	11.29	2.66
5	2	7	13.47	13.44	2.62
5	2	6	6.02	5.75	2.64
5	2	5	8.98	9.18	3.69
5	2	4	1.55*	1.73	0.42
5	2	3	18.40	18.48	2.11
5	2	2	27.22	26.57	1.12
5	2	1	17.51	18.11	2.32
5	2	0	35.09	34.90	0.71
5	2	-1	13.42	12.81	3.38
5	2	-2	28.72	28.42	1.03
5	2	-3	39.50	38.06	0.57
5	2	-4	33.28	33.25	0.78
5	2	-5	11.15	10.69	3.85
5	2	-6	3.05*	2.58	1.35
5	2	-7	25.44	24.30	1.22
5	2	-8	0.95*	0.97	0.14
5	2	-9	10.95	11.09	3.04
5	2	-10	6.41	6.33	2.30
5	2	-11	9.05	9.19	2.56
5	2	-12	1.91*	1.03	0.27
5	2	-13	3.57	4.10	0.79
5	2	-14	2.17*	2.11	0.31
5	2	-15	2.07*	2.34	0.23
5	2	-16	1.36*	0.27	0.08
6	2	-17	1.74*	2.16	0.10
6	2	-16	3.03*	0.28	0.44
6	2	-15	3.76*	4.97	0.42
6	2	-14	2.11*	1.40	0.23
6	2	-13	8.27	8.10	1.82
6	2	-12	2.04*	1.54	0.24
6	2	-11	2.60*	1.89	0.64
6	2	-10	8.54	9.29	2.29
6	2	-9	1.85*	0.89	0.29
6	2	-8	9.28	8.66	3.21
6	2	-7	15.58	15.76	2.44
6	2	-6	10.51	10.69	3.44
6	2	-5	23.01	22.84	1.47
6	2	-4	1.47*	0.52	0.43
6	2	-3	17.33	17.16	2.32
6	2	-2	8.35	8.52	4.01
6	2	-1	11.50	11.86	3.68
6	2	0	34.31	32.73	0.73
6	2	1	4.32	4.88	2.47
6	2	2	16.24	15.62	2.44
6	2	3	17.51	17.73	2.17
6	2	4	9.49	9.10	3.59
6	2	5	9.47	9.62	3.23
6	2	6	10.48	10.48	2.90
6	2	7	7.60	7.67	2.61
6	2	8	12.27	12.54	2.48
6	2	9	2.99*	2.92	0.58
6	2	10	3.00*	2.86	0.68
6	2	11	5.49	5.29	1.30
6	2	12	3.52*	0.26	0.86
6	2	13	4.60*	4.62	0.71
6	2	14	2.32*	1.98	0.19
7	2	13	2.26*	1.06	0.24
7	2	12	2.11*	0.25	0.23
7	2	11	3.95	3.86	0.76
7	2	10	5.41	4.94	1.34
7	2	9	2.73*	2.42	0.42
7	2	8	1.97*	1.08	0.26
7	2	7	9.82	9.84	2.50
7	2	6	8.73	8.77	2.67
7	2	5	3.04*	0.02	1.12
7	2	4	8.63	8.56	3.12
7	2	3	4.37	5.03	1.75
7	2	2	27.00	27.18	1.09
7	2	1	1.68*	0.86	0.35
7	2	0	3.91	3.41	1.75
7	2	-1	3.92	4.78	1.75
7	2	-2	24.12	23.83	1.35
7	2	-3	11.17	10.86	3.42
7	2	-4	8.36	7.98	3.53
7	2	-5	5.22	5.06	2.26
7	2	-6	10.29	10.47	3.13
7	2	-7	1.77*	2.04	0.32
7	2	-8	3.43	3.86	0.95
7	2	-9	1.97*	2.50	0.34
7	2	-10	2.19*	1.16	0.43
7	2	-11	1.92*	0.90	0.27
7	2	-12	1.77*	1.63	0.32
7	2	-13	2.04*	1.89	0.24
7	2	-14	4.35*	4.47	0.75
7	2	-15	2.04*	0.09	0.24
7	2	-16	2.78*	4.79	0.26
7	2	-17	2.28*	1.32	0.19
8	2	-16	2.25*	1.01	0.20
8	2	-15	2.18*	1.20	0.21
8	2	-14	3.33*	3.54	0.49
8	2	-13	3.56*	1.45	0.69
8	2	-12	1.94*	1.67	0.27
8	2	-11	1.43*	1.74	0.18
8	2	-10	11.48	11.98	2.48
8	2	-9	11.53	11.49	2.48
8	2	-8	8.58	8.81	2.61
8	2	-7	20.10	20.63	1.67
8	2	-6	1.93*	0.05	0.27
8	2	-5	1.85*	0.95	0.29
8	2	-4	16.98	16.91	2.15
8	2	-3	5.80	6.88	2.22
8	2	-2	11.93	12.70	3.00
8	2	-1	9.21	9.46	3.08
8	2	0	6.20	6.13	2.49
8	2	1	17.38	17.36	2.02
8	2	2	6.35	6.51	2.33
8	2	3	1.85*	1.77	0.29
8	2	4	7.31	7.72	2.42
8	2	5	9.37	9.06	2.60
8	2	6	7.71	7.83	2.20
8	2	7	10.12	10.06	2.34
8	2	8	5.88	5.87	1.63
8	2	9	2.02*	1.28	0.24
8	2	10	5.13	5.40	1.08
8	2	11	4.12*	4.33	0.59
8	2	12	3.34*	1.28	0.57
9	2	11	4.50*	2.15	0.65
9	2	10	2.13*	2.53	0.22
9	2	9	3.98*	2.53	0.98
9	2	8	2.03*	0.24	0.23
9	2	7	1.93*	0.89	0.27
9	2	6	3.49*	2.46	1.01
9	2	5	4.66	4.48	1.20
9	2	4	4.87	5.18	1.46

h	k	l	Fo	Fc	weight
9	2	3	1.88*	0.21	0.28
9	2	2	8.77	8.69	2.66
9	2	1	3.20	3.39	0.75
9	2	0	5.77	5.87	1.97
9	2	-1	12.38	12.18	2.66
9	2	-2	13.26	13.21	2.55
9	2	-3	13.29	13.16	2.51
9	2	-4	2.80*	2.28	0.49
9	2	-5	9.23	9.27	2.50
9	2	-6	2.47*	1.89	0.32
9	2	-7	11.22	10.66	2.43
9	2	-8	1.35*	2.08	0.13
9	2	-9	1.98*	0.67	0.25
9	2	-10	4.93	5.28	1.19
9	2	-11	2.12*	2.75	0.22
9	2	-12	2.92*	2.14	0.65
9	2	-13	3.16*	2.40	0.81
9	2	-14	2.98*	3.21	0.43
9	2	-15	3.52*	4.93	0.38
9	2	-16	2.29*	1.27	0.19
10	2	-15	2.64*	0.50	0.30
10	2	-14	3.74*	2.61	0.46
10	2	-13	2.23*	1.70	0.20
10	2	-12	5.18	5.69	0.99
10	2	-11	2.06*	0.70	0.24
10	2	-10	5.59	6.25	1.13
10	2	-9	2.11*	1.39	0.22
10	2	-8	3.81*	4.89	0.63
10	2	-7	1.87*	0.18	0.29
10	2	-6	9.92	10.63	2.33
10	2	-5	3.36*	3.19	0.67
10	2	-4	7.32	7.28	2.07
10	2	-3	9.69	10.43	2.42
10	2	-2	2.16*	0.13	0.31
10	2	-1	2.54*	4.22	0.47
10	2	0	15.32	15.03	2.09
10	2	1	2.00*	1.88	0.25
10	2	2	11.29	11.22	2.38
10	2	3	1.83*	1.84	0.37
10	2	4	2.10*	0.22	0.23
10	2	5	1.22*	2.11	0.09
10	2	6	4.07	3.61	0.84
10	2	7	2.43*	0.51	0.43
10	2	8	4.93	4.88	0.89
10	2	9	3.91*	5.48	0.48
10	2	10	2.25*	1.27	0.20
11	2	9	1.76*	0.17	0.12
11	2	8	3.28*	3.18	0.43
11	2	7	2.78*	3.03	0.35
11	2	6	4.54	4.47	0.94
11	2	5	3.15*	2.87	0.62
11	2	4	7.32	6.90	1.63
11	2	3	5.39	5.32	1.22
11	2	2	3.50*	3.02	0.64
11	2	1	9.68	9.46	2.24
11	2	0	2.04*	1.39	0.24
11	2	-1	13.42	13.21	2.19
11	2	-2	8.08	7.68	2.12
11	2	-3	2.68*	3.60	0.39
11	2	-4	2.80*	0.73	0.52
11	2	-5	7.13	7.32	1.74
11	2	-6	13.53	12.74	2.10
11	2	-7	2.17*	3.81	0.21
11	2	-8	1.47*	4.45	0.09
11	2	-9	6.05	5.83	1.26
11	2	-10	5.40	5.06	1.12
11	2	-11	2.12*	0.19	0.22
11	2	-12	2.26*	1.49	0.19
11	2	-13	4.09*	1.84	0.87
11	2	-14	2.44*	3.87	0.17
11	2	-15	2.32*	1.78	0.19
12	2	-14	3.68*	3.42	0.42
12	2	-13	1.72*	2.91	0.09
12	2	-12	5.32	5.45	0.83
12	2	-11	3.53*	2.55	0.52
12	2	-10	7.14	7.05	1.35
12	2	-9	3.21	3.93	0.39
12	2	-8	1.78*	2.27	0.13
12	2	-7	8.92	9.18	1.86
12	2	-6	3.12*	4.59	0.38
12	2	-5	5.03	5.88	1.00
12	2	-4	2.12*	0.75	0.22
12	2	-3	2.10*	0.81	0.23
12	2	-2	2.26*	0.94	0.20
12	2	-1	5.67	5.54	1.22
12	2	0	2.30*	2.24	0.33
12	2	1	2.09*	2.00	0.23
12	2	2	2.12*	0.49	0.22
12	2	3	4.03	3.26	0.73
12	2	4	2.22*	0.56	0.20
12	2	5	3.16*	1.75	0.59
12	2	6	2.19*	1.23	0.21
12	2	7	3.01*	2.25	0.31
13	2	6	2.35*	1.00	0.18
13	2	5	2.39*	0.44	0.17
13	2	4	2.23*	2.77	0.17
13	2	3	3.18*	1.11	0.48
13	2	2	2.27*	2.47	0.19
13	2	1	3.94*	2.34	0.74
13	2	0	2.08*	0.21	0.23
13	2	-1	2.29*	2.81	0.19
13	2	-2	2.38*	1.18	0.22
13	2	-3	8.33	8.05	1.63
13	2	-4	5.28	5.39	0.99
13	2	-5	3.03	3.13	0.41
13	2	-6	3.74*	2.00	0.59
13	2	-7	2.34*	0.40	0.18
13	2	-8	2.42*	4.51	0.17
13	2	-9	3.77*	2.86	0.65
13	2	-10	5.90	5.75	0.96
13	2	-11	1.96*	1.20	0.16
13	2	-12	4.00*	4.11	0.48
13	2	-13	2.24*	2.52	0.14
14	2	-11	2.47*	1.12	0.16
14	2	-10	2.23*	2.17	0.16
14	2	-9	3.54*	2.87	0.38
14	2	-8	4.55*	4.57	0.76
14	2	-7	3.18*	2.42	0.34
14	2	-6	2.45*	2.59	0.17
14	2	-5	2.25*	0.98	0.20
14	2	-4	3.13*	2.78	0.35
14	2	-3	4.23*	4.20	0.57
14	2	-2	6.32	5.70	1.23
14	2	-1	5.47	5.44	0.83
14	2	0	6.74	6.69	1.17
14	2	1	1.38*	2.46	0.06
14	2	2	2.43*	3.11	0.17
14	2	3	3.49*	1.36	0.42
14	2	4	2.47*	0.13	0.16
14	2	5	4.34*	1.45	0.64
15	2	0	2.26*	1.28	0.18
15	2	-1	1.00*	2.10	0.03
15	2	-2	3.86*	2.49	0.46
15	2	-3	1.40*	0.95	0.06
15	2	-4	4.21	3.93	0.50
15	2	-5	2.25*	1.16	0.20
15	2	-6	3.30*	2.18	0.35
15	2	-7	4.49*	3.94	0.46
15	2	-8	1.01*	3.88	0.03
15	2	-9	5.22*	5.37	0.50
15	3	-8	8.21	7.51	1.12
15	3	-7	5.29*	5.05	0.56
15	3	-6	1.43*	1.96	0.06
15	3	-5	2.50*	2.47	0.16
15	3	-4	4.72*	4.28	0.59
15	3	-3	2.36*	0.46	0.18
15	3	-2	5.11	4.88	0.67
15	3	-1	2.40*	2.25	0.17
15	3	0	2.06*	4.09	0.11
14	3	3	2.25*	0.15	0.20
14	3	2	2.23*	0.64	0.20
14	3	1	1.98*	2.59	0.14
14	3	0	1.39*	1.77	0.07
14	3	-1	4.23*	4.10	0.61
14	3	-2	3.20*	2.17	0.31
14	3	-3	2.72*	1.13	0.31
14	3	-4	2.15*	0.48	0.23
14	3	-5	3.47*	1.40	0.47
14	3	-6	3.75*	3.58	0.51
14	3	-7	2.39*	2.09	0.22
14	3	-8	5.17	4.44	0.75
14	3	-9	3.60*	0.04	0.42
14	3	-10	3.20*	1.25	0.36
13	3	-12	3.58	3.16	0.38
13	3	-11	1.41*	2.08	0.06
13	3	-10	2.35*	0.10	0.18
13	3	-9	4.60*	3.53	0.68
13	3	-8	2.33*	0.94	0.18
13	3	-7	6.57	5.60	1.47
13	3	-6	3.70*	0.61	0.72
13	3	-5	1.30*	2.38	0.11
13	3	-4	2.28*	2.80	0.19
13	3	-3	6.87	6.48	1.34
13	3	-2	2.05*	0.17	0.24
13	3	-1	8.06	8.16	1.58
13	3	0	2.58*	2.74	0.29
13	3	1	2.17*	0.11	0.21
13	3	2	3.84*	0.24	0.75
13	3	3	4.02*	3.73	0.61
13	3	4	2.44*	2.13	0.23
13	3	5	2.03*	1.71	0.16
12	3	7	2.32*	0.23	0.19
12	3	6	4.33*	3.37	0.68
12	3	5	1.94*	0.19	0.19
12	3	4	2.23*	3.20	0.20
12	3	3	2.13*	0.13	0.22
12	3	2	2.42*	1.94	0.29
12	3	1	3.60*	1.05	0.65
12	3	0	3.07*	4.57	0.36
12	3	-1	3.62*	3.75	0.54
12	3	-2	2.12*	3.53	0.22
12	3	-3	6.67	6.20	1.55
12	3	-4	4.18*	4.97	0.57
12	3	-5	2.20*	3.11	0.21
12	3	-6	2.93*	3.38	0.46
12	3	-7	2.96*	4.07	0.30
12	3	-8	2.56*	4.43	0.31
12	3	-9	2.44*	4.01	0.25
12	3	-10	1.88*	2.76	0.17
12	3	-11	2.26*	0.85	0.20
12	3	-12	2.49*	1.11	0.27
11	3	-14	2.02*	0.24	0.14
11	3	-13	1.70*	0.68	0.11
11	3	-12	2.34*	1.94	0.27
11	3	-11	2.63*	4.18	0.26
11	3	-10	2.72*	1.33	0.36
11	3	-9	5.61	5.81	1.12
11	3	-8	2.11*	0.76	0.22
11	3	-7	5.14	5.93	1.03
11	3	-6	3.68*	3.22	0.81
11	3	-5	9.17	9.21	2.09
11	3	-4	6.55	7.76	1.58
11	3	-3	6.77	6.34	1.80
11	3	-2	4.23*	3.37	0.90
11	3	-1	11.67	11.94	2.17
11	3	0	11.25	11.03	2.21
11	3	1	3.41*	4.29	0.54
11	3	2	2.13*	0.87	0.32
11	3	3	3.31*	3.22	0.57
11	3	4	7.62	7.74	1.70
11	3	5	3.83	4.50	0.62
11	3	6	2.07*	1.59	0.23
11	3	7	3.24*	2.65	0.53
11	3	8	2.25*	1.55	0.20
10	3	10	2.52*	1.49	0.24
10	3	9	2.81*	0.77	0.38
10	3	8	2.21*	0.66	0.21
10	3	7	2.01*	0.91	0.25
10	3	6	1.99*	1.21	0.25
10	3	5	4.86	4.77	1.20
10	3	4	2.04*	2.31	0.24

h	k	l	Fo	Fc	weight
10	3	3	6.97	6.77	1.95
10	3	2	3.67	3.93	0.76
10	3	1	1.81*	2.64	0.19
10	3	0	3.99*	4.83	0.91
10	3	-1	3.35*	4.62	0.53
10	3	-2	1.96*	0.43	0.26
10	3	-3	1.93*	1.38	0.27
10	3	-4	2.23*	2.41	0.38
10	3	-5	2.86*	1.41	0.87
10	3	-6	2.04*	1.24	0.24
10	3	-7	1.96*	2.17	0.26
10	3	-8	6.39	6.30	1.61
10	3	-9	2.02*	0.28	0.24
10	3	-10	0.88*	1.53	0.04
10	3	-11	2.13*	0.92	0.22
10	3	-12	2.10*	2.01	0.23
10	3	-13	2.27*	2.54	0.19
10	3	-14	4.17*	2.70	0.70
10	3	-15	4.81	4.04	0.64
9	3	-15	3.02*	3.31	0.31
9	3	-14	2.18*	3.28	0.18
9	3	-13	2.22*	1.70	0.20
9	3	-12	2.99*	1.06	0.42
9	3	-11	7.11	7.34	1.74
9	3	-10	1.47*	2.96	0.12
9	3	-9	7.83	7.98	2.06
9	3	-8	8.89	9.15	2.33
9	3	-7	0.78*	2.19	0.04
9	3	-6	7.22	7.43	2.26
9	3	-5	7.57	7.90	2.21
9	3	-4	2.03*	2.31	0.32
9	3	-3	9.89	9.53	2.73
9	3	-2	3.41*	5.38	0.59
9	3	-1	2.11*	0.50	0.42
9	3	0	16.22	17.16	2.04
9	3	1	15.14	15.22	2.18
9	3	2	12.14	12.03	2.42
9	3	3	14.49	14.68	2.15
9	3	4	2.01*	1.76	0.29
9	3	5	2.92*	2.26	0.44
9	3	6	3.90	4.40	0.84
9	3	7	1.96*	1.99	0.26
9	3	8	2.93	2.43	0.51
9	3	9	2.16*	1.46	0.21
9	3	10	2.20*	0.24	0.21
9	3	11	1.02*	1.24	0.04
8	3	12	2.05*	1.98	0.13
8	3	11	3.70*	4.10	0.42
8	3	10	2.70*	1.56	0.43
8	3	9	7.22	6.96	1.63
8	3	8	2.35*	3.01	0.27
8	3	7	3.21	3.38	0.62
8	3	6	2.05*	0.46	0.24
8	3	5	7.15	6.96	2.04
8	3	4	10.45	10.66	2.60
8	3	3	1.94*	0.69	0.26
8	3	2	5.71	5.97	2.01
8	3	1	6.93	6.50	2.69
8	3	0	14.02	13.93	2.53
8	3	-1	3.32	2.40	1.06
8	3	-2	11.07	11.61	3.01
8	3	-3	6.19	6.00	2.45
8	3	-4	3.54	2.75	1.08
8	3	-5	2.96	3.40	0.68
8	3	-6	11.76	11.36	2.70
8	3	-7	1.92*	0.32	0.27
8	3	-8	4.29	4.66	1.18
8	3	-9	1.95*	1.41	0.26
8	3	-10	2.59*	2.55	0.41
8	3	-11	6.46	6.12	1.67
8	3	-12	1.90*	1.23	0.28
8	3	-13	2.23*	0.05	0.31
8	3	-14	2.31*	1.07	0.27
8	3	-15	4.08	3.95	0.65
8	3	-16	2.26*	0.20	0.20
7	3	-16	2.45*	0.46	0.26
7	3	-15	3.02	2.60	0.40
7	3	-14	4.82	4.92	0.83
7	3	-13	2.14*	0.25	0.22
7	3	-12	1.92*	2.94	0.23
7	3	-11	1.97*	2.50	0.26
7	3	-10	3.19*	2.84	0.83
7	3	-9	13.60	13.44	2.38
7	3	-8	7.15	7.03	2.40
7	3	-7	14.80	15.00	2.40
7	3	-6	16.12	16.37	2.22
7	3	-5	1.77*	1.36	0.32
7	3	-4	2.54	2.74	0.75
7	3	-3	2.46	2.30	0.78
7	3	-2	3.88	3.48	1.75
7	3	-1	2.40	2.38	0.74
7	3	0	1.73*	1.24	0.33
7	3	1	21.32	20.31	1.60
7	3	2	2.31*	2.77	0.58
7	3	3	15.72	15.64	2.29
7	3	4	10.49	10.80	2.90
7	3	5	13.11	12.78	2.51
7	3	6	2.74*	1.83	0.69
7	3	7	21.82	22.07	1.37
7	3	8	4.75	4.77	1.24
7	3	9	5.74	6.40	1.61
7	3	10	1.84*	2.82	0.16
7	3	11	4.88	3.83	1.06
7	3	12	6.28	6.01	1.19
6	3	13	1.73*	1.60	0.15
6	3	12	2.88*	1.08	0.63
6	3	11	2.04*	0.55	0.24
6	3	10	5.40	5.24	1.32
6	3	9	3.41*	4.11	0.80
6	3	8	3.22	3.19	0.69
6	3	7	2.30*	2.51	0.45
6	3	6	11.50	11.83	2.78
6	3	5	9.77	9.90	3.06
6	3	4	2.62*	2.86	0.74
6	3	3	15.46	15.57	2.49
6	3	2	1.84*	0.64	0.85
6	3	1	6.83	7.22	3.56
6	3	0	3.36	3.43	1.70
6	3	-1	16.42	16.83	2.40
6	3	-2	13.58	13.34	3.06
6	3	-3	17.48	16.67	2.22
6	3	-4	5.70	5.05	3.04
6	3	-5	3.75	3.63	1.68
6	3	-6	0.95*	0.54	0.13
6	3	-7	16.17	16.18	2.27
6	3	-8	7.20	7.25	2.73
6	3	-9	3.58	3.15	1.01
6	3	-10	2.58*	4.08	0.45
6	3	-11	5.48	5.70	1.67
6	3	-12	2.07*	0.73	0.36
6	3	-13	6.70	6.81	1.62
6	3	-14	5.16	4.82	1.21
6	3	-15	3.53	3.47	0.56
6	3	-16	2.27*	2.21	0.19
5	3	-17	2.29*	2.31	0.21
5	3	-16	2.79*	2.48	0.50
5	3	-15	3.66*	3.17	0.62
5	3	-14	2.56*	1.28	0.64
5	3	-13	3.58*	3.48	0.64
5	3	-12	11.57	12.08	2.35
5	3	-11	6.52	6.80	1.89
5	3	-10	8.09	8.81	2.50
5	3	-9	13.65	13.39	2.55
5	3	-8	13.97	14.26	2.62
5	3	-7	1.75*	0.15	0.33
5	3	-6	16.77	16.59	2.31
5	3	-5	10.83	10.74	3.68
5	3	-4	13.31	14.02	3.21
5	3	-3	13.49	13.35	3.18
5	3	-2	13.57	13.66	3.22
5	3	-1	12.97	12.93	3.36
5	3	0	15.93	16.01	2.63
5	3	1	9.61	9.97	4.06
5	3	2	16.76	16.38	2.41
5	3	3	1.36*	1.25	0.31
5	3	4	10.27	10.55	3.45
5	3	5	1.69*	2.45	0.32
5	3	6	0.72*	2.22	0.07
5	3	7	2.91*	1.77	0.74
5	3	8	9.75	9.60	2.71
5	3	9	2.17*	1.59	0.39
5	3	10	6.77	6.68	1.92
5	3	11	3.47*	0.68	0.94
5	3	12	1.93*	1.10	0.27
5	3	13	2.10*	1.21	0.23
5	3	14	2.15*	1.85	0.22
4	3	15	1.03*	1.79	0.04
4	3	14	4.36	4.09	0.74
4	3	13	3.42*	1.78	0.75
4	3	12	2.03*	3.53	0.24
4	3	11	2.23*	1.80	0.38
4	3	10	3.71*	6.03	0.78
4	3	9	3.27*	1.92	1.03
4	3	8	2.35*	1.40	0.54
4	3	7	16.99	17.18	2.08
4	3	6	2.39*	0.16	1.15
4	3	5	6.65	6.61	3.46
4	3	4	1.55*	1.62	0.41
4	3	3	5.04	5.28	3.57
4	3	2	18.73	17.46	2.10
4	3	1	11.88	11.43	3.77
4	3	0	5.78	5.39	4.32
4	3	-1	8.45	8.77	4.80
4	3	-2	1.52*	2.65	0.43
4	3	-3	11.01	11.36	4.05
4	3	-4	31.87	29.85	0.84
4	3	-5	2.68*	3.16	1.77
4	3	-6	1.98*	1.92	0.81
4	3	-7	3.65	3.44	1.74
4	3	-8	4.67	5.01	2.11
4	3	-9	8.49	9.09	3.00
4	3	-10	6.59	6.39	2.34
4	3	-11	12.60	12.97	2.45
4	3	-12	4.56	4.27	1.24
4	3	-13	0.86*	2.74	0.05
4	3	-14	1.93*	0.92	0.27
4	3	-15	2.83*	2.25	0.42
4	3	-16	6.15	5.91	1.05
3	3	-17	2.29*	0.85	0.33
3	3	-17	3.69*	3.03	0.52
3	3	-16	2.95*	0.84	0.55
3	3	-15	1.94*	0.26	0.27
3	3	-14	2.19*	1.01	0.21
3	3	-13	8.78	8.71	2.21
3	3	-12	1.92*	2.19	0.27
3	3	-11	16.50	17.14	1.98
3	3	-10	9.81	9.88	2.81
3	3	-9	1.68*	0.21	0.35
3	3	-8	8.52	8.87	3.34
3	3	-7	27.71	27.50	1.06
3	3	-6	19.96	18.98	1.86
3	3	-5	1.30*	1.76	0.40
3	3	-4	27.84	28.59	1.08
3	3	-3	52.32	52.43	0.33
3	3	-2	23.45	21.93	1.49
3	3	-1	3.33	2.32	2.59
3	3	0	18.98	18.49	2.15
3	3	1	36.85	36.35	0.65
3	3	2	3.82	3.02	2.84
3	3	3	8.65	8.48	4.46
3	3	4	14.10	13.92	3.05
3	3	5	6.12	6.15	3.67
3	3	6	5.83	6.41	3.14
3	3	7	7.36	7.81	3.17
3	3	8	21.04	21.00	1.56
3	3	9	10.82	11.23	2.70
3	3	10	20.78	20.70	1.50
3	3	11	13.27	13.14	2.23
3	3	12	1.53*	1.41	0.23
3	3	13	2.17*	1.78	0.30
3	3	14	2.11*	2.22	0.23
3	3	15	7.04	6.32	1.41

h	k	l	Fo	Fc	weight
2	3	16	2.53*	2.43	0.26
2	3	15	2.21*	1.29	0.25
2	3	14	3.67*	3.69	0.69
2	3	13	1.92*	0.58	0.27
2	3	12	1.50*	1.38	0.16
2	3	11	11.16	11.16	2.53
2	3	10	13.77	13.68	2.38
2	3	9	12.33	12.26	2.70
2	3	8	3.01*	4.16	0.87
2	3	7	7.42	7.29	3.31
2	3	6	8.21	8.35	4.03
2	3	5	19.48	18.68	1.93
2	3	4	6.17	6.31	4.35
2	3	3	23.94	24.42	1.43
2	3	2	10.12	9.62	4.71
2	3	1	18.44	18.16	2.28
2	3	0	2.34*	3.75	1.84
2	3	-1	10.97	10.82	4.66
2	3	-2	28.87	29.33	1.03
2	3	-3	23.05	22.51	1.54
2	3	-4	9.33	9.09	4.68
2	3	-5	26.93	25.58	1.15
2	3	-6	23.67	22.39	1.42
2	3	-7	7.27	7.01	3.88
2	3	-8	7.92	7.66	3.55
2	3	-9	10.93	11.06	3.04
2	3	-10	8.15	8.37	2.70
2	3	-11	11.22	10.80	2.65
2	3	-12	2.18*	3.24	0.35
2	3	-13	2.59*	2.67	0.41
2	3	-14	3.83*	4.42	0.83
2	3	-15	2.11*	1.99	0.20
2	3	-16	2.79*	2.34	0.50
2	3	-17	1.78*	1.35	0.11
1	3	16	6.68	6.41	1.35
1	3	15	3.43*	0.56	0.69
1	3	14	2.57*	0.46	0.46
1	3	13	5.81	5.40	1.68
1	3	12	1.81*	1.00	0.31
1	3	11	3.15*	2.40	1.00
1	3	10	1.79*	0.07	0.31
1	3	-9	11.69	12.07	3.05
1	3	-8	7.99	7.66	3.53
1	3	-7	1.68*	2.49	0.49
1	3	-6	8.40	8.76	4.43
1	3	-5	33.90	32.06	0.75
1	3	-4	11.98	12.23	4.01
1	3	-3	12.22	11.41	4.00
1	3	-2	4.81	5.08	4.89
1	3	-1	22.36	23.00	1.66
1	3	0	35.04	35.48	0.72
1	3	1	14.80	14.92	3.26
1	3	2	0.86*	0.38	0.28
1	3	3	44.46	43.89	0.45
1	3	4	49.97	48.51	0.36
1	3	5	2.48*	3.39	1.34
1	3	6	24.83	24.04	1.29
1	3	7	11.84	11.94	3.40

h	k	l	Fo	Fc	weight
1	3	8	12.95	13.03	2.85
1	3	9	9.26	9.53	3.01
1	3	10	19.73	20.27	1.65
1	3	11	3.62*	3.06	0.89
1	3	12	10.23	10.35	2.38
1	3	13	1.26*	0.33	0.14
1	3	14	1.86*	1.98	0.25
1	3	15	0.97*	1.50	0.05
1	3	16	1.90*	1.29	0.16
0	3	16	0.55*	1.47	0.01
0	3	15	2.72*	0.58	0.58
0	3	14	1.98*	2.38	0.25
0	3	13	4.47	4.30	1.08
0	3	12	2.05*	0.33	0.33
0	3	11	7.35	7.34	2.46
0	3	10	6.52	6.66	2.43
0	3	9	10.30	9.91	3.18
0	3	8	5.31	5.67	2.71
0	3	7	10.72	10.36	3.68
0	3	6	5.21	5.41	3.74
0	3	5	7.25	7.49	4.68
0	3	4	23.10	21.91	1.53
0	3	3	5.83	6.00	5.40
0	3	2	32.60	33.97	0.82
0	3	1	19.53	20.01	2.11
0	4	0	13.14	11.97	3.53
0	4	1	44.19	43.50	0.46
0	4	2	38.97	36.59	0.58
0	4	3	13.83	14.07	3.21
0	4	4	45.80	44.74	0.42
0	4	5	19.98	19.56	1.85
0	4	6	7.55	7.74	3.77
0	4	7	2.20	2.00	0.75
0	4	8	23.96	25.12	1.30
0	4	9	10.75	10.89	2.84
0	4	10	2.95*	2.59	0.94
0	4	11	6.19	6.02	2.10
0	4	12	1.94*	2.01	0.26
0	4	13	1.78*	1.34	0.24
0	4	14	3.07	2.15	0.56
0	4	15	3.41*	1.83	0.77
0	4	16	2.14*	1.26	0.22
1	4	15	2.11*	0.48	0.22
1	4	14	1.65*	1.98	0.12
1	4	13	2.05*	0.31	0.24
1	4	12	1.96*	3.51	0.24
1	4	11	2.11*	2.20	0.40
1	4	10	1.81*	1.45	0.30
1	4	9	18.21	18.86	1.84
1	4	8	5.36	5.72	2.06
1	4	7	20.07	21.20	1.62
1	4	6	8.16	8.25	3.77
1	4	5	10.36	10.03	3.82
1	4	4	19.87	19.27	1.88
1	4	3	31.85	30.58	0.84
1	4	2	11.09	10.81	4.03
1	4	1	3.05	3.12	2.01
1	4	0	18.45	18.38	2.21

h	k	l	Fo	Fc	weight
1	4	-1	15.82	15.76	2.77
1	4	-2	1.42*	2.13	0.50
1	4	-3	5.59	5.82	4.30
1	4	-4	19.45	19.01	1.95
1	4	-5	4.25	4.60	2.56
1	4	-6	11.04	10.67	3.67
1	4	-7	7.18	7.26	3.38
1	4	-8	4.47	4.93	1.91
1	4	-9	1.05*	3.52	0.09
1	4	-10	2.83	2.47	0.67
1	4	-11	7.37	6.82	2.29
1	4	-12	5.10	5.10	1.44
1	4	-13	4.13	4.07	0.97
1	4	-14	2.05*	0.57	0.24
1	4	-15	2.31*	2.91	0.19
1	4	-16	2.20*	0.07	0.21
2	4	-16	2.58*	4.14	0.15
2	4	-15	1.94*	1.99	0.18
2	4	-14	2.00*	1.08	0.25
2	4	-13	5.33	5.71	1.32
2	4	-12	4.82	4.92	1.22
2	4	-11	7.66	7.62	2.35
2	4	-10	3.01*	3.38	0.79
2	4	-9	8.68	8.72	2.86
2	4	-8	7.64	8.06	2.95
2	4	-7	3.32*	2.75	1.05
2	4	-6	13.51	13.83	2.95
2	4	-5	2.50	2.57	1.15
2	4	-4	20.80	20.14	1.75
2	4	-3	1.40*	0.55	0.51
2	4	-2	25.71	23.62	1.25
2	4	-1	11.36	10.97	4.00
2	4	0	37.84	36.99	0.61
2	4	1	18.15	17.75	2.03
2	4	2	17.37	16.62	2.36
2	4	3	20.32	19.91	1.83
2	4	4	16.30	15.96	2.48
2	4	5	4.12	4.31	2.43
2	4	6	6.68	6.79	3.17
2	4	7	18.46	19.27	1.92
2	4	8	7.68	7.74	2.78
2	4	9	18.26	18.41	1.83
2	4	10	1.81*	0.05	0.31
2	4	11	9.72	10.01	2.36
2	4	12	4.40	4.81	1.05
2	4	13	2.64*	1.07	0.56
2	4	14	2.10*	0.19	0.23
2	4	15	4.30*	4.19	0.60
3	4	15	2.33*	0.86	0.18
3	4	14	6.13	5.43	1.21
3	4	13	2.12*	1.64	0.22
3	4	12	2.42*	3.07	0.34
3	4	11	6.20	6.22	1.70
3	4	10	5.49	5.65	1.69
3	4	9	6.24	6.47	2.28
3	4	8	8.86	9.32	2.67
3	4	7	4.86	4.50	1.92
3	4	6	2.80*	1.42	0.84

h	k	l	Fo	Fc	weight	7
3	4	5	6.81	6.31	3.44	
3	4	4	1.54*	0.98	0.42	
3	4	3	3.29	3.23	1.88	
3	4	2	1.48*	2.03	0.46	
3	4	1	6.51	6.59	4.28	
3	4	0	4.70	5.19	3.30	
3	4	-1	9.61	9.61	4.41	
3	4	-2	1.01*	1.94	0.19	
3	4	-3	1.03*	0.88	0.21	
3	4	-4	6.05	5.92	4.02	
3	4	-5	12.81	12.34	3.23	
3	4	-6	3.14*	0.75	1.47	
3	4	-7	2.65*	4.51	0.59	
3	4	-8	5.06	4.54	2.26	
3	4	-9	2.36*	0.85	0.60	
3	4	-10	9.06	8.77	2.71	
3	4	-11	1.91*	1.82	0.27	
3	4	-12	4.62	4.90	1.27	
3	4	-13	2.81*	2.25	0.69	
3	4	-14	1.31*	0.48	0.10	
3	4	-15	5.06	4.90	0.99	
3	4	-16	2.37*	2.77	0.18	
4	4	-16	2.24*	0.14	0.20	
4	4	-15	2.23*	3.00	0.20	
4	4	-14	7.20	6.61	1.77	
4	4	-13	2.36*	4.24	0.32	
4	4	-12	5.67	5.13	1.64	
4	4	-11	15.35	15.98	2.04	
4	4	-10	14.66	14.57	2.25	
4	4	-9	11.07	11.45	2.79	
4	4	-8	12.72	12.82	2.72	
4	4	-7	20.38	21.01	1.67	
4	4	-6	7.71	6.97	3.53	
4	4	-5	10.18	10.18	3.66	
4	4	-4	27.14	26.94	1.10	
4	4	-3	18.80	18.60	2.03	
4	4	-2	1.48*	1.62	0.46	
4	4	-1	15.42	14.69	2.70	
4	4	0	28.12	27.55	1.04	
4	4	1	1.47*	0.45	0.46	
4	4	2	9.40	8.52	4.01	
4	4	3	14.91	15.66	2.60	
4	4	4	2.52*	3.57	1.00	
4	4	5	6.91	7.27	3.17	
4	4	6	4.69	5.10	1.86	
4	4	7	1.99*	2.61	0.25	
4	4	8	10.70	10.87	2.70	
4	4	9	1.86*	1.66	0.29	
4	4	10	5.20	5.20	1.41	
4	4	11	4.51	4.27	1.04	
4	4	12	2.02*	1.39	0.25	
4	4	13	2.58*	1.08	0.46	
4	4	14	2.33*	2.32	0.18	
4	4	15	3.87*	4.11	0.59	
5	4	12	3.72*	3.57	0.68	
5	4	11	1.94*	0.56	0.27	
5	4	10	3.32*	4.66	0.48	
5	4	9	9.97	9.71	2.45	

h	k	l	Fo	Fc	weight
5	4	8	1.42*	2.04	0.13
5	4	7	7.88	8.22	2.56
5	4	6	9.41	9.67	2.89
5	4	5	3.34*	2.35	1.15
5	4	4	12.55	13.13	2.83
5	4	3	2.82	3.71	1.03
5	4	2	3.98	4.60	1.87
5	4	1	3.40	3.45	1.53
5	4	0	10.29	9.74	3.68
5	4	-1	11.08	11.45	3.66
5	4	-2	6.90	7.27	3.87
5	4	-3	4.77	4.74	3.01
5	4	-4	2.77*	4.10	0.81
5	4	-5	11.10	11.02	3.27
5	4	-6	1.61*	0.33	0.38
5	4	-7	0.71*	0.05	0.06
5	4	-8	5.97	6.27	2.16
5	4	-9	6.65	6.44	2.28
5	4	-10	2.88*	4.44	0.71
5	4	-11	1.97*	0.89	0.26
5	4	-12	2.01*	1.36	0.25
5	4	-13	2.38*	1.83	0.27
5	4	-14	0.93*	1.90	0.05
5	4	-15	2.29*	1.30	0.19
5	4	-16	2.22*	1.16	0.20
6	4	-16	2.49*	2.28	0.44
6	4	-15	2.18*	3.10	0.21
6	4	-14	4.17	4.18	0.75
6	4	-13	2.87*	3.57	0.39
6	4	-12	2.21*	4.10	0.20
6	4	-11	4.05	4.77	0.88
6	4	-10	5.81	6.51	1.68
6	4	-9	1.97*	1.22	0.26
6	4	-8	4.00	4.35	1.23
6	4	-7	1.78*	0.89	0.31
6	4	-6	3.66	3.48	1.27
6	4	-5	8.10	8.73	3.24
6	4	-4	2.36*	1.93	0.71
6	4	-3	2.02*	1.31	0.59
6	4	-2	0.67*	1.07	0.07
6	4	-1	6.59	6.38	3.11
6	4	0	10.35	10.24	3.42
6	4	1	12.98	12.74	2.92
6	4	2	8.25	7.89	3.37
6	4	3	2.31*	2.60	0.60
6	4	4	16.51	17.20	2.11
6	4	5	14.94	15.28	2.25
6	4	6	5.20	4.91	1.81
6	4	7	16.76	16.89	1.91
6	4	8	9.32	9.74	2.21
6	4	9	2.16*	0.41	0.31
6	4	10	2.05*	0.89	0.24
6	4	11	2.14*	2.17	0.22
6	4	12	5.40	4.70	1.00
6	4	13	1.03*	0.04	0.05
7	4	12	1.77*	1.04	0.15
7	4	11	7.53	7.04	1.51
7	4	10	2.01*	0.24	0.25

h	k	l	Fo	Fc	weight
7	4	9	3.03*	0.87	0.76
7	4	8	5.95	6.21	1.54
7	4	7	3.64	3.68	0.89
7	4	6	7.23	7.55	2.03
7	4	5	2.88*	3.34	0.70
7	4	4	1.90*	0.45	0.32
7	4	3	2.71*	0.28	1.04
7	4	2	2.65*	2.38	0.91
7	4	1	5.90	6.20	2.37
7	4	0	4.56	4.04	1.70
7	4	-1	3.38*	2.95	1.03
7	4	-2	1.69*	1.30	0.35
7	4	-3	7.80	7.93	3.00
7	4	-4	1.43*	0.94	0.24
7	4	-5	1.68*	0.16	0.36
7	4	-6	5.73	5.34	1.97
7	4	-7	3.15	3.74	0.70
7	4	-8	1.10*	2.25	0.09
7	4	-9	1.39*	0.46	0.12
7	4	-10	1.89*	1.81	0.28
7	4	-11	2.43*	2.46	0.41
7	4	-12	4.66	4.54	1.07
7	4	-13	7.30	6.66	1.62
7	4	-14	2.15*	2.17	0.22
7	4	-15	5.37	4.94	0.95
7	4	-16	4.11*	3.32	0.71
8	4	-15	4.46	4.56	0.60
8	4	-14	2.13*	0.03	0.22
8	4	-13	3.52	3.64	0.55
8	4	-12	2.88*	4.13	0.33
8	4	-11	3.41*	1.41	0.86
8	4	-10	1.92*	1.95	0.27
8	4	-9	3.88*	5.60	0.74
8	4	-8	10.73	10.65	2.44
8	4	-7	13.45	13.98	2.41
8	4	-6	1.74*	0.46	0.25
8	4	-5	11.38	11.34	2.57
8	4	-4	2.69*	0.16	0.72
8	4	-3	3.23*	0.60	1.02
8	4	-2	1.28*	0.75	0.14
8	4	-1	1.29*	1.29	0.11
8	4	0	8.76	8.77	2.69
8	4	1	12.26	12.57	2.58
8	4	2	1.90*	1.31	0.28
8	4	3	22.50	23.12	1.36
8	4	4	11.93	12.17	2.40
8	4	5	4.38	5.45	1.06
8	4	6	9.94	10.35	2.20
8	4	7	5.71	5.52	1.49
8	4	8	0.92*	1.87	0.05
8	4	9	3.00*	1.31	0.49
8	4	10	1.39*	4.16	0.07
8	4	11	3.22*	0.14	0.49
9	4	10	4.32*	3.51	0.79
9	4	9	2.17*	1.23	0.21
9	4	8	2.01*	0.48	0.25
9	4	7	2.20*	1.56	0.21
9	4	6	1.97*	1.53	0.26

h	k	l	Fo	Fc	weight
9	4	5	2.03*	1.72	0.24
9	4	4	1.92*	0.51	0.27
9	4	3	5.76	6.16	1.61
9	4	2	1.95*	0.51	0.26
9	4	1	11.36	11.52	2.51
9	4	0	1.77*	1.57	0.37
9	4	-1	1.92*	0.49	0.27
9	4	-2	9.61	9.67	2.51
9	4	-3	8.71	8.85	2.48
9	4	-4	10.28	9.81	2.53
9	4	-5	5.37	4.62	1.68
9	4	-6	2.12*	0.92	0.36
9	4	-7	2.03*	0.67	0.24
9	4	-8	2.77*	0.96	0.52
9	4	-9	2.02*	0.62	0.24
9	4-10		5.10	5.50	1.16
9	4-11		2.86*	1.66	0.54
9	4-12		2.20*	0.89	0.21
9	4-13		3.72*	2.69	0.68
9	4-14		0.99*	3.13	0.03
9	4-15		3.97*	2.91	0.60
10	4-14		4.42*	3.66	0.66
10	4-13		1.39*	1.09	0.09
10	4-12		1.67*	1.98	0.12
10	4-11		2.24*	1.89	0.20
10	4-10		3.51*	0.75	0.68
10	4 -9		4.16*	3.43	0.88
10	4 -8		3.25*	2.39	0.66
10	4 -7		9.23	8.97	2.22
10	4 -6		4.85	4.91	1.15
10	4 -5		4.09	4.79	0.91
10	4 -4		3.62	3.49	0.77
10	4 -3		3.38*	4.15	0.58
10	4 -2		10.40	10.18	2.33
10	4 -1		10.01	10.08	2.35
10	4 0		11.97	12.53	2.25
10	4 1		2.97	3.80	0.51
10	4 2		8.25	8.50	2.13
10	4 3		1.95*	3.08	0.21
10	4 4		2.12*	2.73	0.22
10	4 5		2.90*	3.14	0.50
10	4 6		3.26*	1.30	0.62
10	4 7		1.67*	1.63	0.18
10	4 8		2.33*	2.05	0.18
10	4 9		2.35*	1.80	0.18
11	4 8		2.53*	2.61	0.26
11	4 7		3.90*	1.38	0.58
11	4 6		0.98*	1.81	0.04
11	4 5		2.53*	3.97	0.28
11	4 4		5.12	4.70	1.10
11	4 3		5.74	6.24	1.22
11	4 2		3.88	3.56	0.76
11	4 1		2.05*	0.86	0.24
11	4 0		1.96*	2.76	0.31
11	4 -1		7.04	7.16	1.81
11	4 -2		2.73*	0.03	0.47
11	4 -3		1.92*	1.07	0.27
11	4 -4		2.15*	3.85	0.22

h	k	l	Fo	Fc	weight	8
11	4 -5		3.68*	3.99	0.82	
11	4 -6		3.72*	2.08	0.80	
11	4 -7		2.21*	0.49	0.20	
11	4 -8		2.55*	3.85	0.26	
11	4 -9		4.01*	3.08	1.01	
11	4-10		1.88*	3.98	0.14	
11	4-11		2.15*	0.07	0.22	
11	4-12		2.25*	1.30	0.20	
11	4-13		4.40*	2.37	0.63	
12	4-12		2.32*	0.86	0.19	
12	4-11		2.97*	1.96	0.44	
12	4-10		2.24*	2.76	0.20	
12	4 -9		2.34*	1.20	0.25	
12	4 -8		2.20*	1.56	0.21	
12	4 -7		4.03*	0.66	0.84	
12	4 -6		4.10*	4.07	0.67	
12	4 -5		2.14*	0.76	0.22	
12	4 -4		1.81*	3.16	0.16	
12	4 -3		2.56*	5.12	0.30	
12	4 -2		2.24*	1.17	0.27	
12	4 -1		3.41*	1.60	0.81	
12	4 0		3.19*	1.67	0.65	
12	4 1		4.56*	4.89	0.61	
12	4 2		1.89*	2.99	0.18	
12	4 3		2.54*	0.67	0.33	
12	4 4		3.10*	4.15	0.30	
12	4 5		2.50*	2.23	0.16	
12	4 6		2.36*	1.59	0.18	
13	4 4		3.94	4.34	0.44	
13	4 3		2.25*	2.30	0.19	
13	4 2		3.13*	3.25	0.33	
13	4 1		2.26*	2.28	0.20	
13	4 0		3.86*	4.96	0.44	
13	4 -1		2.23*	0.45	0.20	
13	4 -2		7.18	7.01	1.48	
13	4 -3		2.51*	1.01	0.26	
13	4 -4		2.32*	0.44	0.22	
13	4 -5		4.56*	3.88	0.73	
13	4 -6		4.06*	2.90	0.71	
13	4 -7		3.48*	3.85	0.46	
13	4 -8		2.39*	0.41	0.21	
13	4 -9		3.96*	0.24	0.67	
13	4-10		3.18*	0.35	0.39	
13	4-11		1.45*	1.26	0.07	
14	4 -9		3.35*	3.28	0.29	
14	4 -8		2.35*	2.78	0.18	
14	4 -7		7.05	6.43	1.11	
14	4 -6		4.35*	2.32	0.76	
14	4 -5		2.37*	0.92	0.18	
14	4 -4		5.66	5.03	0.88	
14	4 -3		6.92	5.79	1.13	
14	4 -2		3.71	3.68	0.41	
14	4 -1		3.88*	3.94	0.53	
14	4 0		3.92*	0.97	0.65	
14	4 1		2.13*	0.33	0.22	
14	4 2		2.23*	0.80	0.20	
15	4 -4		2.39*	1.39	0.17	
14	5 -1		2.49*	2.53	0.16	

h	k	l	Fo	Fc	weight
14	5	-2	2.29*	3.02	0.19
14	5	-3	2.43*	1.25	0.17
14	5	-4	3.68*	3.71	0.48
14	5	-5	2.35*	0.59	0.18
14	5	-6	2.47*	0.81	0.16
14	5	-7	2.73*	0.24	0.25
13	5	-10	2.54*	2.29	0.16
13	5	-9	4.57	4.55	0.55
13	5	-8	2.26*	0.03	0.20
13	5	-7	3.64	3.26	0.47
13	5	-6	3.27*	1.95	0.44
13	5	-5	2.17*	0.14	0.21
13	5	-4	2.37*	0.65	0.18
13	5	-3	2.18*	2.51	0.21
13	5	-2	3.53*	2.69	0.46
13	5	-1	2.79*	1.73	0.28
13	5	0	3.14*	2.36	0.40
13	5	1	3.10	1.75	0.40
13	5	2	2.88*	1.12	0.35
13	5	3	2.36*	2.16	0.18
12	5	5	4.37*	3.36	0.69
12	5	4	2.35*	1.92	0.18
12	5	3	6.72	6.50	1.20
12	5	2	3.08*	3.56	0.32
12	5	1	2.16*	1.38	0.21
12	5	0	2.33*	1.05	0.33
12	5	-1	3.27*	4.20	0.37
12	5	-2	3.98*	4.36	0.59
12	5	-3	2.48*	0.96	0.34
12	5	-4	4.19*	4.72	0.67
12	5	-5	2.19*	2.92	0.21
12	5	-6	5.74	5.74	1.04
12	5	-7	2.14*	1.71	0.24
12	5	-8	3.12	3.07	0.37
12	5	-9	3.11*	0.17	0.33
12	5	-10	2.24*	2.93	0.18
12	5	-11	5.23	5.21	0.70
11	5	-12	2.20*	1.17	0.21
11	5	-11	3.43*	0.60	0.70
11	5	-10	2.20*	0.98	0.21
11	5	-9	2.28*	0.67	0.19
11	5	-8	2.13*	0.09	0.22
11	5	-7	2.08*	0.87	0.23
11	5	-6	2.19*	0.48	0.21
11	5	-5	4.03*	2.02	0.92
11	5	-4	2.13*	2.04	0.22
11	5	-3	3.69*	3.59	0.61
11	5	-2	2.31*	4.66	0.19
11	5	-1	2.01*	3.21	0.17
11	5	0	6.38	5.81	1.59
11	5	1	2.91*	0.58	0.70
11	5	2	2.80*	1.86	0.39
11	5	3	2.32*	2.50	0.23
11	5	4	1.67*	2.66	0.11
11	5	5	3.56*	1.93	0.61
11	5	6	5.54	4.61	0.97
11	5	7	2.19*	1.02	0.21
10	5	8	1.99*	1.30	0.17
10	5	7	2.11*	1.68	0.22
10	5	6	1.37*	1.40	0.09
10	5	5	2.32*	0.96	0.29
10	5	4	8.42	8.24	1.96
10	5	3	2.16*	1.51	0.21
10	5	2	8.98	9.04	2.08
10	5	1	3.59	3.98	0.72
10	5	0	6.95	7.27	1.73
10	5	-1	7.36	7.67	1.73
10	5	-2	1.48*	1.64	0.15
10	5	-3	5.56	5.41	1.37
10	5	-4	7.80	7.83	1.88
10	5	-5	1.89*	1.36	0.28
10	5	-6	5.15	5.68	1.08
10	5	-7	3.86*	3.83	0.66
10	5	-8	6.00	5.77	1.40
10	5	-9	3.08	2.75	0.43
10	5	-10	2.08*	0.93	0.23
10	5	-11	2.21*	0.24	0.20
10	5	-12	3.42*	2.94	0.53
9	5	-13	1.43*	2.84	0.09
9	5	-14	1.77*	1.84	0.10
9	5	-13	2.80*	0.39	0.35
9	5	-12	2.03*	0.22	0.24
9	5	-11	1.97*	1.05	0.26
9	5	-10	1.74*	2.09	0.17
9	5	-9	1.92*	2.06	0.27
9	5	-8	5.10	5.50	1.13
9	5	-7	3.42*	0.26	0.91
9	5	-6	7.56	7.62	2.05
9	5	-5	1.44*	2.55	0.11
9	5	-4	2.60*	1.14	0.55
9	5	-3	5.08	5.25	1.34
9	5	-2	12.34	12.83	2.20
9	5	-1	2.85*	2.13	0.54
9	5	0	12.56	12.45	2.32
9	5	1	3.46*	4.20	0.70
9	5	2	2.00*	0.87	0.25
9	5	3	3.68*	4.00	0.82
9	5	4	2.17*	2.11	0.29
9	5	5	2.09*	1.23	0.23
9	5	6	1.62*	0.92	0.16
9	5	7	3.46*	0.38	0.87
9	5	8	3.12*	2.38	0.45
9	5	9	2.36*	1.78	0.18
8	5	10	2.32*	1.95	0.19
8	5	9	2.60*	3.16	0.28
8	5	8	3.80*	2.89	0.78
8	5	7	2.26*	0.55	0.38
8	5	6	5.14	4.53	1.41
8	5	5	4.20	4.57	0.94
8	5	4	12.28	12.69	2.25
8	5	3	2.75*	0.69	0.53
8	5	2	16.08	16.35	1.99
8	5	1	8.72	9.16	2.36
8	5	0	1.84*	1.63	0.28
8	5	-1	6.46	7.00	1.87
8	5	-2	5.19	5.06	1.63
8	5	-3	26.01	26.84	1.09
8	5	-4	0.79*	2.25	0.05
8	5	-5	8.21	8.84	2.41
8	5	-6	3.24*	3.01	0.78
8	5	-7	4.12	3.91	1.01
8	5	-8	4.05*	4.07	0.89
8	5	-9	0.86*	0.48	0.06
8	5	-10	3.77*	2.99	0.87
8	5	-11	3.03*	2.30	0.71
8	5	-12	4.42*	3.15	0.82
8	5	-13	2.17*	2.57	0.19
8	5	-14	4.71*	6.36	0.51
8	5	-15	2.33*	1.45	0.18
7	5	-15	2.70*	0.26	0.35
7	5	-14	3.70*	2.85	0.61
7	5	-13	2.13*	0.23	0.22
7	5	-12	3.46*	3.72	0.56
7	5	-11	1.92*	0.23	0.27
7	5	-10	2.00*	1.12	0.25
7	5	-9	4.78	5.59	1.21
7	5	-8	6.74	7.19	2.02
7	5	-7	3.10*	4.10	0.69
7	5	-6	7.34	7.02	2.44
7	5	-5	4.60	4.36	1.42
7	5	-4	6.24	6.00	2.15
7	5	-3	11.67	11.51	2.69
7	5	-2	8.85	9.35	2.61
7	5	-1	14.65	14.81	2.34
7	5	0	4.15*	3.83	1.35
7	5	1	1.88*	1.57	0.31
7	5	2	6.79	7.00	2.21
7	5	3	8.41	8.63	2.60
7	5	4	5.15	5.64	1.41
7	5	5	5.03	5.62	1.50
7	5	6	1.49*	1.84	0.14
7	5	7	1.95*	0.49	0.26
7	5	8	3.31*	0.90	0.81
7	5	9	2.04*	0.21	0.24
7	5	10	2.30*	3.39	0.19
7	5	11	2.48*	0.92	0.31
6	5	12	2.16*	0.40	0.21
6	5	11	0.88*	1.80	0.04
6	5	10	1.65*	0.38	0.19
6	5	9	2.90*	0.93	0.56
6	5	8	3.88	4.41	0.89
6	5	7	6.21	6.07	1.76
6	5	6	6.65	7.22	1.94
6	5	5	3.31*	2.16	1.02
6	5	4	1.90*	2.03	0.28
6	5	3	2.95*	1.42	1.02
6	5	2	1.29*	1.85	0.17
6	5	1	9.28	9.05	2.89
6	5	0	7.64	6.96	2.86
6	5	-1	3.59*	4.22	1.04
6	5	-2	1.76*	0.18	0.35
6	5	-3	1.82*	0.72	0.30
6	5	-4	7.17	7.54	2.61
6	5	-5	3.59	3.37	1.16
6	5	-6	3.39*	2.06	1.07
6	5	-7	5.10	4.74	1.76
6	5	-8	4.02	4.85	1.11
6	5	-9	2.00*	0.90	0.25
6	5	-10	9.78	10.22	2.24
6	5	-11	4.30	4.39	0.95
6	5	-12	2.73*	1.55	0.46
6	5	-13	4.86	4.03	0.98
6	5	-14	1.95*	1.52	0.17
6	5	-15	2.24*	0.54	0.20
5	5	-15	3.55	3.26	0.51
5	5	-14	3.99*	3.40	0.66
5	5	-13	3.62*	3.36	0.68
5	5	-12	2.54*	4.09	0.26
5	5	-11	1.50*	0.18	0.19
5	5	-10	6.21	7.15	1.71
5	5	-9	6.98	6.91	2.27
5	5	-8	6.94	7.24	2.37
5	5	-7	1.82*	1.15	0.30
5	5	-6	4.94	6.18	1.68
5	5	-5	11.56	11.82	2.95
5	5	-4	12.52	13.12	2.85
5	5	-3	7.67	7.45	3.19
5	5	-2	17.21	16.89	2.14
5	5	-1	6.94	6.39	3.32
5	5	0	15.76	15.85	2.34
5	5	1	4.54	4.70	1.93
5	5	2	3.27*	3.52	1.11
5	5	3	2.31*	0.38	0.78
5	5	4	3.36*	0.50	1.33
5	5	5	3.95	3.74	1.25
5	5	6	1.74*	0.44	0.33
5	5	7	3.51*	2.50	1.01
5	5	8	3.09*	0.47	0.86
5	5	9	2.08*	1.86	0.23
5	5	10	3.06*	2.20	0.53
5	5	11	2.18*	0.85	0.21
5	5	12	2.15*	1.53	0.22
5	5	13	2.37*	1.38	0.18
4	5	13	4.61*	5.25	0.69
4	5	12	2.91*	0.24	0.49
4	5	11	1.32*	0.02	0.09
4	5	10	2.98*	3.82	0.50
4	5	9	6.67	6.76	1.91
4	5	8	1.84*	0.34	0.29
4	5	7	0.80*	0.27	0.07
4	5	6	1.89*	2.74	0.37
4	5	5	10.89	10.57	2.86
4	5	4	1.76*	0.82	0.32
4	5	3	5.30	4.85	2.47
4	5	2	7.18	7.40	3.29
4	5	1	6.94	6.99	3.23
4	5	0	4.30	4.48	1.97
4	5	-1	8.49	8.68	3.73
4	5	-2	3.75	3.88	1.85
4	5	-3	5.44	6.03	2.81
4	5	-4	9.45	9.61	3.46
4	5	-5	9.34	9.19	3.28

h	k	l	Fo	Fc	weight
4	5	-6	11.13	11.61	2.94
4	5	-7	1.82*	1.58	0.34
4	5	-8	6.24	5.77	2.20
4	5	-9	7.31	7.64	2.37
4	5	-10	6.30	6.02	1.97
4	5	-11	1.87*	0.92	0.29
4	5	-12	1.55*	2.26	0.17
4	5	-13	6.25	6.57	1.37
4	5	-14	1.93*	1.77	0.19
4	5	-15	2.45*	1.64	0.21
3	5	-15	3.61*	0.91	0.88
3	5	-14	3.85*	2.39	0.81
3	5	-13	2.00*	1.76	0.25
3	5	-12	2.00*	0.32	0.25
3	5	-11	4.30	4.56	1.05
3	5	-10	8.92	9.81	2.46
3	5	-9	7.27	7.77	2.38
3	5	-8	7.93	7.88	2.70
3	5	-7	3.52*	2.89	1.29
3	5	-6	12.06	12.39	2.99
3	5	-5	1.72*	2.78	0.34
3	5	-4	16.56	16.54	2.30
3	5	-3	10.14	10.49	3.55
3	5	-2	0.91*	1.70	0.14
3	5	-1	5.38	5.68	3.09
3	5	0	6.63	6.82	3.52
3	5	1	8.86	8.08	3.96
3	5	2	5.76	5.21	3.42
3	5	3	5.74	6.07	2.94
3	5	4	4.60	4.87	2.19
3	5	5	11.65	11.55	2.91
3	5	6	4.78	4.83	1.92
3	5	7	12.76	12.63	2.60
3	5	8	7.95	7.82	2.39
3	5	9	4.86	4.67	1.38
3	5	10	1.52*	0.99	0.20
3	5	11	3.87*	3.23	0.83
3	5	12	3.67*	3.54	0.59
3	5	13	3.12*	3.04	0.49
3	5	14	2.90*	2.76	0.34
2	5	14	4.04	4.39	0.61
2	5	13	5.82	5.65	1.22
2	5	12	2.78*	2.84	0.45
2	5	11	3.09*	3.49	0.58
2	5	10	2.54*	3.22	0.47
2	5	9	2.97*	2.50	0.66
2	5	8	16.32	16.95	2.02
2	5	7	8.84	8.66	2.81
2	5	6	17.65	18.43	1.98
2	5	5	5.89	6.06	2.77
2	5	4	11.16	10.62	3.28
2	5	3	1.82*	3.08	0.54
2	5	2	1.47*	0.79	0.46
2	5	1	23.22	22.80	1.44
2	5	0	16.31	15.83	2.44
2	5	-1	22.64	22.11	1.51
2	5	-2	7.86	7.88	3.87
2	5	-3	2.95*	3.66	1.70
2	5	-4	3.79	5.00	1.83
2	5	-5	7.34	7.34	3.31
2	5	-6	1.64*	2.25	0.37
2	5	-7	3.66	4.16	1.22
2	5	-8	4.19	4.65	1.39
2	5	-9	5.62	5.08	1.97
2	5	-10	3.07*	2.92	0.83
2	5	-11	2.26*	0.38	0.60
2	5	-12	2.18*	1.53	0.35
2	5	-13	2.62*	0.23	0.53
2	5	-14	2.37*	2.19	0.28
2	5	-15	2.46*	0.36	0.42
1	5	-15	2.10*	0.79	0.23
1	5	-14	2.11*	1.32	0.23
1	5	-13	1.99*	1.34	0.25
1	5	-12	2.87*	1.60	0.54
1	5	-11	2.13*	1.61	0.22
1	5	-10	3.40*	4.84	0.73
1	5	-9	2.96*	2.92	0.62
1	5	-8	11.35	11.68	2.77
1	5	-7	1.63*	1.51	0.37
1	5	-6	3.46	3.86	1.44
1	5	-5	7.02	7.09	3.43
1	5	-4	3.21*	3.95	1.38
1	5	-3	5.81	6.13	3.57
1	5	-2	2.33	2.50	1.00
1	5	-1	20.23	19.83	1.81
1	5	0	7.32	7.38	4.39
1	5	1	10.01	9.50	4.02
1	5	2	2.45*	1.37	1.22
1	5	3	3.33	3.95	1.89
1	5	4	1.89*	3.43	0.52
1	5	5	4.73	4.74	2.26
1	5	6	5.98	5.57	2.70
1	5	7	17.54	17.88	1.97
1	5	8	3.91	4.12	1.18
1	5	9	15.84	16.01	2.06
1	5	10	3.14	2.60	0.80
1	5	11	1.96*	0.92	0.26
1	5	12	2.02*	2.07	0.24
1	5	13	3.57*	4.49	0.48
1	5	14	2.13*	0.20	0.22
1	5	15	1.03*	3.13	0.04
0	5	15	1.44*	1.07	0.09
0	5	14	3.80	3.77	0.66
0	5	13	2.31*	2.27	0.43
0	5	12	2.73	1.82	0.52
0	5	11	1.85*	0.99	0.29
0	5	10	7.11	7.29	2.30
0	5	9	7.72	7.83	2.46
0	5	8	17.46	17.86	1.91
0	5	7	16.87	17.14	2.06
0	5	6	15.66	15.90	2.40
0	5	5	8.07	8.16	3.63
0	5	4	1.55*	0.85	0.42
0	5	3	24.48	24.73	1.32
0	5	2	8.20	7.49	4.28
0	5	1	23.00	22.38	1.48
0	6	0	8.61	8.33	3.63
0	6	1	13.68	14.18	2.78
0	6	2	5.89	6.03	3.01
0	6	3	13.51	13.79	2.77
0	6	4	5.44	5.42	2.66
0	6	5	5.77	6.22	2.57
0	6	6	2.85*	4.82	0.67
0	6	7	7.18	7.36	2.53
0	6	8	1.41*	0.02	0.18
0	6	9	4.61	4.46	1.40
0	6	10	3.71*	3.04	1.16
0	6	11	2.03*	0.15	0.24
0	6	12	3.53*	0.35	0.82
0	6	13	6.51	6.25	1.36
0	6	14	2.17*	0.33	0.21
1	6	14	2.72*	0.47	0.42
1	6	13	2.17*	2.88	0.21
1	6	12	2.03*	0.55	0.24
1	6	11	4.06	2.65	0.94
1	6	10	2.35*	2.66	0.41
1	6	9	1.21*	0.19	0.13
1	6	8	7.55	7.73	2.47
1	6	7	6.23	5.75	2.19
1	6	6	4.70	4.67	1.73
1	6	5	5.14	5.41	2.11
1	6	4	2.18*	0.23	0.72
1	6	3	1.55*	0.44	0.42
1	6	2	4.49	4.55	2.11
1	6	1	1.19*	0.91	0.23
1	6	0	5.42	5.52	2.85
1	6	-1	3.80	3.58	1.77
1	6	-2	4.78	4.86	2.28
1	6	-3	1.86*	2.09	0.49
1	6	-4	4.63	5.59	1.82
1	6	-5	2.44*	2.43	0.57
1	6	-6	2.77	2.26	0.75
1	6	-7	5.53	5.90	1.95
1	6	-8	6.07	6.47	1.97
1	6	-9	4.90	5.05	1.30
1	6	-10	1.50*	2.60	0.19
1	6	-11	3.82*	2.30	1.09
1	6	-12	2.81*	0.57	0.41
1	6	-13	3.63*	2.61	0.91
1	6	-14	2.02*	0.01	0.18
2	6	-15	2.38*	1.19	0.18
2	6	-14	3.64	3.04	0.51
2	6	-13	3.35*	1.90	0.75
2	6	-12	2.00*	0.99	0.25
2	6	-11	1.99*	0.18	0.25
2	6	-10	2.14*	3.04	0.31
2	6	-9	3.13	3.64	0.64
2	6	-8	8.62	8.06	2.58
2	6	-7	10.33	9.83	2.66
2	6	-6	9.39	9.34	2.93
2	6	-5	8.31	8.24	3.05
2	6	-4	4.20	3.75	1.68
2	6	-3	8.07	8.80	3.16
2	6	-2	2.96*	4.10	0.89
2	6	-1	3.15	3.11	1.35
2	6	0	3.71	3.40	1.74
2	6	1	3.82	3.95	1.64
2	6	2	2.65*	0.99	1.06
2	6	3	9.38	9.21	3.17
2	6	4	3.84	4.03	1.52
2	6	5	2.40*	0.38	0.77
2	6	6	7.06	8.32	2.30
2	6	7	1.78*	1.09	0.32
2	6	8	1.82*	1.91	0.30
2	6	9	3.01*	0.49	1.01
2	6	10	3.37*	3.07	0.74
2	6	11	3.24*	1.85	0.80
2	6	12	2.21*	0.41	0.21
2	6	13	1.42*	3.35	0.09
2	6	14	7.01	6.27	1.17
3	6	13	2.04*	2.14	0.24
3	6	12	2.09*	1.27	0.23
3	6	11	5.51	4.86	1.20
3	6	10	1.30*	0.21	0.13
3	6	9	1.98*	0.03	0.27
3	6	8	5.26	6.06	1.42
3	6	7	2.74*	1.57	0.95
3	6	6	10.19	9.95	2.66
3	6	5	3.04	3.58	0.74
3	6	4	6.11	6.13	2.28
3	6	3	2.86*	3.48	0.89
3	6	2	1.65*	0.23	0.37
3	6	1	9.60	10.11	3.26
3	6	0	6.18	5.46	2.86
3	6	-1	9.24	10.19	3.37
3	6	-2	1.59*	1.42	0.37
3	6	-3	17.01	17.45	2.13
3	6	-4	4.71	4.04	1.73
3	6	-5	16.97	16.71	2.09
3	6	-6	4.75	5.41	1.56
3	6	-7	1.96*	1.08	0.26
3	6	-8	12.70	12.64	2.45
3	6	-9	8.53	8.29	2.50
3	6	-10	9.96	9.65	2.28
3	6	-11	2.64*	3.60	0.44
3	6	-12	2.64*	2.80	0.37
3	6	-13	1.37*	1.87	0.09
3	6	-14	2.24*	1.79	0.21
3	6	-15	2.40*	2.07	0.17
4	6	-15	3.75*	0.08	0.69
4	6	-14	3.50	2.89	0.47
4	6	-13	3.99*	0.24	0.98
4	6	-12	2.80*	0.73	0.44
4	6	-11	2.39*	1.59	0.37
4	6	-10	2.76*	3.93	0.38
4	6	-9	1.46*	3.07	0.16
4	6	-8	7.19	7.37	2.13
4	6	-7	16.94	17.05	1.96
4	6	-6	2.05*	0.14	0.39
4	6	-5	0.76*	1.12	0.05
4	6	-4	16.58	17.24	2.10
4	6	-3	23.43	23.81	1.34

h	k	l	Fo	Fc	weight
4	6	-2	2.91*	3.70	0.71
4	6	-1	9.23	9.39	3.04
4	6	0	10.87	11.21	3.08
4	6	1	8.77	8.90	3.13
4	6	2	1.83*	3.57	0.29
4	6	3	4.47	4.30	1.60
4	6	4	0.78*	3.63	0.05
4	6	5	5.11	5.17	1.69
4	6	6	1.84*	1.07	0.28
4	6	7	1.87*	0.75	0.29
4	6	8	5.36	4.98	1.37
4	6	9	2.03*	1.84	0.24
4	6	10	2.30*	0.40	0.34
4	6	11	4.67*	5.47	0.68
4	6	12	5.07	4.76	0.83
5	6	12	3.26*	0.11	0.45
5	6	11	3.86*	2.69	0.72
5	6	10	2.23*	0.79	0.20
5	6	9	5.19	5.06	1.21
5	6	8	2.05*	1.04	0.24
5	6	7	1.51*	2.33	0.13
5	6	6	10.32	10.50	2.39
5	6	5	2.85*	1.29	0.77
5	6	4	17.60	17.17	1.89
5	6	3	2.94*	1.57	0.78
5	6	2	9.76	9.85	2.76
5	6	1	10.82	11.64	2.70
5	6	0	3.60*	3.54	0.98
5	6	-1	27.26	27.26	1.04
5	6	-2	4.23	4.55	1.39
5	6	-3	12.58	13.22	2.68
5	6	-4	16.16	16.89	2.08
5	6	-5	0.77*	2.03	0.06
5	6	-6	16.48	16.02	2.02
5	6	-7	1.93*	0.27	0.27
5	6	-8	3.29	3.04	0.72
5	6	-9	2.57*	2.21	0.56
5	6-10		1.95*	2.49	0.26
5	6-11		4.60	4.28	1.11
5	6-12		2.15*	0.78	0.22
5	6-13		2.13*	3.70	0.22
5	6-14		1.43*	1.28	0.10
5	6-15		2.33*	0.26	0.18
6	6-14		3.15*	2.95	0.35
6	6-13		2.85*	2.67	0.36
6	6-12		2.86*	0.06	0.40
6	6-11		4.01	4.05	0.93
6	6-10		2.87*	2.84	0.57
6	6	-9	2.03*	2.52	0.24
6	6	-8	11.67	12.03	2.31
6	6	-7	3.61*	0.15	1.01
6	6	-6	9.27	9.22	2.49
6	6	-5	7.26	8.44	2.28
6	6	-4	11.11	11.39	2.57
6	6	-3	15.76	16.24	2.09
6	6	-2	17.11	17.80	1.95
6	6	-1	3.70	3.85	1.01
6	6	0	7.84	7.93	2.49
6	6	1	4.61	4.91	1.59
6	6	2	7.61	7.55	2.26
6	6	3	3.90*	4.93	0.97
6	6	4	8.44	8.16	2.33
6	6	5	2.02*	0.14	0.25
6	6	6	2.48*	0.91	0.59
6	6	7	6.06	5.74	1.61
6	6	8	1.32*	2.54	0.11
6	6	9	2.35*	1.10	0.35
6	6	10	3.84*	2.15	0.82
6	6	11	2.23*	1.86	0.20
7	6	10	2.27*	0.54	0.19
7	6	9	1.71*	1.56	0.14
7	6	8	2.16*	0.80	0.21
7	6	7	2.64*	1.51	0.57
7	6	6	6.82	6.91	1.76
7	6	5	2.34*	2.09	0.45
7	6	4	7.20	7.28	1.96
7	6	3	3.74	2.75	0.95
7	6	2	2.99*	1.58	0.73
7	6	1	7.06	7.44	1.95
7	6	0	0.81*	2.52	0.07
7	6	-1	12.15	12.01	2.51
7	6	-2	3.59*	0.77	1.12
7	6	-3	2.41*	1.40	0.67
7	6	-4	2.81*	0.34	0.91
7	6	-5	2.03*	3.13	0.24
7	6	-6	6.60	5.57	2.00
7	6	-7	1.95*	1.03	0.26
7	6	-8	1.92*	1.08	0.27
7	6	-9	3.21*	3.01	0.76
7	6-10		2.89*	0.48	0.62
7	6-11		2.19*	1.45	0.21
7	6-12		1.27*	1.11	0.08
7	6-13		3.15*	1.74	0.42
7	6-14		2.35*	1.87	0.18
8	6-14		3.46*	1.88	0.45
8	6-13		2.03*	1.84	0.16
8	6-12		6.35	5.70	1.11
8	6-11		2.15*	2.63	0.22
8	6-10		3.73*	2.22	0.77
8	6	-9	3.76*	3.19	0.90
8	6	-8	1.54*	1.03	0.13
8	6	-7	6.04	6.14	1.55
8	6	-6	2.85*	0.37	0.88
8	6	-5	2.24*	3.37	0.23
8	6	-4	10.68	10.79	2.35
8	6	-3	4.13	4.21	1.08
8	6	-2	13.37	13.60	2.23
8	6	-1	8.84	8.87	2.19
8	6	0	2.05*	0.10	0.24
8	6	1	1.85*	0.96	0.29
8	6	2	3.86*	5.56	0.62
8	6	3	6.23	6.17	1.58
8	6	4	1.79*	3.38	0.19
8	6	5	2.03*	1.17	0.24
8	6	6	2.12*	0.22	0.22
8	6	7	2.25*	2.49	0.20
8	6	8	2.22*	0.84	0.26
9	6	9	1.45*	1.82	0.07
9	6	8	2.33*	2.08	0.18
9	6	7	2.65*	2.27	0.29
9	6	6	2.14*	1.41	0.22
9	6	5	3.81*	2.14	1.05
9	6	4	2.28*	1.18	0.32
9	6	3	1.99*	2.37	0.25
9	6	2	2.54*	1.14	0.38
9	6	1	7.38	7.45	1.84
9	6	0	3.16*	1.64	0.97
9	6	-1	7.26	6.89	1.88
9	6	-2	3.19	2.83	0.65
9	6	-3	2.00*	0.98	0.25
9	6	-4	6.26	6.24	1.61
9	6	-5	3.51*	3.52	0.87
9	6	-6	3.87*	3.82	1.03
9	6	-7	3.90	4.36	0.74
9	6	-8	2.25*	1.21	0.39
9	6	-9	4.08*	4.46	0.71
9	6-10		1.35*	0.44	0.10
9	6-11		2.77*	0.53	0.34
9	6-12		4.50*	2.43	0.79
9	6-13		1.03*	3.03	0.03
10	6-12		2.22*	0.09	0.20
10	6-11		1.42*	2.19	0.07
10	6-10		2.19*	0.73	0.21
10	6	-9	2.06*	0.28	0.24
10	6	-8	2.21*	3.38	0.20
10	6	-7	2.06*	1.45	0.24
10	6	-6	2.11*	2.51	0.22
10	6	-5	2.29*	2.32	0.30
10	6	-4	1.28*	1.25	0.08
10	6	-3	2.02*	3.29	0.26
10	6	-2	3.38*	0.61	0.73
10	6	-1	3.62	3.50	0.69
10	6	0	2.04*	2.14	0.20
10	6	1	4.03*	4.45	0.73
10	6	2	2.65*	0.50	0.52
10	6	3	2.17*	2.13	0.21
10	6	4	4.00*	3.27	0.79
10	6	5	7.07	6.65	1.28
10	6	6	4.30*	3.22	0.72
10	6	7	3.88*	2.66	0.59
11	6	5	2.21*	1.09	0.20
11	6	4	3.19*	1.44	0.47
11	6	3	4.28	4.29	0.60
11	6	2	4.37*	4.76	0.68
11	6	1	2.20*	1.82	0.21
11	6	0	2.98	1.93	0.46
11	6	-1	2.10*	0.37	0.23
11	6	-2	3.26*	4.75	0.41
11	6	-3	5.41	5.30	1.05
11	6	-4	4.11*	3.29	0.92
11	6	-5	6.76	6.01	1.40
11	6	-6	2.12*	1.39	0.22
11	6	-7	2.36*	2.27	0.28
11	6	-8	2.33*	0.91	0.18
11	6	-9	2.22*	3.65	0.18
11	6-10		4.29*	3.06	0.72
11	6-11		3.42*	1.50	0.49
12	6-10		2.55*	0.70	0.15
12	6	-9	2.41*	2.32	0.17
12	6	-8	2.37*	1.56	0.18
12	6	-7	3.32*	0.74	0.41
12	6	-6	2.26*	1.49	0.20
12	6	-5	2.32*	2.19	0.18
12	6	-4	2.25*	1.44	0.20
12	6	-3	3.39*	1.49	0.40
12	6	-2	0.98*	1.20	0.03
12	6	-1	2.61*	2.68	0.25
12	6	0	3.85*	2.34	0.68
12	6	1	2.66*	1.81	0.32
12	6	2	2.25*	0.28	0.20
12	6	3	3.68	3.18	0.44
13	6	0	5.28	4.90	0.74
13	6	-1	2.30*	1.69	0.19
13	6	-2	4.22*	3.11	0.72
13	6	-3	2.46*	2.39	0.17
13	6	-4	3.23*	0.30	0.41
13	6	-5	4.58*	4.24	0.57
13	6	-6	3.85*	1.60	0.75
13	6	-7	4.27*	4.66	0.41
12	7	1	1.48*	1.42	0.07
12	7	0	2.34*	0.40	0.18
12	7	-1	3.56*	1.25	0.57
12	7	-2	3.39*	0.43	0.62
12	7	-3	3.06*	0.08	0.49
12	7	-4	2.50*	0.01	0.21
12	7	-5	2.35*	0.16	0.18
12	7	-6	1.78*	1.99	0.11
12	7	-7	1.04*	0.81	0.03
11	7	-8	2.29*	0.88	0.19
11	7	-8	3.53*	1.32	0.58
11	7	-7	3.63*	2.30	0.52
11	7	-6	1.73*	1.39	0.11
11	7	-5	2.19*	0.40	0.21
11	7	-4	4.37	4.47	0.64
11	7	-3	4.40*	4.32	0.57
11	7	-2	1.71*	0.21	0.15
11	7	-1	1.88*	0.67	0.17
11	7	0	4.39	2.94	0.77
11	7	1	7.44	6.53	1.32
11	7	2	2.32*	0.89	0.19
11	7	3	6.28	5.48	0.98
10	7	5	4.00*	1.19	0.68
10	7	4	2.48*	0.42	0.34
10	7	3	1.84*	2.40	0.13
10	7	2	3.80*	1.55	0.66
10	7	1	2.19*	0.38	0.21
10	7	0	2.05*	1.33	0.24
10	7	-1	4.26*	3.67	0.88
10	7	-2	3.67	3.47	0.65
10	7	-3	5.60	5.16	1.25
10	7	-4	1.90*	4.08	0.14
10	7	-5	1.98*	1.47	0.25
10	7	-6	3.30	3.16	0.48
10	7	-7	2.17*	1.73	0.21
10	7	-8	5.87	5.85	0.93
10	7	-9	2.28*	0.00	0.19
10	7-10		1.83*	1.56	0.13
10	7-11		2.56*	0.42	0.28
9	7-11		2.30*	1.80	0.19
9	7-10		4.47*	2.76	0.80
9	7	-9	3.40*	2.18	0.49
9	7	-8	2.22*	2.01	0.20
9	7	-7	3.81	3.84	0.59
9	7	-6	2.14*	0.84	0.22
9	7	-5	1.92*	1.00	0.27
9	7	-4	2.76*	1.22	0.55
9	7	-3	2.90*	0.24	0.57
9	7	-2	0.92*	0.42	0.07
9	7	-1	2.09*	0.36	0.23
9	7	0	2.60*	2.22	0.39
9	7	1	2.13*	1.31	0.22
9	7	2	3.66*	3.35	0.46
9	7	3	3.84*	1.34	0.83
9	7	4	3.00*	2.66	0.40
9	7	5	6.47	5.34	1.29
8	7	6	2.25*	0.64	0.20
9	7	7	5.15	5.02	0.73
8	7	8	2.32*	1.12	0.18
8	7	7	2.19*	1.06	0.21
8	7	6	2.13*	0.59	0.22
8	7	5	2.36*	1.71	0.27
8	7	4	2.08*	1.02	0.23
8	7	3	0.93*	1.18	0.06
8	7	2	3.98*	0.72	1.05
8	7	1	2.38*	0.44	0.40
8	7	0	4.69	4.85	1.20
8	7	-1	1.97*	1.13	0.26
8	7	-2	3.46	4.09	0.66
8	7	-3	3.55*	0.06	0.97
8	7	-4	1.91*	0.52	0.27
8	7	-5	3.50	3.17	0.76
8	7	-6	5.66	5.48	1.26
8	7	-7	5.40	5.14	1.23
8	7	-8	5.37	5.60	0.87
8	7	-9	4.06*	2.57	0.91
8	7-10		2.19*	2.88	0.21
8	7-11		3.47*	0.69	0.76
8	7-12		2.17*	1.10	0.21
7	7-13		6.62	4.82	1.13
7	7-12		2.26*	1.79	0.22
7	7-11		9.51	8.18	1.71
7	7-10		4.75	3.25	1.00
7	7	-9	2.96*	2.95	0.43
7	7	-8	5.71	5.57	1.24
7	7	-7	2.02*	2.03	0.24
7	7	-6	2.06*	2.59	0.23
7	7	-5	3.60*	3.35	0.59
7	7	-4	1.86*	1.42	0.26
7	7	-3	4.37	4.55	1.14
7	7	-2	1.91*	1.84	0.28
7	7	-1	6.95	7.17	1.94
7	7	0	8.69	8.65	2.22
7	7	1	1.90*	0.56	0.28
7	7	2	3.94*	5.70	0.77
7	7	3	3.50	3.70	0.71
7	7	4	1.29*	0.43	0.12
7	7	5	5.23	4.34	1.26
7	7	6	1.97*	0.12	0.26
7	7	7	5.75	5.07	1.14
7	7	8	4.02*	2.68	0.95
7	7	9	2.51*	2.08	0.27
6	7	10	2.53*	0.05	0.33
6	7	9	2.17*	0.44	0.21
6	7	8	3.52*	2.51	0.78
6	7	7	2.51*	1.07	0.36
6	7	6	1.81*	1.50	0.23
6	7	5	2.00*	3.84	0.25
6	7	4	2.20*	3.86	0.21
6	7	3	6.40	7.18	1.74
6	7	2	1.92*	1.89	0.27
6	7	1	3.57	3.94	0.84
6	7	0	3.45*	3.64	0.86
6	7	-1	1.83*	1.85	0.30
6	7	-2	5.06	5.30	1.53
6	7	-3	7.11	7.00	2.28
6	7	-4	4.33	4.68	1.08
6	7	-5	2.79	2.33	0.62
6	7	-6	2.73*	0.48	0.88
6	7	-7	5.10	4.55	1.35
6	7	-8	3.11*	0.52	0.87
6	7	-9	1.80*	0.91	0.31
6	7-10		2.67*	0.51	0.48
6	7-11		3.22*	0.01	0.49
6	7-12		3.00*	2.74	0.33
6	7-13		3.25*	1.91	0.40
5	7-13		3.67*	0.64	0.72
5	7-12		2.19*	1.76	0.21
5	7-11		2.15*	0.03	0.26
5	7-10		2.09*	1.71	0.23
5	7	-9	2.87*	4.06	0.44
5	7	-8	3.14	3.63	0.61
5	7	-7	14.64	14.45	2.01
5	7	-6	5.90	4.98	1.79
5	7	-5	14.68	15.08	2.13
5	7	-4	2.32*	3.85	0.41
5	7	-3	1.15*	2.99	0.12
5	7	-2	2.29*	0.04	0.39
5	7	-1	7.91	8.04	2.38
5	7	0	10.47	10.28	2.59
5	7	1	8.11	8.41	2.35
5	7	2	8.05	8.34	2.30
5	7	3	5.03	4.92	1.50
5	7	4	1.81*	1.81	0.31
5	7	5	2.63*	1.77	0.78
5	7	6	5.28	4.73	1.44
5	7	7	2.12*	0.62	0.22
5	7	8	4.81	4.47	0.97
5	7	9	4.98	4.26	1.07
5	7	10	2.67*	1.66	0.40
4	7	11	5.67	3.84	1.08
4	7	10	3.42*	2.81	0.67
4	7	9	2.14*	2.69	0.28
4	7	8	1.96*	1.20	0.26
4	7	7	1.27*	2.43	0.12
4	7	6	2.86	2.47	0.63
4	7	5	3.20*	0.94	0.94
4	7	4	2.51*	2.68	0.47
4	7	3	5.78	5.93	1.79
4	7	2	7.39	7.37	2.50
4	7	1	1.68*	0.84	0.35
4	7	0	2.37*	2.08	0.55
4	7	-1	4.40	4.98	1.27
4	7	-2	13.93	14.15	2.35
4	7	-3	4.96	4.43	1.63
4	7	-4	11.82	11.92	2.56
4	7	-5	2.00*	1.16	0.35
4	7	-6	1.91*	2.08	0.27
4	7	-7	6.43	6.24	1.89
4	7	-8	1.51*	1.45	0.14
4	7	-8	4.01*	3.60	1.00
4	7-10		2.01*	0.23	0.25
4	7-11		2.08*	0.90	0.23
4	7-12		3.11*	2.48	0.50
4	7-13		2.04*	0.07	0.24
4	7-14		2.31*	0.23	0.19
3	7-14		2.77*	1.27	0.45
3	7-13		2.02*	0.94	0.24
3	7-12		3.78*	0.87	0.95
3	7-11		5.59	4.54	1.45
3	7-10		7.14	6.76	1.72
3	7	-9	1.95*	0.63	0.26
3	7	-8	4.18	3.93	0.94
3	7	-7	3.65	2.84	0.93
3	7	-6	7.29	7.28	2.14
3	7	-5	5.78	6.15	1.91
3	7	-4	12.19	12.03	2.43
3	7	-3	13.67	12.82	2.36
3	7	-2	10.08	10.60	2.76
3	7	-1	3.09*	3.18	0.76
3	7	0	8.81	9.37	2.71
3	7	1	7.84	7.58	2.45
3	7	2	5.73	5.58	1.91
3	7	3	1.83*	1.72	0.30
3	7	4	3.16*	3.50	0.77
3	7	5	2.00*	2.11	0.25
3	7	6	3.09*	4.18	0.59
3	7	7	3.74*	4.11	0.95
3	7	8	2.72*	1.33	0.62
3	7	9	1.84*	1.18	0.30
3	7	10	2.90*	4.81	0.30
3	7	11	2.30*	0.77	0.18
3	7	12	5.48	4.75	0.96
2	7	12	3.37*	0.86	0.48
2	7	11	3.93*	5.45	0.49
2	7	10	2.03*	0.67	0.24
2	7	9	5.32	5.42	1.38
2	7	8	2.06*	1.97	0.24
2	7	7	4.81	5.24	1.39
2	7	6	7.75	7.38	2.36
2	7	5	3.28*	0.29	1.22
2	7	4	3.11*	1.95	0.80
2	7	3	13.32	14.20	2.46
2	7	2	3.28	3.45	0.88
2	7	1	13.20	13.32	2.56
2	7	0	3.32*	3.98	0.85
2	7	-1	2.64*	2.79	0.63
2	7	-2	3.16*	2.85	1.14
2	7	-3	13.41	13.56	2.46
2	7	-4	1.91*	0.73	0.27
2	7	-5	3.67*	3.37	1.07
2	7	-6	5.61	5.38	1.63
2	7	-7	6.61	6.67	2.06
2	7	-8	1.91*	1.07	0.27
2	7	-9	3.21*	4.69	0.72
2	7-10		1.93*	0.04	0.27
2	7-11		3.91*	3.75	0.70
2	7-12		1.90*	1.33	0.28
2	7-13		2.27*	0.80	0 19
1	7-13		2.24*	0.77	0.20
1	7-12		4.25	3.80	0.76
1	7-11		3.81*	2.07	0.79
1	7-10		1.85*	0.75	0.29
1	7	-9	3.22*	1.90	1.13
1	7	-8	3.35*	0.18	0.91
1	7	-7	2.00*	4.16	0.25
1	7	-6	3.66*	3.11	0.83
1	7	-5	5.66	5.09	1.98
1	7	-4	9.73	10.06	2.71
1	7	-3	11.74	12.09	2.63
1	7	-2	5.13	5.06	1.92
1	7	-1	22.02	21.79	1.45
1	7	0	15.93	16.40	2.20
1	7	1	2.15*	2.73	0.46
1	7	2	22.42	22.89	1.41
1	7	3	9.22	8.86	2.85
1	7	4	2.26*	3.15	0.47
1	7	5	2.29*	2.00	0.53
1	7	6	5.81	6.02	1.92
1	7	7	2.56*	4.12	0.47
1	7	8	3.41*	4.95	0.74
1	7	9	1.57*	0.22	0.23
1	7	10	3.25*	2.91	0.74
1	7	11	0.97*	1.54	0.05
1	7	12	1.42*	3 15	0.08
1	7	13	2.18*	1.06	0.21
0	7	13	2.11*	1.15	0.22
0	7	12	2.28*	0.15	0.19
0	7	11	2.06*	3.09	0.24
0	7	10	2.62*	3.11	0.46
0	7	9	1.27*	1.14	0.14
0	7	8	3.26*	1.68	0.97
0	7	7	1.89*	0.94	0.28
0	7	6	2.96*	2.51	0.75

h	k	l	Fo	Fc	weight
0	7	5	2.66*	2.67	0.64
0	7	4	11.25	11.47	2.70
0	7	3	7.14	6.88	2.62
0	7	2	9.24	8.96	2.89
0	7	1	4.69	5.27	1.65
0	8	0	9.16	8.75	2.54
0	8	1	13.40	12.84	2.34
0	8	2	1.90*	0.20	0.28
0	8	3	22.02	22.56	1.36
0	8	4	1.20*	3.29	0.09
0	8	5	7.38	8.42	2.07
0	8	6	1.88*	0.89	0.28
0	8	7	2.02*	2.62	0.32
0	8	8	1.94*	0.92	0.27
0	8	9	2.10*	3.05	0.23
0	8	10	1.98*	0.94	0.26
0	8	11	4.28*	2.96	0.83
0	8	12	1.80*	0.59	0.19
1	8	11	4.58	3.90	0.85
1	8	10	3.13*	2.14	0.46
1	8	9	2.72*	1.97	0.59
1	8	8	3.62*	0.56	0.89
1	8	7	2.04*	0.11	0.29
1	8	6	6.05	5.33	1.54
1	8	5	5.89	6.00	1.61
1	8	4	4.10*	4.90	0.82
1	8	3	1.91*	2.66	0.27
1	8	2	2.76*	3.44	0.60
1	8	1	7.68	7.67	2.35
1	8	0	5.96	6.54	1.93
1	8	-1	2.47*	3.52	0.44
1	8	-2	4.48	4.62	1.37
1	8	-3	2.05*	3.36	0.36
1	8	-4	5.29	5.15	1.53
1	8	-5	1.83*	0.70	0.30
1	8	-6	1.91*	1.51	0.27
1	8	-7	2.84*	3.26	0.45
1	8	-8	4.12*	3.49	0.85
1	8	-9	2.01*	0.83	0.25
1	8	-10	3.89*	1.08	1.01
1	8	-11	2.67*	1.95	0.37
1	8	-12	2.26*	0.54	0.20
2	8	-12	2.13*	1.22	0.22
2	8	-11	3.46*	1.88	0.47
2	8	-10	3.36*	3.59	0.53
2	8	-9	3.27*	2.38	0.73
2	8	-8	1.30*	1.85	0.13
2	8	-7	4.26	4.09	0.92
2	8	-6	1.99*	0.21	0.25
2	8	-5	3.66*	1.12	1.06
2	8	-4	6.74	6.16	2.01
2	8	-3	1.88*	1.51	0.24
2	8	-2	7.98	7.46	2.53
2	8	-1	5.49	5.46	1.64
2	8	0	1.84*	0.07	0.30
2	8	1	6.97	7.54	2.10
2	8	2	10.37	11.02	2.35
2	8	3	3.71*	4.63	0.87

h	k	l	Fo	Fc	weight
2	8	4	8.70	9.27	2.22
2	8	5	4.75	3.57	1.30
2	8	6	1.96*	1.30	0.26
2	8	7	1.94*	1.71	0.27
2	8	8	2.15*	3.89	0.22
2	8	9	1.38*	2.21	0.10
2	8	10	1.42*	2.16	0.12
2	8	11	2.11*	1.29	0.23
3	8	11	2.09*	2.95	0.20
3	8	10	2.22*	0.64	0.20
3	8	9	1.47*	2.95	0.10
3	8	8	1.36*	1.54	0.10
3	8	7	1.62*	1.50	0.17
3	8	6	1.29*	2.69	0.10
3	8	5	2.04*	0.28	0.24
3	8	4	4.30	3.90	1.12
3	8	3	3.35*	3.98	0.66
3	8	2	2.66*	1.02	0.50
3	8	1	5.59	5.35	1.74
3	8	0	1.19*	0.18	0.15
3	8	-1	2.22*	3.24	0.44
3	8	-2	2.66*	0.04	0.73
3	8	-3	1.86*	2.10	0.29
3	8	-4	1.95*	0.24	0.26
3	8	-5	4.59	4.04	1.31
3	8	-6	1.25*	1.38	0.10
3	8	-7	1.87*	1.54	0.29
3	8	-8	2.19*	0.37	0.21
3	8	-9	1.64*	1.45	0.19
3	8	-10	2.08*	0.52	0.23
3	8	-11	3.61*	2.16	0.61
3	8	-12	2.28*	1.26	0.19
4	8	-12	2.20*	0.10	0.21
4	8	-11	2.17*	2.31	0.21
4	8	-10	2.22*	1.75	0.20
4	8	-9	2.86*	1.32	0.56
4	8	-8	2.08*	1.51	0.32
4	8	-7	3.41*	2.02	0.69
4	8	-6	3.09*	5.29	0.48
4	8	-5	5.59	5.62	1.54
4	8	-4	3.12	3.85	0.62
4	8	-3	3.54*	3.74	1.17
4	8	-2	1.91*	0.45	0.38
4	8	-1	3.08*	1.22	0.78
4	8	0	1.97*	2.83	0.27
4	8	1	2.98*	0.20	0.88
4	8	2	3.48*	2.82	0.76
4	8	3	2.03*	3.55	0.24
4	8	4	4.30*	3.49	0.81
4	8	5	1.83*	1.85	0.25
4	8	6	2.12*	2.52	0.22
4	8	7	2.14*	0.47	0.30
4	8	8	2.60*	2.95	0.42
4	8	9	2.10*	0.17	0.23
4	8	10	4.15*	3.02	0.77
5	8	9	2.23*	0.55	0.20
5	8	8	2.01*	1.08	0.22
5	8	7	2.06*	1.02	0.23

h	k	l	Fo	Fc	weight
5	8	6	1.35*	0.39	0.10
5	8	5	2.09*	2.62	0.23
5	8	4	2.16*	0.48	0.21
5	8	3	2.01*	1.01	0.25
5	8	2	3.44*	2.19	0.81
5	8	1	3.73*	2.40	0.86
5	8	0	2.90*	2.05	0.74
5	8	-1	1.51*	0.44	0.18
5	8	-2	1.74*	0.84	0.24
5	8	-3	1.75*	1.43	0.22
5	8	-4	3.53*	2.87	0.78
5	8	-5	2.02*	0.89	0.24
5	8	-6	2.11*	1.52	0.22
5	8	-7	2.61*	1.28	0.59
5	8	-8	0.94*	1.56	0.05
5	8	-9	1.92*	0.44	0.20
5	8	-10	2.11*	0.03	0.23
5	8	-11	2.25*	1.99	0.20
5	8	-12	3.89*	2.44	0.74
6	8	-12	1.05*	3.20	0.03
6	8	-11	3.82*	3.19	0.71
6	8	-10	4.77	4.17	0.85
6	8	-9	2.11*	1.01	0.22
6	8	-8	1.91*	1.64	0.20
6	8	-7	2.12*	2.34	0.22
6	8	-6	1.30*	0.76	0.13
6	8	-5	2.41*	0.49	0.46
6	8	-4	2.02*	1.59	0.25
6	8	-3	1.88*	0.72	0.28
6	8	-2	4.06	3.73	0.85
6	8	-1	2.19*	2.12	0.32
6	8	0	4.66	4.85	1.18
6	8	1	2.71*	2.20	0.58
6	8	2	2.04*	2.31	0.29
6	8	3	2.02*	1.08	0.25
6	8	4	2.05*	1.15	0.24
6	8	5	2.39*	2.51	0.30
6	8	6	3.25*	1.25	0.59
6	8	7	2.23*	1.12	0.20
6	8	8	2.52*	1.11	0.31
7	8	7	3.85*	2.35	0.75
7	8	6	2.18*	0.66	0.21
7	8	5	3.27*	1.37	0.68
7	8	4	0.97*	1.85	0.05
7	8	3	3.81*	1.28	0.85
7	8	2	1.99*	1.48	0.25
7	8	1	3.40	3.31	0.66
7	8	0	2.17*	2.92	0.21
7	8	-1	2.25*	2.11	0.39
7	8	-2	1.85*	1.35	0.21
7	8	-3	2.75*	0.02	0.52
7	8	-4	4.02*	3.29	0.82
7	8	-5	2.30*	1.64	0.30
7	8	-6	4.11*	4.78	0.71
7	8	-7	2.34*	0.33	0.47
7	8	-8	2.31*	3.90	0.19
7	8	-9	1.98*	1.62	0.15
7	8	-10	2.38*	3.74	0.18

h	k	l	Fo	Fc	weight 13
7	8	-11	2.93*	2.81	0.43
8	8	-10	3.71*	2.40	0.51
8	8	-9	2.19*	0.50	0.21
8	8	-8	4.83	4.57	0.76
8	8	-7	3.08*	2.23	0.34
8	8	-6	6.74	6.34	1.31
8	8	-5	3.02*	1.30	0.50
8	8	-4	3.55*	2.09	0.72
8	8	-3	2.88*	2.74	0.51
8	8	-2	2.83*	1.95	0.44
8	8	-1	1.95*	0.66	0.26
8	8	0	3.91*	2.87	0.96
8	8	1	2.44*	1.13	0.40
8	8	2	3.06*	1.57	0.52
8	8	3	3.67*	3.81	0.63
8	8	4	3.31*	0.41	0.53
8	8	5	2.87*	3.10	0.38
8	8	6	4.63*	3.27	0.75
8	8	7	2.35*	1.69	0.18
9	8	4	1.78*	1.28	0.15
9	8	3	2.48*	0.26	0.28
9	8	2	2.11*	0.02	0.22
9	8	1	3.42*	0.95	0.72
9	8	0	2.77*	3.33	0.34
9	8	-1	1.69*	3.20	0.12
9	8	-2	1.98*	1.88	0.26
9	8	-3	2.10*	1.85	0.24
9	8	-4	2.18*	1.65	0.21
9	8	-5	3.40*	1.97	0.80
9	8	-6	4.40	3.72	0.75
9	8	-7	3.17*	2.83	0.40
9	8	-8	1.76*	2.54	0.14
9	8	-9	2.39*	2.35	0.17
10	8	-8	2.46*	0.25	0.17
10	8	-7	4.59	3.70	0.73
10	8	-6	2.31*	0.50	0.19
10	8	-5	2.26*	0.42	0.20
10	8	-4	3.08*	3.07	0.37
10	8	-3	2.01*	3.02	0.18
10	8	-2	3.17*	3.29	0.34
10	8	-1	2.12*	0.58	0.22
10	8	0	2.26*	0.97	0.20
10	8	1	4.55	3.21	0.81
10	8	2	3.27*	3.50	0.38
10	8	3	2.31*	1.26	0.19
11	8	0	2.40*	1.81	0.17
11	8	-1	1.80*	0.33	0.13
11	8	-2	1.04*	1.32	0.05
11	8	-3	2.23*	2.21	0.20
11	8	-4	2.84*	0.49	0.40
11	8	-5	4.42*	3.90	0.65
11	8	-6	2.38*	1.52	0.18
9	9	-6	2.09*	0.29	0.14
9	9	-5	6.96	6.43	1.11
9	9	-4	2.17*	0.36	0.21
9	9	-3	2.72*	2.83	0.28
9	9	-2	2.40*	0.42	0.17
9	9	-1	3.09*	1.26	0.48

h	k	l	Fo	Fc	weight
9	9	0	2.31*	2.23	0.19
9	9	1	2.38*	0.23	0.18
8	9	3	3.18	2.58	0.38
8	9	2	2.29*	0.39	0.19
8	9	1	2.27*	0.96	0.19
8	9	0	2.46*	1.90	0.28
8	9	-1	2.24*	1.50	0.26
8	9	-2	2.00*	1.93	0.18
8	9	-3	1.73*	0.03	0.16
8	9	-4	3.76*	2.06	0.68
8	9	-5	2.02*	0.24	0.19
8	9	-6	2.04*	0.92	0.20
8	9	-7	2.92*	1.47	0.37
8	9	-8	3.47*	1.00	0.56
7	9	-9	2.96*	0.12	0.36
7	9	-8	2.91*	1.29	0.28
7	9	-7	4.05*	2.91	0.66
7	9	-6	6.04	5.55	1.14
7	9	-5	3.57*	4.46	0.47
7	9	-4	4.39*	4.56	0.75
7	9	-3	2.04*	2.94	0.24
7	9	-2	2.14*	1.22	0.22
7	9	-1	2.93*	1.24	0.43
7	9	0	3.53*	0.90	0.79
7	9	1	3.82*	2.45	0.75
7	9	2	3.86*	2.32	0.73
7	9	3	3.62	3.17	0.51
7	9	4	3.24*	4.06	0.38
7	9	5	3.60*	0.63	0.87
6	9	6	2.93*	1.38	0.40
6	9	5	3.05*	0.01	0.43
6	9	4	2.45*	2.48	0.25
6	9	3	0.98*	1.15	0.07
6	9	2	2.65*	2.19	0.37
6	9	1	2.06*	0.57	0.23
6	9	0	3.03*	0.30	0.61
6	9	-1	2.19*	1.53	0.19
6	9	-2	2.86*	1.45	0.52
6	9	-3	2.87*	0.15	0.48
6	9	-4	2.04*	0.19	0.24
6	9	-5	1.94*	1.74	0.17
6	9	-6	2.94*	0.87	0.49
6	9	-7	0.99*	0.28	0.04
6	9	-8	2.11*	1.03	0.22
6	9	-9	2.37*	0.22	0.18
5	9	-10	2.26*	1.12	0.20
5	9	-9	2.12*	1.89	0.22
5	9	-8	2.26*	2.16	0.20
5	9	-7	2.60*	1.84	0.34
5	9	-6	2.06*	1.74	0.23
5	9	-5	2.09*	2.63	0.23
5	9	-4	2.06*	0.65	0.24
5	9	-3	1.94*	0.58	0.26
5	9	-2	0.93*	1.31	0.07
5	9	-1	2.14*	2.18	0.22
5	9	0	0.94*	0.57	0.05
5	9	1	2.07*	2.71	0.23
5	9	2	0.95*	1.40	0.05

h	k	l	Fo	Fc	weight
5	9	3	3.33*	1.93	0.66
5	9	4	3.65*	2.97	0.64
5	9	5	2.08*	0.58	0.23
5	9	6	2.26*	1.79	0.22
5	9	7	2.73*	1.20	0.35
4	9	8	2.28*	2.19	0.19
4	9	7	2.03*	3.22	0.18
4	9	6	1.72*	1.70	0.12
4	9	5	2.57*	1.92	0.37
4	9	4	2.53*	2.82	0.41
4	9	3	0.94*	2.65	0.04
4	9	2	2.28*	1.51	0.33
4	9	1	3.20*	3.22	0.62
4	9	0	1.98*	1.14	0.25
4	9	-1	1.95*	1.22	0.26
4	9	-2	2.43*	0.52	0.42
4	9	-3	4.03*	3.08	0.91
4	9	-4	1.86*	1.35	0.24
4	9	-5	1.99*	0.24	0.25
4	9	-6	2.02*	1.12	0.24
4	9	-7	2.17*	0.95	0.38
4	9	-8	4.32	3.99	0.75
4	9	-9	3.19*	0.78	0.60
4	9	-10	4.26*	2.59	0.76
3	9	-10	2.18*	0.75	0.21
3	9	-9	2.17*	1.93	0.21
3	9	-8	3.81*	1.42	0.95
3	9	-7	0.96*	2.21	0.05
3	9	-6	2.03*	0.54	0.24
3	9	-5	1.93*	1.84	0.27
3	9	-4	4.18	3.69	0.92
3	9	-3	1.29*	0.30	0.10
3	9	-2	3.51*	1.20	0.83
3	9	-1	3.14*	2.98	0.65
3	9	0	1.99*	0.31	0.25
3	9	1	4.46	2.87	1.26
3	9	2	1.84*	1.34	0.23
3	9	3	3.88	3.88	0.83
3	9	4	3.26*	1.40	0.69
3	9	5	7.04	6.62	1.58
3	9	6	2.23*	0.88	0.20
3	9	7	5.14	4.48	1.04
3	9	8	2.23*	1.09	0.20
3	9	9	2.90*	2.06	0.31
2	9	9	1.46*	1.23	0.13
2	9	8	2.24*	2.72	0.20
2	9	7	3.11*	3.20	0.63
2	9	6	3.19*	2.23	0.71
2	9	5	2.05*	1.21	0.24
2	9	4	1.88*	0.31	0.28
2	9	3	1.59*	0.48	0.18
2	9	2	2.11*	1.92	0.22
2	9	1	2.85*	0.52	0.50
2	9	0	4.11*	3.71	0.99
2	9	-1	1.92*	0.80	0.27
2	9	-2	1.80*	0.23	0.26
2	9	-3	2.14*	3.48	0.22
2	9	-4	3.00	2.64	0.60

h	k	l	Fo	Fc	weight
2	9	-5	1.99*	1.69	0.25
2	9	-6	2.08*	3.27	0.23
2	9	-7	4.38	4.26	0.91
2	9	-8	0.98*	1.94	0.05
2	9	-9	4.79	4.01	0.90
2	9	-10	3.98*	2.05	0.54
1	9	-10	2.52*	0.81	0.31
1	9	-9	3.01*	2.36	0.47
1	9	-8	2.29*	2.38	0.19
1	9	-7	2.35*	2.89	0.17
1	9	-6	3.72	3.81	0.71
1	9	-5	1.60*	2.79	0.13
1	9	-4	3.42*	1.31	0.96
1	9	-3	2.05*	2.49	0.24
1	9	-2	3.35*	0.97	1.00
1	9	-1	2.52*	1.73	0.58
1	9	0	1.78*	2.74	0.20
1	9	1	2.36*	0.26	0.51
1	9	2	2.04*	2.88	0.24
1	9	3	2.87*	1.13	0.63
1	9	4	8.14	8.25	2.04
1	9	5	4.23	4.17	0.82
1	9	6	1.65*	2.71	0.18
1	9	7	3.89*	4.61	0.58
0	9	8	3.97*	0.09	0.69
0	9	9	4.53	2.75	0.95
0	9	10	3.46*	1.18	0.52
0	9	10	2.74*	1.96	0.35
0	9	9	2.47*	0.15	0.38
0	9	8	4.07*	3.76	0.83
0	9	7	3.20*	1.10	0.77
0	9	6	1.64*	2.68	0.12
0	9	5	1.94*	0.54	0.27
0	9	4	2.08*	1.88	0.23
0	9	3	2.02*	0.21	0.24
0	9	2	1.79*	2.32	0.23
0	9	1	4.08*	4.24	0.91
0	10	0	6.00	4.97	1.47
0	10	1	2.06*	0.16	0.23
0	10	2	2.89*	1.05	0.45
0	10	3	1.96*	0.15	0.26
0	10	4	2.53*	3.27	0.30
0	10	5	4.25	4.23	0.78
0	10	6	3.03*	2.79	0.38
0	10	7	7.35	6.25	1.51
0	10	8	2.35*	0.53	0.18
1	10	7	1.98*	0.48	0.25
1	10	6	1.43*	0.66	0.08
1	10	5	1.00*	0.35	0.05
1	10	4	3.94*	1.23	0.74
1	10	3	0.97*	0.38	0.05
1	10	2	0.97*	1.33	0.04
1	10	1	1.36*	1.16	0.11
1	10	0	1.98*	1.31	0.25
1	10	-1	2.01*	0.53	0.25
1	10	-2	1.84*	0.67	0.27
1	10	-3	1.84*	1.30	0.23
1	10	-4	2.10*	1.01	0.23

h	k	l	Fo	Fc	weight 14
1	10	-5	2.05*	1.52	0.24
1	10	-6	1.74*	1.00	0.12
1	10	-7	2.37*	0.62	0.18
1	10	-8	2.26*	1.88	0.20
2	10	-8	2.32*	2.54	0.19
2	10	-7	4.22*	2.27	0.89
2	10	-6	3.80*	1.13	0.77
2	10	-5	2.12*	0.24	0.22
2	10	-4	0.98*	0.73	0.06
2	10	-3	2.08*	1.05	0.23
2	10	-2	2.08*	0.74	0.23
2	10	-1	2.05*	1.03	0.24
2	10	0	2.06*	0.24	0.23
2	10	1	3.49*	0.17	0.81
2	10	2	1.91*	0.30	0.28
2	10	3	2.60*	2.82	0.39
2	10	4	2.15*	0.39	0.22
2	10	5	5.58	5.44	0.98
2	10	6	6.27	5.46	1.26
2	10	7	3.35	3.13	0.41
3	10	6	2.32*	0.71	0.22
3	10	5	2.27*	1.27	0.19
3	10	4	1.74*	1.45	0.13
3	10	3	1.72*	2.09	0.13
3	10	2	2.78*	2.38	0.52
3	10	1	2.76*	3.18	0.45
3	10	0	1.88*	1.08	0.28
3	10	-1	3.77*	3.55	0.64
3	10	-2	3.77*	1.27	0.64
3	10	-3	2.18*	2.11	0.21
3	10	-4	2.61*	1.65	0.38
3	10	-5	2.44*	0.93	0.31
3	10	-6	2.86*	0.02	0.26
3	10	-7	3.70*	2.08	0.66
3	10	-8	3.30*	0.11	0.42
4	10	-8	5.30	4.68	0.82
4	10	-7	2.13*	0.33	0.22
4	10	-6	2.25*	1.21	0.20
4	10	-5	2.11*	1.57	0.19
4	10	-4	2.82*	2.34	0.31
4	10	-3	2.42*	1.83	0.29
4	10	-2	0.99*	0.51	0.06
4	10	-1	2.18*	1.34	0.21
4	10	0	3.42*	1.30	0.63
4	10	1	2.17*	1.60	0.21
4	10	2	2.16*	0.63	0.21
4	10	3	2.02*	1.13	0.24
4	10	4	3.23*	1.23	0.64
4	10	5	2.06*	0.58	0.24
5	10	4	2.18*	2.22	0.21
5	10	3	1.78*	2.08	0.12
5	10	2	2.68*	0.13	0.37
5	10	1	2.23*	2.72	0.20
5	10	0	2.00*	1.94	0.17
5	10	-1	2.83*	2.24	0.40
5	10	-2	3.60*	2.94	0.61
5	10	-3	2.39*	2.36	0.26
5	10	-4	3.03*	0.65	0.55

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight 15
5	10	-5	1.76*	2.95	0.10																		
5	10	-6	2.20*	0.30	0.21																		
5	10	-7	2.55*	1.58	0.36																		
6	10	-6	1.81*	0.16	0.14																		
6	10	-5	2.31*	1.76	0.20																		
6	10	-4	3.69*	1.45	0.72																		
6	10	-3	2.21*	2.00	0.20																		
6	10	-2	2.25*	0.17	0.20																		
6	10	-1	2.32*	2.75	0.19																		
6	10	0	1.77*	1.02	0.14																		
6	10	1	2.32*	0.45	0.19																		
6	10	2	3.43*	1.50	0.57																		
6	10	3	2.66*	3.31	0.21																		
7	10	1	2.27*	0.70	0.19																		
7	10	0	2.76*	0.32	0.41																		
7	10	-1	2.32*	1.85	0.18																		
7	10	-2	1.80*	1.59	0.16																		
7	10	-3	3.29*	0.97	0.52																		
7	10	-4	2.09*	2.36	0.13																		
7	10	-5	3.40	3.23	0.38																		
4	11	-1	2.33*	0.17	0.18																		
4	11	-2	1.49*	1.55	0.07																		
3	11	-3	3.47*	0.57	0.56																		
3	11	-2	5.47	4.66	0.91																		
3	11	-1	2.33*	1.33	0.22																		
3	11	0	6.06	5.18	1.11																		
3	11	1	2.22*	1.70	0.20																		
3	11	2	4.20*	3.65	0.62																		
2	11	3	3.32*	2.13	0.41																		
2	11	2	3.45*	1.03	0.46																		
2	11	1	2.07*	0.33	0.23																		
2	11	0	2.34*	0.94	0.18																		
2	11	-1	2.31*	0.27	0.21																		
2	11	-2	2.31*	0.39	0.24																		
2	11	-3	2.08*	0.01	0.21																		
2	11	-4	1.05*	0.34	0.04																		
1	11	-4	1.48*	0.89	0.09																		
1	11	-3	2.41*	1.65	0.17																		
1	11	-2	3.33	2.65	0.42																		
1	11	-1	3.85*	1.36	0.76																		
1	11	0	3.25*	0.49	0.70																		
1	11	1	2.73*	3.73	0.22																		
1	11	2	2.22*	0.67	0.20																		
1	11	3	3.80*	4.23	0.35																		
1	11	4	2.21*	2.97	0.21																		
0	11	4	2.21*	1.37	0.20																		
0	11	3	2.54*	1.26	0.33																		
0	11	2	2.92*	1.41	0.43																		
0	11	1	2.22*	0.21	0.20																		

3297 reflections

1,2,3,5,6,8-hexamethyl-4-mesyl-7-hydroxy-tetracyclo[4.2.1.1.^{2,5} 0^{3,7}]decane

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	1
-11	5	1	3.64	3.64	4.27	-11	0	2	7.17	7.25	3.70	-10	4	5	4.43	4.70	4.14	-9	8	3	9.85	9.66	3.21	
-11	5	2	5.19	5.02	4.02	-10	0	2	11.64	11.86	2.86	-10	4	6	3.46	3.61	4.30	-9	8	2	4.87	4.50	4.07	
-11	5	3	6.01	5.45	3.89	-10	0	4	8.69	8.40	3.43	-10	4	7	5.01	5.86	4.05	-9	8	1	8.43	8.73	3.48	
-11	5	4	4.05	3.82	4.20	-10	0	6	4.97	5.31	4.06	-10	4	8	1.75*	0.12	4.61	-9	7	1	8.15	7.77	3.53	
-11	5	5	1.97*	1.22	4.57	-10	0	8	4.70	4.49	4.10	-10	4	9	1.96*	0.24	4.57	-9	7	2	5.81	5.70	3.92	
-11	5	6	2.46*	2.33	4.48	-10	0	10	8.75	7.60	3.42	-10	4	10	8.02	7.40	3.55	-9	7	3	9.22	9.80	3.33	
-11	5	7	1.21*	1.24	4.73	-10	0	12	5.96	6.06	3.90	-10	4	11	1.54*	1.10	4.66	-9	7	4	1.79*	2.30	4.61	
-11	5	8	2.51*	0.33	4.47	-10	0	14	7.15	6.17	3.70	-10	4	12	3.01	2.66	4.38	-9	7	5	8.79	8.39	3.41	
-11	4	10	6.30	4.63	4.01	-10	0	16	5.01	5.22	4.05	-10	4	13	1.24*	1.83	4.72	-9	7	6	2.39*	2.20	4.49	
-11	4	9	1.26*	1.15	4.72	-10	1	15	1.24*	0.87	4.72	-10	4	14	4.79	4.43	4.09	-9	7	7	1.39*	0.64	4.69	
-11	4	8	12.56	11.97	2.67	-10	1	14	1.24*	1.15	4.72	-10	5	13	7.79	7.27	3.59	-9	7	8	8.34	8.58	3.50	
-11	4	7	3.84	3.66	4.24	-10	1	13	2.73	1.85	4.43	-10	5	12	3.62	3.12	4.27	-9	7	9	2.62*	1.90	4.45	
-11	4	6	2.28*	2.90	4.51	-10	1	12	2.80	2.66	4.41	-10	5	11	2.36*	1.66	4.49	-9	7	10	4.98	4.42	4.06	
-11	4	5	2.19*	1.04	4.53	-10	1	11	2.55	2.74	4.46	-10	5	10	6.59	6.94	3.80	-9	7	11	1.21*	0.07	4.73	
-11	4	4	6.98	5.52	3.90	-10	1	10	0.83*	0.04	4.82	-10	5	9	2.03*	1.98	4.56	-9	7	12	5.28	5.41	4.01	
-11	4	3	1.19*	0.03	4.73	-10	1	9	5.48	5.25	3.98	-10	5	8	0.86*	1.11	4.81	-9	7	13	1.26*	0.50	4.72	
-11	4	2	3.95	3.57	4.22	-10	1	8	3.37	3.18	4.32	-10	5	7	2.77	2.27	4.42	-9	6	14	1.26*	2.55	4.72	
-11	4	1	9.85	9.67	3.21	-10	1	7	5.50	5.85	3.97	-10	5	6	4.87	4.22	4.07	-9	6	13	2.71	2.95	4.43	
-11	3	1	1.18*	1.83	4.73	-10	1	6	2.61	2.90	4.45	-10	5	5	7.60	7.30	3.63	-9	6	12	1.21*	1.55	4.73	
-11	3	2	5.16	5.08	4.03	-10	1	5	8.67	9.25	3.44	-10	5	4	8.81	9.15	3.41	-9	6	11	4.00	3.39	4.21	
-11	3	3	2.38*	1.07	4.49	-10	1	4	2.79	2.57	4.42	-10	5	3	7.72	7.93	3.61	-9	6	10	5.87	5.51	3.81	
-11	3	4	3.32	2.68	4.32	-10	1	3	9.50	9.72	3.28	-10	5	2	4.15	3.91	4.19	-9	6	9	1.13*	0.81	4.75	
-11	3	5	1.85*	1.59	4.59	-10	1	2	0.66*	1.97	4.86	-10	5	1	7.42	6.43	3.66	-9	6	8	0.68*	2.24	4.85	
-11	3	6	4.57	3.91	4.12	-10	1	1	9.87	9.81	3.19	-10	6	1	1.72*	0.57	4.62	-9	6	7	6.89	6.97	3.73	
-11	3	7	3.03	3.23	4.37	-10	2	1	3.41	3.24	4.31	-10	6	2	4.27	4.03	4.17	-9	6	6	0.67*	1.96	4.85	
-11	3	8	1.15*	0.03	4.74	-10	2	2	1.40*	0.24	4.69	-10	6	3	2.40*	0.35	4.49	-9	6	5	2.43*	3.42	4.48	
-11	3	9	1.02*	1.11	4.77	-10	2	3	2.42	2.39	4.48	-10	6	4	1.58*	0.15	4.65	-9	6	4	0.88*	0.22	4.80	
-11	3	10	8.52	7.98	3.46	-10	2	4	1.09*	0.31	4.75	-10	6	5	4.57	4.75	4.12	-9	6	3	6.38	6.06	3.83	
-11	3	11	4.55	3.93	4.12	-10	2	5	0.89*	0.22	4.78	-10	6	6	6.17	5.81	3.87	-9	6	2	2.34*	1.47	4.50	
-11	2	12	1.99*	0.84	4.57	-10	2	6	9.20	9.13	3.34	-10	6	7	1.29*	1.01	4.71	-9	6	1	8.16	8.42	3.53	
-11	2	11	2.45*	2.29	4.48	-10	2	7	2.77	3.07	4.42	-10	6	8	1.20*	1.56	4.73	-9	5	1	14.75	14.47	2.24	
-11	2	10	2.04*	2.20	4.55	-10	2	8	2.65	3.31	4.44	-10	6	9	0.96*	1.18	4.79	-9	5	2	10.55	11.20	3.08	
-11	2	9	9.39	8.85	3.30	-10	2	9	0.75*	1.87	4.83	-10	6	10	1.27*	2.04	4.71	-9	5	3	7.58	7.63	3.63	
-11	2	8	4.17	3.79	4.18	-10	2	10	2.14	2.78	4.54	-10	6	11	3.57	3.47	4.28	-9	5	4	1.69*	2.63	4.63	
-11	2	7	4.13	4.34	4.19	-10	2	11	3.40	3.51	4.31	-10	7	9	3.58	2.99	4.28	-9	5	5	2.62	2.04	4.45	
-11	2	6	1.14*	0.16	4.74	-10	2	12	6.93	7.30	3.74	-10	7	8	1.25*	2.09	4.72	-9	5	6	2.24*	1.90	4.52	
-11	2	5	4.83	4.64	4.08	-10	2	13	1.16*	0.76	4.74	-10	7	7	2.48*	2.64	4.47	-9	5	7	1.51*	0.28	4.66	
-11	2	4	1.18*	0.68	4.73	-10	2	14	2.42*	2.84	4.48	-10	7	6	1.93*	0.19	4.58	-9	5	8	7.34	7.73	3.67	
-11	2	3	1.14*	0.20	4.74	-10	2	15	1.72*	2.31	4.62	-10	7	5	2.35	2.48	4.50	-9	5	9	8.22	7.77	3.52	
-11	2	2	9.80	9.50	3.22	-10	3	15	2.10*	1.45	4.54	-10	7	4	4.96	4.93	4.06	-9	5	10	3.82	2.92	4.24	
-11	2	1	4.98	4.62	4.05	-10	3	14	3.12	2.40	4.36	-10	7	3	5.44	5.29	3.98	-9	5	11	0.84*	1.52	4.81	
-11	1	1	5.11	5.20	4.04	-10	3	13	2.56*	2.30	4.46	-10	7	2	4.04	3.78	4.21	-9	5	12	1.10*	2.80	4.75	
-11	1	2	2.61	1.76	4.45	-10	3	12	6.79	6.65	3.76	-10	7	1	3.31	2.76	4.33	-9	5	13	1.21*	1.61	4.73	
-11	1	3	12.70	12.16	2.64	-10	3	11	4.01	3.02	4.21	-9	9	1	5.52	6.26	3.97	-9	5	14	2.13*	1.26	4.54	
-11	1	4	1.13*	0.14	4.75	-10	3	10	4.48	4.36	4.13	-9	9	2	7.33	7.39	3.67	-9	5	15	5.95	5.54	3.90	
-11	1	5	5.11	5.10	4.04	-10	3	9	5.25	5.54	4.01	-9	9	3	7.72	7.59	3.60	-9	4	16	5.62	4.78	3.95	
-11	1	6	3.09	2.82	4.36	-10	3	8	0.76*	0.96	4.83	-9	9	4	4.69	4.92	4.10	-9	4	15	5.52	5.23	3.97	
-11	1	7	9.04	8.52	3.37	-10	3	7	1.12*	0.98	4.75	-9	9	5	2.48	2.20	4.47	-9	4	14	4.61	4.02	4.11	
-11	1	8	1.06*	1.04	4.76	-10	3	6	4.82	4.49	4.08	-9	9	6	0.74*	1.43	4.84	-9	4	13	3.65	4.15	4.27	
-11	1	9	3.08	3.58	4.36	-10	3	5	2.87	2.50	4.40	-9	9	7	1.26*	1.12	4.72	-9	4	12	4.87	4.72	4.07	
-11	1	10	1.16*	0.22	4.74	-10	3	4	2.18*	1.47	4.53	-9	8	11	6.38	5.48	3.83	-9	4	11	5.97	5.46	3.90	
-11	1	11	8.76	8.36	3.42	-10	3	3	5.77	5.56	3.93	-9	8	10	5.28	4.90	4.01	-9	4	10	2.17*	1.14	4.53	
-11	1	12	1.27*	2.01	4.71	-10	3	2	1.53*	1.07	4.66	-9	8	9	3.35	3.51	4.32	-9	4	9	1.43*	2.07	4.68	
-11	0	12	4.36	3.73	4.15	-10	3	1	6.65	6.45	3.79	-9	8	8	2.55*	1.68	4.46	-9	4	8	3.81	3.25	4.24	
-11	0	10	4.31	4.30	4.16	-10	4	1	2.61	2.57	4.45	-9	8	7	5.47	5.31	3.98	-9	4	7	5.56	5.52	3.96	
-11	0	8	1.06*	0.70	4.76	-10	4	2	1.22*	0.92	4.72	-9	8	6	1.88	1.66	4.59	-9	4	6	7.96	7.50	3.56	
-11	0	6	2.47*	2.38	4.47	-10	4	3	5.96	6.24	3.90	-9	8	5	7.20	6.82	3.69	-9	4	5	10.67	11.44	3.05	
-11	0	4	1.60*	1.33	4.64	-10	4	4	6.89	6.76	3.75	-9	8	4	1.18*	2.62	4.74	-9	4	4	3.60	3.38	4.28	

h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	h	k	l	Fo	Fc	weight	2
-9	4	3	10.58	10.68	3.07	-9	0	10	4.93	5.53	4.06	-8	3	12	4.19	3.48	4.18	-8	6	12	1.15*	0.50	4.74	
-9	4	2	5.97	5.50	3.90	-9	0	8	7.11	5.77	3.71	-8	3	11	2.34*	2.15	4.50	-8	6	13	6.67	5.91	3.78	
-9	4	1	5.30	5.47	4.01	-9	0	6	12.90	14.01	2.60	-8	3	10	2.68	2.75	4.44	-8	6	14	1.21*	0.10	4.73	
-9	3	1	9.14	9.25	3.35	-9	0	4	7.17	6.71	3.70	-8	3	9	6.00	6.10	3.89	-8	6	15	2.13*	2.38	4.54	
-9	3	2	4.55	5.08	4.12	-9	0	2	17.31	17.06	1.77	-8	3	8	3.01	2.70	4.38	-8	6	16	1.37*	1.40	4.69	
-9	3	3	4.13	4.15	4.19	-8	0	2	16.74	17.42	1.87	-8	3	7	13.14	13.42	2.56	-8	7	15	1.61*	1.17	4.64	
-9	3	4	1.76*	2.04	4.61	-8	0	4	19.44	20.73	1.45	-8	3	6	6.81	6.69	3.76	-8	7	14	8.12	7.46	3.53	
-9	3	5	3.74	3.71	4.25	-8	0	6	4.85	4.28	4.08	-8	3	5	11.91	12.36	2.81	-8	7	13	1.23*	0.49	4.72	
-9	3	6	3.49	2.69	4.30	-8	0	8	22.04	23.08	1.12	-8	3	4	2.84	3.48	4.41	-8	7	12	2.85	3.15	4.41	
-9	3	7	8.70	9.58	3.43	-8	0	10	1.59*	3.96	4.65	-8	3	3	12.16	12.24	2.76	-8	7	11	1.81*	0.07	4.60	
-9	3	8	3.21	3.14	4.34	-8	0	12	3.72	3.76	4.26	-8	3	2	3.09	2.48	4.36	-8	7	10	7.67	7.55	3.61	
-9	3	9	5.83	5.50	3.92	-8	0	14	2.16*	0.43	4.53	-8	3	1	11.13	11.74	2.96	-8	7	9	1.39*	2.19	4.69	
-9	3	10	4.81	4.73	4.08	-8	0	16	1.15*	1.08	4.74	-8	4	1	13.64	13.88	2.46	-8	7	8	1.05*	1.48	4.76	
-9	3	11	2.29*	1.35	4.51	-8	0	18	2.64	2.80	4.44	-8	4	2	13.00	13.09	2.58	-8	7	7	3.51	3.30	4.29	
-9	3	12	1.15*	1.88	4.74	-8	1	19	2.27*	2.17	4.51	-8	4	3	16.46	17.12	1.92	-8	7	6	12.58	12.28	2.67	
-9	3	13	2.21*	0.94	4.52	-8	1	18	2.09*	0.83	4.55	-8	4	4	9.27	8.51	3.32	-8	7	5	4.20	4.03	4.18	
-9	3	14	4.09	3.38	4.20	-8	1	17	8.00	7.38	3.56	-8	4	5	5.84	6.18	3.82	-8	7	4	2.13*	1.18	4.54	
-9	3	15	2.38*	2.20	4.49	-8	1	16	1.16*	0.18	4.74	-8	4	6	0.42*	0.08	4.92	-8	7	3	3.55	3.16	4.29	
-9	3	16	1.40*	1.41	4.69	-8	1	15	2.29*	2.15	4.51	-8	4	7	3.62	3.64	4.27	-8	7	2	0.80*	1.81	4.82	
-9	3	17	0.37*	1.88	4.93	-8	1	14	6.27	6.17	3.85	-8	4	8	1.22*	1.92	4.73	-8	7	1	10.08	10.03	3.17	
-9	2	17	2.51*	1.83	4.47	-8	1	13	11.09	11.29	2.97	-8	4	9	6.03	5.62	3.89	-8	8	1	18.60	18.40	1.57	
-9	2	16	2.09	1.50	4.55	-8	1	12	6.73	7.28	3.77	-8	4	10	2.26*	0.52	4.51	-8	8	2	2.64*	3.35	4.44	
-9	2	15	1.22*	1.55	4.73	-8	1	11	5.21	4.24	4.02	-8	4	11	3.98	4.30	4.22	-8	8	3	6.33	6.10	3.84	
-9	2	14	6.52	6.58	3.81	-8	1	10	1.04*	1.86	4.77	-8	4	12	1.45*	2.21	4.67	-8	8	4	2.11*	0.32	4.54	
-9	2	13	4.82	4.41	4.08	-8	1	9	1.03*	1.93	4.77	-8	4	13	6.14	5.26	3.87	-8	8	5	8.84	8.88	3.41	
-9	2	12	1.76*	0.72	4.61	-8	1	8	1.05*	1.50	4.76	-8	4	14	4.73	4.49	4.10	-8	8	6	1.80*	0.68	4.60	
-9	2	11	1.11*	0.22	4.75	-8	1	7	18.80	19.00	1.54	-8	4	15	6.24	6.03	3.85	-8	8	7	3.18	3.20	4.35	
-9	2	10	12.32	12.36	2.72	-8	1	6	10.50	11.15	3.08	-8	4	16	1.27*	1.83	4.71	-8	8	8	4.33	3.79	4.16	
-9	2	9	1.10*	1.91	4.75	-8	1	5	4.89	5.40	4.07	-8	4	17	2.55*	2.28	4.46	-8	8	9	8.81	7.82	3.41	
-9	2	8	1.05*	0.35	4.76	-8	1	4	2.11*	2.00	4.54	-8	4	18	1.22*	0.81	4.73	-8	8	10	3.63	3.37	4.27	
-9	2	7	3.85	4.06	4.24	-8	1	3	26.55	27.34	0.72	-8	5	17	2.61	2.20	4.45	-8	8	11	4.57	5.11	4.12	
-9	2	6	1.04*	1.47	4.77	-8	1	2	2.38	2.70	4.48	-8	5	16	2.75	3.35	4.42	-8	8	12	3.39	3.12	4.31	
-9	2	5	5.28	5.92	4.01	-8	1	1	10.42	10.75	3.10	-8	5	15	1.83*	1.27	4.60	-8	8	13	1.37*	0.60	4.69	
-9	2	4	9.00	8.87	3.37	-8	2	1	3.96	3.59	4.22	-8	5	14	1.86*	1.51	4.59	-8	9	11	2.84	2.50	4.46	
-9	2	3	2.10*	1.50	4.54	-8	2	2	9.31	9.62	3.32	-8	5	13	7.60	7.22	3.63	-8	9	10	0.96*	2.03	4.78	
-9	2	2	1.57*	2.68	4.65	-8	2	3	6.02	5.85	3.89	-8	5	12	2.71	3.93	4.43	-8	9	9	1.23*	1.42	4.72	
-9	2	1	2.84	3.00	4.41	-8	2	4	7.60	7.33	3.63	-8	5	11	1.90*	1.58	4.58	-8	9	8	2.23*	0.41	4.52	
-9	1	1	16.50	16.87	1.91	-8	2	5	9.92	10.30	3.20	-8	5	10	10.99	10.94	2.99	-8	9	7	5.06	5.05	4.04	
-9	1	2	1.56*	1.44	4.65	-8	2	6	1.38*	1.35	4.69	-8	5	9	4.48	4.87	4.14	-8	9	6	1.50*	0.33	4.67	
-9	1	3	15.52	16.69	2.09	-8	2	7	11.73	12.64	2.84	-8	5	8	1.07*	0.48	4.76	-8	9	5	2.34	1.43	4.50	
-9	1	4	1.75*	1.41	4.61	-8	2	8	6.24	6.06	3.85	-8	5	7	4.65	4.55	4.11	-8	9	4	1.18*	0.41	4.74	
-9	1	5	12.84	13.11	2.62	-8	2	9	2.13	1.71	4.54	-8	5	6	15.41	15.90	2.11	-8	9	3	6.58	7.00	3.80	
-9	1	6	1.03*	0.52	4.77	-8	2	10	6.65	8.61	3.78	-8	5	5	8.60	8.84	3.45	-8	9	2	7.22	7.03	3.69	
-9	1	7	1.04*	1.80	4.77	-8	2	11	1.10*	2.21	4.75	-8	5	4	6.02	5.96	3.89	-8	9	1	0.88*	1.50	4.80	
-9	1	8	4.05	4.48	4.21	-8	2	12	16.06	15.97	1.99	-8	5	3	5.55	5.06	3.96	-8	10	1	5.00	4.87	4.05	
-9	1	9	12.31	12.55	2.72	-8	2	13	1.61*	0.20	4.64	-8	5	2	1.87	2.38	4.59	-8	10	2	0.36*	1.06	4.93	
-9	1	10	6.74	6.39	3.77	-8	2	14	1.14*	2.31	4.74	-8	5	1	7.93	7.88	3.57	-8	10	3	7.13	7.15	3.71	
-9	1	11	1.10*	0.90	4.75	-8	2	15	1.16*	1.04	4.74	-8	6	1	9.43	9.11	3.29	-8	10	4	1.25*	0.04	4.72	
-9	1	12	6.54	6.37	3.81	-8	2	16	3.78	3.51	4.25	-8	6	2	1.93	2.48	4.58	-8	10	5	11.49	11.19	2.89	
-9	1	13	5.43	4.72	3.98	-8	2	17	0.35*	1.63	4.94	-8	6	3	8.60	8.29	3.45	-8	10	6	1.23*	1.33	4.72	
-9	1	14	1.17*	1.68	4.74	-8	2	18	3.59	3.48	4.28	-8	6	4	6.56	6.65	3.80	-8	10	7	1.52*	2.01	4.66	
-9	1	15	7.39	7.74	3.66	-8	2	19	6.28	6.61	3.85	-8	6	5	15.59	15.54	2.08	-8	10	8	2.53	2.65	4.46	
-9	1	16	3.85	3.64	4.24	-8	3	18	1.24*	1.00	4.72	-8	6	6	2.55	2.59	4.46	-7	11	1	1.26*	1.01	4.72	
-9	1	17	3.13	2.45	4.36	-8	3	17	8.81	9.16	3.22	-8	6	7	1.50*	0.15	4.66	-7	11	2	10.54	10.86	3.08	
-9	0	18	1.05*	0.35	4.76	-8	3	16	1.17*	0.11	4.74	-8	6	8	1.11*	0.08	4.75	-7	11	3	1.26*	0.83	4.72	
-9	0	16	5.93	4.45	3.90	-8	3	15	3.63	4.09	4.27	-8	6	9	1.76	2.98	4.61	-7	11	4	7.69	7.78	3.61	
-9	0	14	2.62*	3.17	4.45	-8	3	14	2.15*	2.25	4.53	-8	6	10	1.72*	1.24	4.62	-7	11	5	7.23	6.96	3.69	
-9	0	12	12.22	10.78	2.74	-8	3	13	4.59	4.35	4.12	-8	6	11	8.45	8.97	3.29	-7	11	6	8.90	8.60	3.91	

h	k	l	Fo	Fc	weight
-7	11	7	4.85	4.67	4.08
-7	11	8	7.46	7.23	3.65
-7	10	11	6.83	6.43	3.76
-7	10	10	2.09*	0.11	4.54
-7	10	9	2.23	2.04	4.52
-7	10	8	3.99	4.20	4.21
-7	10	7	3.29	3.64	4.33
-7	10	6	8.20	8.23	3.52
-7	10	5	3.09	3.21	4.36
-7	10	4	3.80	3.38	4.24
-7	10	3	7.30	7.05	3.68
-7	10	2	1.19*	1.91	4.73
-7	10	1	2.72	2.44	4.43
-7	9	1	6.74	6.24	3.94
-7	9	2	2.65	2.99	4.44
-7	9	3	1.18*	2.89	4.74
-7	9	4	3.79	3.59	4.25
-7	9	5	6.10	6.28	3.88
-7	9	6	7.39	7.48	3.66
-7	9	7	2.12*	2.30	4.54
-7	9	8	4.84	4.80	4.08
-7	9	9	5.03	4.74	4.05
-7	9	10	2.60*	3.59	4.45
-7	9	11	1.91*	1.91	4.58
-7	9	12	2.68	2.73	4.43
-7	9	13	2.62*	1.83	4.45
-7	8	15	1.98*	0.59	4.57
-7	8	14	2.73	1.86	4.43
-7	8	13	8.05	7.96	3.55
-7	8	12	0.78*	1.18	4.83
-7	8	11	5.56	4.88	3.96
-7	8	10	1.15*	0.28	4.74
-7	8	9	6.73	6.63	3.77
-7	8	8	1.36*	0.58	4.69
-7	8	7	8.78	8.23	3.42
-7	8	6	1.12*	1.80	4.75
-7	8	5	6.34	6.63	3.84
-7	8	4	0.91*	1.30	4.80
-7	8	3	13.12	13.92	2.56
-7	8	2	3.41	3.08	4.31
-7	8	1	2.63	2.35	4.44
-7	7	1	0.53*	1.53	4.89
-7	7	2	5.48	5.62	3.98
-7	7	3	9.45	8.76	3.29
-7	7	4	4.91	4.61	4.07
-7	7	5	1.83*	1.16	4.60
-7	7	6	4.23	4.46	4.18
-7	7	7	1.86*	2.73	4.58
-7	7	8	12.40	12.05	2.71
-7	7	9	1.76*	2.42	4.61
-7	7	10	5.57	5.68	3.96
-7	7	11	6.51	6.03	3.81
-7	7	12	6.44	5.78	3.82
-7	7	13	1.23*	1.34	4.72
-7	7	14	5.38	5.73	3.99
-7	7	15	0.62*	0.44	4.87
-7	7	16	2.03*	0.18	4.56
-7	6	17	6.26	5.61	3.85
-7	6	16	2.61*	1.93	4.45
-7	6	15	5.65	5.91	3.95
-7	6	14	1.17*	1.17	4.74
-7	6	13	6.72	6.78	3.78
-7	6	12	1.11*	0.27	4.75
-7	6	11	4.12	2.82	4.19
-7	6	10	7.66	7.60	3.62
-7	6	9	24.84	25.34	0.85
-7	6	8	0.87*	0.10	4.81
-7	6	7	1.07*	0.50	4.76
-7	6	6	5.12	5.34	4.03
-7	6	5	18.72	18.94	1.55
-7	6	4	5.71	5.46	3.78
-7	6	3	17.74	18.27	1.70
-7	6	2	7.95	8.34	3.56
-7	6	1	19.09	18.54	1.50
-7	5	0	10.01	10.44	3.18
-7	5	2	8.96	9.46	3.38
-7	5	3	24.84	25.70	0.85
-7	5	4	21.12	21.65	1.23
-7	5	5	2.28*	3.00	4.51
-7	5	6	4.81	4.57	4.08
-7	5	7	19.06	19.90	1.50
-7	5	8	12.58	11.68	2.67
-7	5	9	3.66	3.97	4.27
-7	5	10	3.02	4.09	4.38
-7	5	11	3.13	3.98	4.36
-7	5	12	5.85	5.18	3.82
-7	5	13	1.55*	0.51	4.65
-7	5	14	3.55	4.01	4.29
-7	5	15	5.85	5.41	3.82
-7	5	16	3.15	3.10	4.35
-7	5	17	4.56	3.75	4.12
-7	5	18	1.86*	0.16	4.59
-7	4	19	4.17	3.67	4.19
-7	4	18	5.84	5.66	3.92
-7	4	17	1.15*	0.24	4.74
-7	4	16	2.56	2.73	4.46
-7	4	15	1.66*	0.29	4.63
-7	4	14	1.58*	1.62	4.65
-7	4	13	5.58	5.84	3.96
-7	4	12	4.53	4.18	4.13
-7	4	11	2.93	2.06	4.39
-7	4	10	19.18	18.48	1.48
-7	4	9	6.19	6.44	3.86
-7	4	8	19.65	19.80	1.42
-7	4	7	3.81	4.34	4.24
-7	4	6	7.52	7.83	3.64
-7	4	5	5.77	6.25	3.93
-7	4	4	17.37	17.26	1.77
-7	4	3	7.20	7.40	3.70
-7	4	2	21.00	21.44	1.24
-7	4	1	6.97	7.43	3.73
-7	3	1	14.84	15.41	2.22
-7	3	2	6.96	7.09	3.73
-7	3	3	2.13	1.48	4.54
-7	3	4	11.43	11.75	2.90
-7	3	5	15.08	15.41	2.18
-7	3	6	14.22	14.95	2.34
-7	3	7	8.70	8.12	3.43
-7	3	8	18.91	19.09	1.52
-7	3	9	3.33	3.09	4.32
-7	3	10	4.82	5.08	4.08
-7	3	11	1.49*	0.50	4.67
-7	3	12	2.25*	2.95	4.51
-7	3	13	1.16*	2.92	4.74
-7	3	14	0.45*	0.95	4.91
-7	3	15	4.70	4.29	4.10
-7	3	16	1.11*	1.25	4.75
-7	3	17	1.50*	0.93	4.66
-7	3	18	1.87*	0.90	4.59
-7	3	19	6.67	5.84	3.78
-7	2	20	3.02	2.58	4.38
-7	2	19	3.35	3.13	4.32
-7	2	18	1.40*	2.11	4.69
-7	2	17	1.16*	2.34	4.74
-7	2	16	2.55	3.07	4.46
-7	2	15	2.28*	0.64	4.51
-7	2	14	8.12	7.65	3.53
-7	2	13	7.45	6.83	3.65
-7	2	12	12.57	13.88	2.67
-7	2	11	0.29*	2.68	4.95
-7	2	10	17.51	17.14	1.74
-7	2	9	1.59*	1.40	4.65
-7	2	8	18.00	19.88	1.66
-7	2	7	0.97*	1.10	4.78
-7	2	6	11.67	11.04	2.85
-7	2	5	6.04	5.33	3.88
-7	2	4	12.02	11.52	2.78
-7	2	3	4.44	4.83	4.14
-7	2	2	9.37	9.63	3.31
-7	2	1	11.42	11.81	2.90
-7	1	1	26.98	28.01	0.69
-7	1	2	9.82	10.51	3.22
-7	1	3	13.27	13.76	2.53
-7	1	4	1.92*	2.87	4.58
-7	1	5	16.55	17.01	1.90
-7	1	6	6.91	7.58	3.74
-7	1	7	26.14	26.95	0.75
-7	1	8	5.24	5.32	4.01
-7	1	9	9.20	8.18	3.34
-7	1	10	11.22	12.04	2.94
-7	1	11	17.98	17.96	1.66
-7	1	12	14.60	14.78	2.27
-7	1	13	2.25*	0.88	4.51
-7	1	14	3.73	4.01	4.26
-7	1	15	10.59	9.82	3.07
-7	1	16	1.08*	0.09	4.76
-7	1	17	3.26	3.68	4.33
-7	1	18	4.57	4.47	4.12
-7	1	19	0.71*	0.55	4.84
-7	1	20	2.48*	2.32	4.47
-7	0	20	1.24*	1.74	4.72
-7	0	18	1.16*	1.39	4.74
-7	0	16	4.63	4.48	4.11
-7	0	14	5.37	6.00	3.89
-7	0	12	3.94	3.14	4.22
-7	0	10	10.17	9.44	3.15
-7	0	8	23.95	25.27	0.93
-7	0	6	22.79	22.42	1.04
-7	0	4	13.84	14.64	2.42
-7	0	2	18.37	17.59	1.60
-6	0	2	6.69	7.16	3.78
-6	0	4	16.16	17.53	1.97
-6	0	6	31.22	32.08	0.47
-6	0	8	7.88	6.86	3.58
-6	0	10	10.94	11.31	3.00
-6	0	12	36.54	38.40	0.30
-6	0	14	6.82	6.75	3.76
-6	0	16	8.46	8.17	3.47
-6	0	18	0.95*	0.11	4.79
-6	0	20	7.96	7.75	3.56
-6	1	21	4.33	3.10	4.16
-6	1	20	5.06	4.42	4.04
-6	1	19	4.93	4.58	4.06
-6	1	18	4.16	3.71	4.19
-6	1	17	5.67	4.84	3.95
-6	1	16	2.87	2.87	4.40
-6	1	15	2.22*	3.05	4.52
-6	1	14	12.66	13.20	2.65
-6	1	13	13.91	13.64	2.40
-6	1	12	9.03	9.31	3.37
-6	1	11	2.66	3.71	4.44
-6	1	10	13.59	14.26	2.47
-6	1	9	22.78	23.30	1.04
-6	1	8	5.94	6.29	3.90
-6	1	7	5.15	5.22	4.03
-6	1	6	2.80	2.43	4.41
-6	1	5	33.88	34.44	0.38
-6	1	4	8.63	8.83	3.44
-6	1	3	4.28	4.33	4.17
-6	1	2	5.66	5.01	3.95
-6	1	1	18.18	17.82	1.63
-6	2	1	7.01	7.32	3.73
-6	2	2	20.00	19.76	1.37
-6	2	3	1.09*	0.20	4.76
-6	2	4	26.53	27.52	0.72
-6	2	5	8.35	8.26	3.49
-6	2	6	22.68	23.17	1.05
-6	2	7	1.94*	2.21	4.57
-6	2	8	1.57*	0.85	4.65
-6	2	9	16.50	17.06	1.91
-6	2	10	22.28	23.80	1.09
-6	2	11	16.78	16.68	1.87
-6	2	12	14.64	15.03	2.26
-6	2	13	6.87	7.46	3.75
-6	2	14	10.55	11.02	3.08
-6	2	15	7.23	6.95	3.69
-6	2	16	5.66	5.36	3.95
-6	2	17	1.36*	0.08	4.69
-6	2	18	9.18	7.97	3.34
-6	2	19	1.20*	0.51	4.73
-6	2	20	1.94*	2.03	4.57
-6	2	21	1.25*	0.32	4.72

h	k	l	Fo	Fc	weight
-6	3	20	2.18*	1.72	4.53
-6	3	19	2.12	2.15	4.54
-6	3	18	1.13*	0.40	4.75
-6	3	17	1.97*	1.01	4.57
-6	3	16	2.90	2.59	4.40
-6	3	15	4.17	4.21	4.19
-6	3	14	3.54	3.28	4.29
-6	3	13	1.48*	0.54	4.67
-6	3	12	1.69*	0.22	4.62
-6	3	11	20.39	21.12	1.32
-6	3	10	6.96	6.89	3.73
-6	3	9	13.83	14.73	2.42
-6	3	8	15.95	16.60	2.01
-6	3	7	6.82	6.83	3.76
-6	3	6	16.50	16.69	1.91
-6	3	5	15.31	15.38	2.13
-6	3	4	17.25	17.96	1.79
-6	3	3	6.59	6.46	3.80
-6	3	2	3.25	2.37	4.34
-6	3	1	9.67	9.38	3.25
-6	4	1	4.65	5.43	4.11
-6	4	2	11.57	12.34	2.87
-6	4	3	3.91	4.37	4.23
-6	4	4	1.67	2.13	4.63
-6	4	5	4.66	4.41	4.11
-6	4	6	26.98	27.55	0.69
-6	4	7	1.41*	2.32	4.68
-6	4	8	39.05	39.97	0.25
-6	4	9	6.09	6.58	3.88
-6	4	10	5.90	6.55	3.91
-6	4	11	2.14*	0.33	4.53
-6	4	12	11.08	10.39	2.97
-6	4	13	1.46*	1.84	4.67
-6	4	14	5.80	6.09	3.92
-6	4	15	1.00*	1.08	4.78
-6	4	16	3.06	2.96	4.37
-6	4	17	4.57	4.24	4.12
-6	4	18	5.57	5.41	3.96
-6	4	19	2.00*	2.48	4.56
-6	4	20	0.37*	1.00	4.93
-6	5	19	1.93*	2.57	4.58
-6	5	18	1.21*	1.56	4.73
-6	5	17	1.14*	0.04	4.74
-6	5	16	1.26*	0.93	4.72
-6	5	15	4.75	4.71	4.09
-6	5	14	1.57*	0.21	4.65
-6	5	13	1.59*	0.42	4.65
-6	5	12	11.80	12.37	2.83
-6	5	11	3.82	3.17	4.24
-6	5	10	9.14	9.37	3.35
-6	5	9	21.77	22.79	1.15
-6	5	8	13.45	13.72	2.49
-6	5	7	1.04*	0.57	4.77
-6	5	6	12.44	11.82	2.70
-6	5	5	28.16	28.56	0.62
-6	5	4	19.49	18.68	1.44
-6	5	3	12.73	12.78	2.64
-6	5	2	12.56	12.01	2.67
-6	5	1	1.91*	2.72	4.58
-6	6	1	23.35	24.32	0.88
-6	6	2	8.94	9.21	3.39
-6	6	3	17.84	18.17	1.69
-6	6	4	16.87	17.61	1.85
-6	6	5	1.04*	2.10	4.77
-6	6	6	4.86	4.80	4.07
-6	6	7	34.90	35.78	0.35
-6	6	8	2.76	2.34	4.42
-6	6	9	3.44	2.88	4.30
-6	6	10	3.23	3.34	4.34
-6	6	11	16.24	16.36	1.96
-6	6	12	7.04	7.02	3.72
-6	6	13	4.54	5.21	4.13
-6	6	14	5.66	5.40	3.95
-6	6	15	4.81	4.67	4.08
-6	6	16	1.16*	1.23	4.74
-6	6	17	8.60	8.13	3.45
-6	6	18	2.21*	0.73	4.52
-6	7	17	2.40	2.58	4.49
-6	7	16	6.15	5.74	3.87
-6	7	15	4.34	3.93	4.16
-6	7	14	0.68*	0.94	4.85
-6	7	13	5.00	5.12	4.05
-6	7	12	10.84	11.28	3.02
-6	7	11	1.15*	2.04	4.74
-6	7	10	1.08*	0.41	4.76
-6	7	9	6.39	6.01	3.83
-6	7	8	9.02	9.57	3.37
-6	7	7	17.48	18.28	1.75
-6	7	6	13.82	13.78	2.42
-6	7	5	10.28	10.29	3.13
-6	7	4	14.46	14.65	2.29
-6	7	3	4.29	4.06	4.17
-6	7	2	17.83	17.48	1.69
-6	7	1	0.88*	1.32	4.80
-6	8	1	9.87	10.46	3.21
-6	8	2	3.81	4.34	4.24
-6	8	3	13.82	14.43	2.42
-6	8	4	2.91	2.82	4.40
-6	8	5	0.81*	2.65	4.82
-6	8	6	2.05*	2.15	4.55
-6	8	7	6.37	6.33	3.83
-6	8	8	1.07*	0.76	4.76
-6	8	9	2.82	3.72	4.41
-6	8	10	4.37	3.88	4.15
-6	8	11	8.09	7.97	3.54
-6	8	12	4.98	4.80	4.06
-6	8	13	3.50	3.87	4.29
-6	8	14	3.82	3.40	4.24
-6	8	15	8.78	8.19	3.42
-6	8	16	1.29*	1.52	4.71
-6	8	17	1.27*	2.23	4.71
-6	9	14	3.24	2.58	4.34
-6	9	13	7.43	6.86	3.65
-6	9	12	8.44	8.75	3.48
-6	9	11	0.60*	1.27	4.87
-6	9	10	8.41	7.88	3.48
-6	9	9	1.80*	0.51	4.60
-6	9	8	3.27	2.82	4.33
-6	9	7	5.27	4.70	4.01
-6	9	6	12.35	12.93	2.72
-6	9	5	1.02*	0.67	4.77
-6	9	4	0.85*	1.38	4.81
-6	9	3	8.57	8.84	3.45
-6	9	2	11.79	11.98	2.83
-6	9	1	6.24	6.39	3.85
-6	10	1	5.03	5.38	4.05
-6	10	2	8.15	7.90	3.53
-6	10	3	4.29	3.89	4.17
-6	10	4	1.34*	2.67	4.70
-6	10	5	1.12*	0.47	4.75
-6	10	6	1.12*	0.39	4.75
-6	10	7	1.45*	1.62	4.67
-6	10	8	1.95*	2.18	4.57
-6	10	9	1.75*	1.69	4.61
-6	10	10	2.40*	2.37	4.49
-6	10	11	1.08*	2.37	4.76
-6	10	12	5.83	5.67	3.92
-6	10	13	3.28	3.34	4.33
-6	11	10	5.40	4.92	3.99
-6	11	9	9.49	9.58	3.28
-6	11	8	1.20*	1.68	4.73
-6	11	7	2.18	2.52	4.53
-6	11	6	10.88	10.37	3.01
-6	11	5	4.66	4.40	4.11
-6	11	4	10.07	10.33	3.17
-6	11	3	1.17*	0.24	4.74
-6	11	2	9.00	9.31	3.37
-6	11	1	1.89*	2.22	4.58
-6	12	1	8.60	8.55	3.45
-6	12	2	7.52	7.88	3.64
-6	12	3	2.75*	3.35	4.42
-6	12	4	1.22*	1.33	4.72
-6	12	5	1.85*	3.07	4.59
-6	12	6	1.29*	1.22	4.71
-5	12	9	5.99	5.87	3.89
-5	12	8	4.27	4.32	4.17
-5	12	7	1.23*	0.26	4.72
-5	12	6	4.60	4.01	4.12
-5	12	5	1.21*	0.72	4.73
-5	12	4	4.91	4.50	4.07
-5	12	3	4.92	5.25	4.06
-5	12	2	6.89	6.97	3.75
-5	12	1	9.03	8.90	3.37
-5	11	1	1.48*	1.16	4.67
-5	11	2	10.10	10.09	3.17
-5	11	3	2.65*	2.84	4.44
-5	11	4	5.15	4.82	4.03
-5	11	5	5.39	4.73	3.99
-5	11	6	3.39	3.62	4.31
-5	11	7	10.30	10.32	3.13
-5	11	8	1.53*	0.20	4.66
-5	11	9	1.23*	2.59	4.72
-5	11	10	11.79	11.29	2.83
-5	11	11	5.71	5.23	3.94
-5	11	12	9.34	8.69	3.31
-5	10	14	8.75	8.59	3.42
-5	10	13	1.22*	0.97	4.73
-5	10	12	2.59	2.44	4.45
-5	10	11	6.98	7.04	3.73
-5	10	10	2.43*	3.01	4.48
-5	10	9	5.61	5.83	3.96
-5	10	8	1.14*	0.59	4.74
-5	10	7	3.23	3.39	4.34
-5	10	6	8.64	9.07	3.44
-5	10	5	16.00	15.74	2.00
-5	10	4	3.70	3.37	4.26
-5	10	3	7.86	7.56	3.58
-5	10	2	4.19	3.78	4.18
-5	10	1	9.11	8.93	3.35
-5	9	1	7.56	7.72	3.63
-5	9	2	6.09	6.42	3.88
-5	9	3	5.47	5.42	3.98
-5	9	4	13.28	14.29	2.53
-5	9	5	1.08*	0.18	4.76
-5	9	6	7.66	7.54	3.62
-5	9	7	8.28	8.41	3.51
-5	9	8	6.45	6.15	3.82
-5	9	9	5.08	5.04	4.04
-5	9	10	7.65	7.96	3.62
-5	9	11	1.92*	1.56	4.58
-5	9	12	0.59*	1.16	4.87
-5	9	13	2.28*	1.30	4.51
-5	9	14	4.37	4.14	4.15
-5	9	15	5.80	5.34	3.93
-5	9	16	9.30	9.08	3.32
-5	8	17	2.11*	1.87	4.54
-5	8	16	4.25	3.61	4.17
-5	8	15	6.63	6.59	3.79
-5	8	14	1.78*	0.64	4.61
-5	8	13	5.99	5.53	3.90
-5	8	12	9.78	9.16	3.23
-5	8	11	6.97	7.29	3.73
-5	8	10	2.34*	3.48	4.50
-5	8	9	10.34	10.38	3.12
-5	8	8	9.30	9.40	3.32
-5	8	7	29.40	30.08	0.56
-5	8	6	7.31	7.50	3.68
-5	8	5	2.18*	1.86	4.53
-5	8	4	12.52	12.68	2.68
-5	8	3	5.07	5.08	4.04
-5	8	2	29.02	29.65	0.58
-5	8	1	27.88	28.37	0.63
-5	7	1	1.46*	2.17	4.67
-5	7	2	31.43	32.03	0.46
-5	7	3	9.60	8.78	3.26
-5	7	4	18.62	18.63	1.57
-5	7	5	6.85	7.49	3.75
-5	7	6	28.34	28.72	0.61
-5	7	7	8.01	7.48	3.55
-5	7	8	11.31	10.98	2.93
-5	7	9	3.67	4.10	4.27
-5	7	10	19.55	20.08	1.43

h	k	l	Fo	Fc	weight
-5	7	11	7.98	6.95	3.56
-5	7	12	1.12*	0.52	4.75
-5	7	13	3.04	3.07	4.37
-5	7	14	4.63	4.34	4.11
-5	7	15	6.05	6.48	3.89
-5	7	16	5.80	6.10	3.93
-5	7	17	5.89	5.27	3.91
-5	7	18	4.75	3.78	4.09
-5	6	19	2.67*	0.44	4.44
-5	6	18	1.22*	0.50	4.73
-5	6	17	1.20*	1.34	4.73
-5	6	16	2.87	2.51	4.40
-5	6	15	7.41	7.03	3.66
-5	6	14	2.68	2.95	4.44
-5	6	13	1.08*	0.08	4.76
-5	6	12	10.83	11.01	3.02
-5	6	11	11.37	11.95	2.91
-5	6	10	6.44	6.51	3.82
-5	6	9	11.13	11.33	2.96
-5	6	8	15.80	16.27	2.04
-5	6	7	0.63*	0.89	4.86
-5	6	6	1.92*	0.34	4.58
-5	6	5	30.74	30.64	0.49
-5	6	4	4.12	4.09	4.19
-5	6	3	18.51	17.81	1.58
-5	6	2	16.47	17.17	1.92
-5	6	1	7.29	7.35	3.68
-5	5	1	9.78	10.97	3.23
-5	5	2	26.37	26.46	0.74
-5	5	3	7.47	6.91	3.65
-5	5	4	17.16	17.33	1.80
-5	5	5	0.90*	0.23	4.80
-5	5	6	28.43	29.20	0.61
-5	5	7	17.38	17.26	1.76
-5	5	8	14.98	15.84	2.19
-5	5	9	3.44	3.32	4.30
-5	5	10	20.07	21.22	1.36
-5	5	11	0.70*	2.13	4.85
-5	5	12	6.51	6.75	3.81
-5	5	13	4.34	4.23	4.16
-5	5	14	4.67	5.09	4.11
-5	5	15	0.32*	0.60	4.95
-5	5	16	3.19	3.23	4.35
-5	5	17	3.26	3.39	4.33
-5	5	18	1.17*	0.53	4.74
-5	5	19	5.81	5.78	3.92
-5	5	20	5.98	5.91	3.90
-5	4	20	1.26*	2.61	4.72
-5	4	19	0.70*	0.60	4.85
-5	4	18	1.74*	0.23	4.61
-5	4	17	1.40*	0.38	4.68
-5	4	16	4.61	4.42	4.11
-5	4	15	4.71	4.80	4.10
-5	4	14	1.02*	0.34	4.77
-5	4	13	9.00	8.66	3.37
-5	4	12	4.93	4.02	4.06
-5	4	11	8.68	9.33	3.43
-5	4	10	20.68	20.94	1.28
-5	4	9	5.22	5.02	4.02
-5	4	8	18.81	19.46	1.54
-5	4	7	20.57	20.33	1.29
-5	4	6	4.94	5.01	4.06
-5	4	5	17.29	17.12	1.78
-5	4	4	23.85	23.84	0.84
-5	4	3	5.77	5.14	3.83
-5	4	2	27.96	25.23	0.63
-5	4	1	7.79	8.01	3.59
-5	3	1	2.82	2.98	4.41
-5	3	2	2.78	2.05	4.42
-5	3	3	36.04	35.99	0.32
-5	3	4	24.53	24.31	0.88
-5	3	5	1.71	1.79	4.62
-5	3	6	3.55	3.89	4.29
-5	3	7	4.85	5.15	4.08
-5	3	8	7.10	7.01	3.71
-5	3	9	22.46	22.84	1.07
-5	3	10	3.95	4.46	4.22
-5	3	11	6.86	6.04	3.74
-5	3	12	6.80	7.11	3.76
-5	3	13	5.65	6.13	3.95
-5	3	14	5.89	6.25	3.89
-5	3	15	3.58	3.86	4.28
-5	3	16	4.21	3.72	4.18
-5	3	17	7.40	7.15	3.66
-5	3	18	2.30*	1.69	4.50
-5	3	19	2.02*	0.02	4.56
-5	3	20	1.16*	0.82	4.74
-5	3	21	4.00	3.33	4.21
-5	2	21	1.23*	0.22	4.72
-5	2	20	2.35*	0.46	4.50
-5	2	19	5.55	5.18	3.96
-5	2	18	1.88*	1.55	4.59
-5	2	17	2.27*	2.02	4.51
-5	2	16	5.43	4.94	3.99
-5	2	15	2.90	3.31	4.40
-5	2	14	4.32	5.03	4.16
-5	2	13	0.49*	0.81	4.90
-5	2	12	11.58	11.99	2.87
-5	2	11	6.41	7.98	3.83
-5	2	10	14.43	14.72	2.30
-5	2	9	0.92*	0.58	4.79
-5	2	8	41.17	42.75	0.22
-5	2	7	3.81	4.15	4.24
-5	2	6	2.48	3.04	4.47
-5	2	5	23.92	24.22	0.93
-5	2	4	26.24	25.73	0.74
-5	2	3	12.44	12.71	2.70
-5	2	2	10.81	11.77	3.03
-5	1	1	15.81	15.85	2.04
-5	1	1	28.06	26.95	0.63
-5	1	2	8.70	7.87	3.43
-5	1	3	12.44	11.12	2.70
-5	1	4	19.99	19.01	1.37
-5	1	5	26.39	27.01	0.73
-5	1	6	4.86	4.66	4.08
-5	1	7	6.99	7.99	3.73
-5	1	8	7.86	7.75	3.58
-5	1	9	23.11	23.84	1.01
-5	1	10	4.19	4.32	4.18
-5	1	11	5.43	5.52	3.98
-5	1	12	15.82	17.80	2.04
-5	1	13	3.72	3.11	4.26
-5	1	14	3.21	3.21	4.34
-5	1	15	1.52*	1.74	4.66
-5	1	16	4.66	4.38	4.11
-5	1	17	1.50*	1.37	4.67
-5	1	18	1.16*	1.90	4.74
-5	1	19	1.80*	2.26	4.60
-5	1	20	6.16	5.68	3.87
-5	1	21	1.23*	0.64	4.72
-5	0	20	2.13*	1.94	4.54
-5	0	18	14.32	13.21	2.32
-5	0	16	3.24	2.37	4.34
-5	0	14	15.58	16.59	2.08
-5	0	12	5.85	6.06	3.92
-5	0	10	6.97	8.08	3.73
-5	0	8	45.32	46.33	0.16
-5	0	6	25.56	25.35	0.79
-5	0	4	54.08	53.67	0.10
-5	0	2	41.21	41.23	0.21
-4	0	2	52.49	54.34	0.10
-4	0	4	49.15	49.25	0.13
-4	0	6	43.11	43.67	0.19
-4	0	8	36.71	35.24	0.30
-4	0	10	14.08	14.68	2.37
-4	0	12	4.61	5.04	4.11
-4	0	14	8.73	8.65	3.42
-4	0	16	7.85	6.05	3.58
-4	0	18	4.37	3.34	4.15
-4	0	20	11.41	10.59	2.91
-4	0	22	2.59*	1.26	4.45
-4	1	22	1.78*	1.25	4.61
-4	1	21	2.24*	2.26	4.52
-4	1	20	1.25*	2.84	4.72
-4	1	19	4.28	3.83	4.17
-4	1	18	2.07*	1.65	4.55
-4	1	17	6.69	7.07	3.78
-4	1	16	1.41*	1.42	4.68
-4	1	15	14.06	14.69	2.37
-4	1	14	8.47	8.64	3.47
-4	1	13	18.71	19.17	1.55
-4	1	12	6.14	6.80	3.87
-4	1	11	25.25	26.55	0.82
-4	1	10	13.58	13.44	2.47
-4	1	9	16.85	17.17	1.85
-4	1	8	8.82	8.79	3.41
-4	1	7	32.73	33.60	0.42
-4	1	6	11.03	12.06	2.98
-4	1	5	5.49	3.13	3.97
-4	1	4	14.07	13.18	2.37
-4	1	3	33.05	33.71	0.40
-4	1	2	37.57	36.94	0.28
-4	1	1	7.74	5.56	3.60
-4	2	1	3.59	4.46	4.28
-4	2	2	17.49	18.41	1.74
-4	2	3	4.74	4.14	4.09
-4	2	4	6.43	5.93	3.82
-4	2	5	12.77	12.41	2.63
-4	2	6	59.47	61.55	0.07
-4	2	7	23.29	22.30	0.99
-4	2	8	15.56	15.67	2.08
-4	2	9	7.03	6.92	3.72
-4	2	10	0.84*	1.34	4.81
-4	2	11	18.38	19.52	1.60
-4	2	12	1.08*	2.12	4.76
-4	2	13	15.00	15.29	2.19
-4	2	14	15.10	15.52	2.17
-4	2	15	5.06	6.07	4.04
-4	2	16	1.00*	0.93	4.78
-4	2	17	2.58	1.17	4.45
-4	2	18	1.06*	0.55	4.76
-4	2	19	2.81	2.61	4.41
-4	2	20	2.66*	2.69	4.44
-4	2	21	4.01	3.55	4.21
-4	2	22	2.32*	1.20	4.80
-4	3	21	5.20	4.73	4.02
-4	3	20	1.19*	0.02	4.73
-4	3	19	9.70	8.98	3.24
-4	3	18	2.17*	2.61	4.53
-4	3	17	5.23	4.75	4.02
-4	3	16	3.61	3.99	4.28
-4	3	15	5.78	4.84	3.93
-4	3	14	13.64	15.00	2.46
-4	3	13	0.97*	0.25	4.78
-4	3	12	6.77	6.84	3.77
-4	3	11	5.34	5.71	4.00
-4	3	10	1.89*	1.31	4.58
-4	3	9	0.54*	0.95	4.89
-4	3	8	0.81*	1.74	4.82
-4	3	7	2.47	2.20	4.47
-4	3	6	0.80*	0.74	4.82
-4	3	5	27.88	28.73	0.64
-4	3	4	20.20	19.68	1.34
-4	3	3	3.41	4.90	4.31
-4	3	2	25.25	23.79	0.82
-4	3	1	39.36	39.34	0.25
-4	4	1	13.85	14.51	2.41
-4	4	2	21.82	21.93	1.14
-4	4	3	22.91	21.74	1.03
-4	4	4	11.81	11.25	2.83
-4	4	5	22.04	22.11	1.12
-4	4	6	19.37	19.03	1.46
-4	4	7	10.47	10.87	3.09
-4	4	8	12.21	11.64	2.74
-4	4	9	4.45	4.43	4.14
-4	4	10	8.50	9.12	3.47
-4	4	11	13.17	12.73	2.55
-4	4	12	18.31	19.24	1.61
-4	4	13	5.87	5.90	3.91
-4	4	14	6.38	6.32	3.83
-4	4	15	2.75	2.15	4.42
-4	4	16	5.61	5.47	3.96

h	k	l	Fo	Fc	weight
-4	4	17	1.10*	0.22	4.75
-4	4	18	2.99	2.28	4.38
-4	4	19	4.62	5.13	4.11
-4	4	20	2.63*	2.46	4.44
-4	4	21	4.87	4.72	4.07
-4	5	20	4.31	3.24	4.16
-4	5	19	4.30	3.65	4.16
-4	5	18	6.47	5.85	3.82
-4	5	17	1.99*	1.10	4.56
-4	5	16	1.50*	0.99	4.66
-4	5	15	5.85	6.10	3.92
-4	5	14	7.95	8.62	3.57
-4	5	13	2.31	2.60	4.50
-4	5	12	3.62	4.26	4.28
-4	5	11	0.96*	0.17	4.79
-4	5	10	1.96*	2.40	4.57
-4	5	9	8.37	9.04	3.49
-4	5	8	22.10	22.89	1.11
-4	5	7	11.85	11.71	2.82
-4	5	6	3.00	3.23	4.38
-4	5	5	9.05	8.15	3.37
-4	5	4	13.40	13.47	2.50
-4	5	3	0.83*	1.31	4.81
-4	5	2	0.83*	1.27	4.82
-4	5	1	41.63	41.09	0.21
-4	6	1	23.57	24.22	0.96
-4	6	2	5.77	5.83	3.93
-4	6	3	26.43	26.61	0.73
-4	6	4	0.92*	0.47	4.80
-4	6	5	12.75	12.98	2.63
-4	6	6	11.75	11.63	2.84
-4	6	7	15.13	14.82	2.17
-4	6	8	6.35	6.48	3.64
-4	6	9	14.89	15.34	2.21
-4	6	10	1.09*	0.98	4.76
-4	6	11	9.79	9.84	3.22
-4	6	12	2.17*	0.35	4.63
-4	6	13	19.20	19.46	1.48
-4	6	14	9.62	9.56	3.26
-4	6	15	12.86	12.78	2.61
-4	6	16	5.63	4.62	3.95
-4	6	17	9.32	9.03	3.31
-4	6	18	1.05*	1.51	4.76
-4	6	19	1.22*	1.73	4.73
-4	6	20	2.42	2.01	4.48
-4	7	19	2.32*	1.15	4.50
-4	7	18	5.58	5.24	3.96
-4	7	17	4.93	4.92	4.06
-4	7	16	1.18*	0.03	4.73
-4	7	15	11.08	10.85	2.97
-4	7	14	1.16*	2.12	4.74
-4	7	13	8.29	8.90	3.50
-4	7	12	7.24	6.86	3.69
-4	7	11	17.61	17.33	1.72
-4	7	10	4.54	4.45	4.13
-4	7	9	2.71	2.75	4.43
-4	7	8	21.70	22.38	1.16
-4	7	7	1.95	2.08	4.57
-4	7	6	5.10	5.58	4.04
-4	7	5	21.19	20.63	1.22
-4	7	4	45.46	47.31	0.16
-4	7	3	14.95	14.73	2.20
-4	7	2	17.08	17.61	1.81
-4	7	1	11.65	10.67	2.86
-4	8	1	4.71	5.78	4.10
-4	8	2	18.75	19.32	1.55
-4	8	3	4.48	3.49	4.14
-4	8	4	12.49	13.04	2.69
-4	8	5	36.42	36.28	0.31
-4	8	6	13.10	13.01	2.56
-4	8	7	2.27*	2.92	4.51
-4	8	8	10.28	11.13	3.13
-4	8	9	16.19	16.63	1.97
-4	8	10	4.49	4.20	4.13
-4	8	11	9.59	9.83	3.26
-4	8	12	2.04	1.59	4.55
-4	8	13	14.59	14.23	2.27
-4	8	14	3.28	3.13	4.33
-4	8	15	2.20*	1.46	4.52
-4	8	16	4.03	4.06	4.21
-4	8	17	0.81*	1.98	4.82
-4	8	18	3.61	3.40	4.28
-4	9	16	2.45*	0.52	4.48
-4	9	15	2.69*	3.21	4.43
-4	9	14	15.56	15.58	2.08
-4	9	13	2.30	2.65	4.51
-4	9	12	3.59	3.24	4.28
-4	9	11	8.39	8.52	3.49
-4	9	10	5.17	5.92	4.03
-4	9	9	10.62	11.27	3.06
-4	9	8	12.21	12.09	2.74
-4	9	7	13.60	13.42	2.46
-4	9	6	5.25	5.21	4.01
-4	9	5	17.12	17.33	1.81
-4	9	4	16.74	17.77	1.87
-4	9	3	3.53	2.96	4.29
-4	9	2	2.18	2.68	4.53
-4	9	1	14.66	14.37	2.26
-4	10	1	7.22	6.93	3.69
-4	10	2	3.09	3.13	4.36
-4	10	3	19.07	19.16	1.50
-4	10	4	11.37	12.27	2.91
-4	10	5	11.81	11.55	2.82
-4	10	6	1.92*	1.19	4.58
-4	10	7	7.41	7.48	3.66
-4	10	8	8.40	8.23	3.48
-4	10	9	6.02	5.71	3.89
-4	10	10	1.15*	1.39	4.74
-4	10	11	1.19*	0.15	4.73
-4	10	12	4.18	3.94	4.18
-4	10	13	7.76	7.40	3.60
-4	10	14	1.45*	1.17	4.67
-4	10	15	4.57	4.39	4.12
-4	11	13	1.85*	3.39	4.59
-4	11	12	8.90	8.36	3.39
-4	11	11	2.15*	2.09	4.53
-4	11	10	2.78*	3.61	4.42
-4	11	9	8.18	8.23	3.52
-4	11	8	1.91*	1.81	4.58
-4	11	7	7.55	7.45	3.64
-4	11	6	6.82	6.80	3.76
-4	11	5	5.95	6.21	3.90
-4	11	4	10.37	10.47	3.11
-4	11	3	8.39	8.28	3.49
-4	11	2	8.76	8.90	3.42
-4	11	1	0.93*	1.76	4.79
-4	12	1	1.18*	0.11	4.73
-4	12	2	10.55	10.67	3.08
-4	12	3	7.24	7.34	3.69
-4	12	4	6.18	6.20	3.86
-4	12	5	3.21	3.24	4.34
-4	12	6	5.96	5.93	3.90
-4	12	7	11.23	11.31	2.94
-4	12	8	2.70*	2.99	4.43
-4	12	9	1.50*	0.34	4.66
-4	12	10	2.69*	1.46	4.43
-4	13	6	1.34*	0.55	4.70
-4	13	5	1.97*	2.50	4.57
-4	13	4	3.18	2.98	4.35
-4	13	3	11.72	12.01	2.84
-4	13	2	4.23	4.99	4.18
-4	13	1	6.68	7.25	3.78
-3	13	1	13.75	14.29	2.43
-3	13	2	6.00	6.07	3.89
-3	13	3	1.26*	0.64	4.72
-3	13	4	4.36	4.53	4.15
-3	13	5	18.49	18.80	1.59
-3	13	6	3.42	3.62	4.31
-3	13	7	6.58	7.09	3.80
-3	13	8	4.52	4.75	4.13
-3	12	11	11.57	11.56	2.87
-3	12	10	3.20	3.31	4.35
-3	12	9	1.94*	1.59	4.58
-3	12	8	2.97	3.25	4.38
-3	12	7	2.39	2.30	4.49
-3	12	6	4.59	4.64	4.10
-3	12	5	7.39	7.22	3.66
-3	12	4	7.06	7.07	3.72
-3	12	3	3.61	3.81	4.28
-3	12	2	0.59*	0.67	4.88
-3	11	1	8.61	8.25	3.45
-3	11	1	6.14	5.67	3.87
-3	11	2	10.76	11.42	3.04
-3	11	3	2.33*	1.90	4.50
-3	11	4	12.29	11.98	2.73
-3	11	5	5.06	4.30	4.04
-3	11	6	2.28*	2.36	4.51
-3	11	7	3.50	3.63	4.30
-3	11	8	12.15	12.09	2.76
-3	11	9	3.80	4.34	4.25
-3	11	10	5.68	5.62	3.94
-3	11	11	2.92	3.04	4.39
-3	11	12	1.48*	1.06	4.67
-3	11	13	2.17*	3.20	4.53
-3	10	15	4.00	3.56	4.21
-3	10	14	2.18*	1.81	4.53
-3	10	13	3.88	4.06	4.23
-3	10	12	1.33*	0.67	4.70
-3	10	11	7.74	7.39	3.60
-3	10	10	1.33*	0.37	4.70
-3	10	9	4.22	3.84	4.18
-3	10	8	4.70	5.00	4.10
-3	10	7	12.08	12.29	2.77
-3	10	6	8.67	9.06	3.40
-3	10	5	2.37*	1.56	4.49
-3	10	4	8.61	8.46	3.45
-3	10	3	20.92	20.74	1.25
-3	10	2	2.11*	2.86	4.54
-3	10	1	7.27	7.26	3.68
-3	9	1	1.58*	1.46	4.65
-3	9	2	19.77	20.55	1.40
-3	9	3	5.10	5.62	4.04
-3	9	4	5.28	4.78	4.01
-3	9	5	10.53	10.38	3.08
-3	9	6	7.19	6.98	3.70
-3	9	7	21.49	21.81	1.18
-3	9	8	12.92	13.06	2.60
-3	9	9	16.11	16.33	1.98
-3	9	10	6.55	6.31	3.80
-3	9	11	6.34	6.90	3.84
-3	9	12	9.74	10.08	3.24
-3	9	13	5.11	4.82	4.04
-3	9	14	2.10*	1.10	4.54
-3	9	15	4.12	3.85	4.19
-3	9	16	9.93	9.61	3.20
-3	9	17	1.34*	0.52	4.70
-3	8	18	2.87	3.43	4.40
-3	8	17	8.05	8.14	3.55
-3	8	16	4.10	3.92	4.20
-3	8	15	5.50	5.00	3.97
-3	8	14	8.63	8.39	3.44
-3	8	13	5.23	5.64	4.02
-3	8	12	1.78*	0.27	4.61
-3	8	11	12.52	12.78	2.68
-3	8	10	6.87	6.67	3.91
-3	8	9	17.65	18.88	1.72
-3	8	8	3.11	2.98	4.36
-3	8	7	32.73	32.42	0.42
-3	8	6	8.03	7.02	3.55
-3	8	5	11.43	11.62	2.90
-3	8	4	20.50	20.97	1.30
-3	8	3	43.46	43.13	0.18
-3	8	2	10.64	10.27	3.06
-3	8	1	11.83	12.20	2.82
-3	7	1	7.57	7.89	3.63
-3	7	2	34.27	33.96	0.37
-3	7	3	8.34	8.12	3.49
-3	7	4	13.43	12.54	2.50
-3	7	5	7.54	7.65	3.64
-3	7	6	28.42	28.24	0.61
-3	7	7	4.61	5.03	4.11
-3	7	8	11.82	11.45	2.82

h	k	l	Fo	Fc	weight
-3	7	9	11.70	11.54	2.85
-3	7	10	11.13	11.06	2.96
-3	7	11	7.14	7.34	3.70
-3	7	12	1.42*	0.19	4.68
-3	7	13	15.53	15.41	2.09
-3	7	14	6.56	7.04	3.80
-3	7	15	8.20	8.18	3.52
-3	7	16	2.16*	2.35	4.53
-3	7	17	1.20*	1.43	4.73
-3	7	18	1.21*	1.74	4.73
-3	7	19	1.24*	0.47	4.72
-3	6	20	2.49	2.24	4.47
-3	6	19	1.20*	1.33	4.73
-3	6	18	6.96	6.10	3.73
-3	6	17	10.45	10.52	3.10
-3	6	16	2.92	2.79	4.39
-3	6	15	10.76	10.61	3.04
-3	6	14	2.12	3.83	4.54
-3	6	13	13.94	14.28	2.40
-3	6	12	0.96*	2.19	4.78
-3	6	11	20.33	21.26	1.33
-3	6	10	6.56	6.15	3.80
-3	6	9	2.80	2.74	4.41
-3	6	8	1.79	0.71	4.60
-3	6	7	15.26	16.06	2.14
-3	6	6	15.92	15.49	2.02
-3	6	5	27.75	26.89	0.65
-3	6	4	9.71	8.80	3.24
-3	6	3	25.79	25.77	0.78
-3	6	2	23.70	23.18	0.85
-3	6	1	13.08	13.12	2.57
-3	5	1	7.87	8.49	3.58
-3	5	2	10.27	10.88	3.13
-3	5	3	2.28	2.30	4.51
-3	5	4	23.84	22.76	0.94
-3	5	5	16.14	15.50	1.98
-3	5	6	24.26	24.36	0.90
-3	5	7	33.96	33.79	0.37
-3	5	8	19.51	19.85	1.44
-3	5	9	19.11	19.82	1.49
-3	5	10	11.95	11.66	2.80
-3	5	11	1.15*	0.19	4.74
-3	5	12	10.45	10.97	3.10
-3	5	13	0.64*	2.23	4.86
-3	5	14	3.23	3.39	4.34
-3	5	15	3.42	3.37	4.31
-3	5	16	7.07	6.18	3.72
-3	5	17	0.85*	1.25	4.81
-3	5	18	1.77*	2.52	4.61
-3	5	19	3.19	2.78	4.35
-3	5	20	1.49*	0.68	4.67
-3	4	21	7.72	7.52	3.61
-3	4	20	4.60	4.59	4.12
-3	4	19	1.14*	0.40	4.74
-3	4	18	2.33*	0.97	4.50
-3	4	17	1.09*	0.88	4.76
-3	4	16	1.06*	1.19	4.76
-3	4	15	1.94*	0.95	4.57
-3	4	14	13.84	14.74	2.42
-3	4	13	1.72*	1.82	4.62
-3	4	12	9.48	8.91	3.29
-3	4	11	14.01	14.55	2.38
-3	4	10	2.47	2.17	4.47
-3	4	9	3.68	3.61	4.26
-3	4	8	11.98	12.04	2.79
-3	4	7	15.61	15.41	2.07
-3	4	6	14.20	14.30	2.35
-3	4	5	13.42	14.03	2.50
-3	4	4	14.96	14.62	2.20
-3	4	3	18.69	18.29	1.56
-3	4	2	14.02	11.21	2.38
-3	4	1	25.56	25.03	0.79
-3	3	1	14.45	15.48	2.30
-3	3	2	16.39	15.06	1.93
-3	3	3	11.72	12.37	2.84
-3	3	4	31.92	30.84	0.44
-3	3	5	27.66	28.07	0.65
-3	3	6	9.71	9.56	3.24
-3	3	7	5.49	5.65	3.98
-3	3	8	20.66	20.10	1.28
-3	3	9	14.60	14.37	2.27
-3	3	10	10.69	11.29	3.05
-3	3	11	8.45	8.36	3.48
-3	3	12	12.81	13.10	2.62
-3	3	13	1.49	0.62	4.67
-3	3	14	3.84	3.60	4.24
-3	3	15	10.61	10.83	3.06
-3	3	16	8.45	8.87	3.48
-3	3	17	9.87	9.04	3.21
-3	3	18	3.72	3.40	4.26
-3	3	19	3.25	3.40	4.34
-3	3	20	7.07	6.87	3.72
-3	3	21	2.78*	2.76	4.42
-3	2	22	5.21	5.09	4.02
-3	2	21	1.43*	1.47	4.68
-3	2	20	2.05*	2.26	4.55
-3	2	19	3.83	3.41	4.24
-3	2	18	1.72*	2.15	4.62
-3	2	17	1.36*	1.49	4.70
-3	2	16	5.74	6.31	3.93
-3	2	15	1.56*	2.24	4.65
-3	2	14	19.50	20.84	1.44
-3	2	13	13.22	13.51	2.54
-3	2	12	17.50	19.03	1.74
-3	2	11	5.82	5.45	3.92
-3	2	10	24.37	24.84	0.89
-3	2	9	29.98	29.28	0.53
-3	2	8	21.70	22.68	1.16
-3	2	7	2.94	4.35	4.39
-3	2	6	29.46	29.19	0.55
-3	2	5	5.92	4.49	3.91
-3	2	4	50.12	51.35	0.12
-3	2	3	0.64*	0.47	4.86
-3	2	2	58.76	58.81	0.07
-3	2	1	42.04	40.22	0.20
-3	1	1	36.91	40.07	0.30
-3	1	2	7.98	8.47	3.56
-3	1	3	10.61	11.39	3.07
-3	1	4	49.78	50.02	0.12
-3	1	5	29.50	30.99	0.55
-3	1	6	7.33	8.08	3.67
-3	1	7	15.57	14.42	2.08
-3	1	8	0.82*	3.41	4.82
-3	1	9	61.46	62.52	0.06
-3	1	10	3.14	3.96	4.35
-3	1	11	14.37	14.88	2.31
-3	1	12	6.74	7.25	3.77
-3	1	13	17.15	16.49	1.80
-3	1	14	7.53	7.88	3.64
-3	1	15	16.38	17.10	1.93
-3	1	16	3.48	3.17	4.30
-3	1	17	7.47	7.44	3.65
-3	1	18	1.32*	0.48	4.70
-3	1	19	7.68	7.94	3.61
-3	1	20	1.17*	1.01	4.74
-3	1	21	2.25*	0.08	4.51
-3	1	22	1.25*	1.67	4.72
-3	0	22	2.38*	2.09	4.49
-3	0	20	7.76	7.86	3.60
-3	0	18	4.72	4.39	4.10
-3	0	16	4.91	6.06	4.07
-3	0	14	16.52	16.76	1.91
-3	0	12	10.98	11.14	2.99
-3	0	10	25.05	25.04	0.83
-3	0	8	52.89	56.87	0.10
-3	0	6	39.03	42.36	0.25
-3	0	4	26.45	28.10	0.73
-3	0	2	10.86	9.94	3.02
-2	0	2	67.17	72.27	0.05
-2	0	4	47.11	50.80	0.14
-2	0	6	81.77	84.95	0.03
-2	0	8	43.25	40.03	0.19
-2	0	10	22.34	21.74	1.09
-2	0	12	21.48	22.80	1.18
-2	0	14	20.48	20.83	1.31
-2	0	16	13.50	13.53	2.48
-2	0	18	8.15	8.54	3.53
-2	0	20	4.32	4.04	4.16
-2	0	22	5.95	5.56	3.90
-2	1	22	4.49	4.22	4.13
-2	1	21	5.56	5.70	3.96
-2	1	20	1.89	0.92	4.58
-2	1	19	2.27*	2.11	4.51
-2	1	18	1.81*	0.41	4.60
-2	1	17	11.19	11.08	2.95
-2	1	16	1.11*	1.95	4.75
-2	1	15	9.97	10.01	3.19
-2	1	14	15.68	16.86	2.06
-2	1	13	38.69	40.03	0.26
-2	1	12	0.93*	0.20	4.79
-2	1	11	20.20	20.58	1.34
-2	1	10	25.96	23.91	0.76
-2	1	9	25.43	26.17	0.80
-2	1	8	23.92	23.42	0.93
-2	1	7	84.54	85.64	0.02
-2	1	6	41.01	41.29	0.22
-2	1	5	0.67*	1.34	4.86
-2	1	4	9.59	10.53	3.26
-2	1	3	57.54	59.62	0.08
-2	1	2	1.98	2.02	4.57
-2	1	1	18.57	18.00	1.57
-2	2	1	31.78	31.15	0.45
-2	2	2	65.61	67.40	0.05
-2	2	3	11.26	11.50	2.94
-2	2	4	2.50	2.36	4.47
-2	2	5	11.69	12.15	2.85
-2	2	6	32.68	31.46	0.42
-2	2	7	64.48	61.67	0.06
-2	2	8	20.30	19.89	1.33
-2	2	9	13.10	12.27	2.56
-2	2	10	5.19	4.61	4.02
-2	2	11	8.63	8.56	3.44
-2	2	12	0.25*	0.54	4.96
-2	2	13	7.67	8.21	3.61
-2	2	14	11.71	11.77	2.84
-2	2	15	1.07*	0.20	4.76
-2	2	16	3.49	4.49	4.30
-2	2	17	6.67	6.38	3.78
-2	2	18	9.20	9.35	3.34
-2	2	19	1.11*	1.44	4.75
-2	2	20	1.17*	0.08	4.74
-2	2	21	1.39*	3.09	4.69
-2	2	22	1.21*	0.20	4.73
-2	3	21	0.63*	1.03	4.87
-2	3	20	1.75*	1.13	4.61
-2	3	19	5.23	5.22	4.02
-2	3	18	7.34	6.97	3.67
-2	3	17	11.15	11.01	2.96
-2	3	16	4.23	4.46	4.18
-2	3	15	15.68	15.59	2.06
-2	3	14	22.88	24.19	1.03
-2	3	13	14.12	14.60	2.36
-2	3	12	2.53	2.58	4.46
-2	3	11	3.59	3.47	4.28
-2	3	10	3.87	2.99	4.23
-2	3	9	15.72	14.64	2.05
-2	3	8	27.29	26.86	0.67
-2	3	7	0.74*	2.43	4.84
-2	3	6	1.82	1.68	4.60
-2	3	5	39.16	38.53	0.25
-2	3	4	33.29	33.44	0.40
-2	3	3	46.89	47.43	0.15
-2	3	2	7.19	7.06	3.70
-2	3	1	44.40	43.95	0.17
-2	4	1	52.54	51.97	0.10
-2	4	2	13.75	12.70	2.44
-2	4	3	41.69	39.82	0.21
-2	4	4	20.19	19.38	1.34
-2	4	5	10.79	10.51	3.03
-2	4	6	18.36	17.14	1.60
-2	4	7	12.56	11.52	2.67
-2	4	8	3.28	2.71	4.33

h	k	l	Fo	Fc	weight
-2	4	9	36.77	36.82	0.30
-2	4	10	7.65	8.04	3.62
-2	4	11	11.45	11.85	2.90
-2	4	12	18.16	18.05	1.64
-2	4	13	1.93	2.63	4.58
-2	4	14	2.50	1.98	4.47
-2	4	15	8.84	9.25	3.40
-2	4	16	2.07*	2.56	4.55
-2	4	17	1.09*	0.38	4.75
-2	4	18	3.78	4.50	4.25
-2	4	19	5.15	5.58	4.03
-2	4	20	7.43	6.92	3.66
-2	4	21	3.62	3.61	4.28
-2	5	21	5.36	5.07	4.00
-2	5	20	4.65	4.58	4.11
-2	5	19	1.95*	0.91	4.57
-2	5	18	6.57	6.27	3.80
-2	5	17	2.07*	0.51	4.55
-2	5	16	2.03*	2.71	4.56
-2	5	15	9.71	10.04	3.24
-2	5	14	5.24	4.01	4.02
-2	5	13	13.85	13.55	2.41
-2	5	12	13.00	12.72	2.58
-2	5	11	6.58	6.71	3.80
-2	5	10	7.67	8.18	3.61
-2	5	9	8.61	9.01	3.45
-2	5	8	22.82	22.76	1.04
-2	5	7	17.13	16.82	1.81
-2	5	6	19.09	18.76	1.50
-2	5	5	25.69	25.00	0.78
-2	5	4	20.24	20.57	1.34
-2	5	3	9.46	6.79	3.29
-2	5	2	44.90	43.02	0.17
-2	5	1	42.09	39.38	0.20
-2	6	1	42.61	41.90	0.19
-2	6	2	8.20	9.58	3.52
-2	6	3	1.83	2.02	4.60
-2	6	4	29.17	28.66	0.57
-2	6	5	40.98	41.19	0.22
-2	6	6	9.12	8.99	3.35
-2	6	7	18.89	18.32	1.52
-2	6	8	0.36*	0.15	4.94
-2	6	9	0.69*	0.87	4.85
-2	6	10	5.86	5.73	3.92
-2	6	11	25.20	25.34	0.82
-2	6	12	2.26	3.01	4.51
-2	6	13	11.92	12.13	2.80
-2	6	14	0.92*	1.69	4.79
-2	6	15	13.95	13.93	2.39
-2	6	16	7.87	6.97	3.58
-2	6	17	1.01*	0.64	4.77
-2	6	18	2.41*	2.79	4.49
-2	6	19	8.08	7.96	3.54
-2	6	20	1.11*	0.20	4.75
-2	7	19	1.23*	1.10	4.72
-2	7	18	4.40	4.52	4.15
-2	7	17	4.51	4.37	4.13
-2	7	16	7.85	8.34	3.58
-2	7	15	3.74	3.99	4.25
-2	7	14	4.63	4.70	4.11
-2	7	13	8.54	8.26	3.46
-2	7	12	13.45	13.84	2.49
-2	7	11	11.63	11.46	2.86
-2	7	10	1.57*	0.25	4.65
-2	7	9	17.28	17.09	1.78
-2	7	8	0.94*	1.25	4.79
-2	7	7	9.07	8.65	3.36
-2	7	6	26.00	26.25	0.76
-2	7	5	6.67	7.23	3.78
-2	7	4	27.05	26.94	0.69
-2	7	3	3.80	3.53	4.25
-2	7	2	13.20	12.30	2.84
-2	7	1	3.78	3.62	4.25
-2	8	1	45.65	45.58	0.16
-2	8	2	17.25	16.63	1.78
-2	8	3	1.29*	0.08	4.71
-2	8	4	3.41	4.03	4.31
-2	8	5	29.25	28.62	0.56
-2	8	6	1.02*	0.72	4.77
-2	8	7	26.70	26.04	0.71
-2	8	8	5.02	5.59	4.05
-2	8	9	15.07	15.27	2.18
-2	8	10	10.73	10.99	3.04
-2	8	11	10.47	11.03	3.09
-2	8	12	7.88	7.94	3.58
-2	8	13	1.16*	1.36	4.74
-2	8	14	3.48	3.27	4.30
-2	8	15	10.64	10.66	3.06
-2	8	16	8.93	8.72	3.39
-2	8	17	5.34	4.55	4.00
-2	8	18	0.95*	0.08	4.79
-2	9	17	1.26*	0.55	4.72
-2	9	16	6.00	6.27	3.89
-2	9	15	6.63	6.54	3.79
-2	9	14	10.06	9.85	3.17
-2	9	13	7.43	7.24	3.66
-2	9	12	10.59	10.23	3.07
-2	9	11	3.11	3.81	4.36
-2	9	10	10.63	10.90	3.06
-2	9	9	10.32	10.76	3.12
-2	9	8	1.06*	0.87	4.76
-2	9	7	12.89	12.62	2.61
-2	9	6	12.97	13.28	2.59
-2	9	5	24.63	24.17	0.87
-2	9	4	1.58*	1.14	4.65
-2	9	3	1.55*	2.15	4.65
-2	9	2	19.78	19.28	1.40
-2	9	1	9.03	9.09	3.37
-2	10	1	9.34	9.57	3.31
-2	10	2	4.05	4.07	4.20
-2	10	3	4.98	5.49	4.06
-2	10	4	5.86	5.36	3.92
-2	10	5	17.00	17.26	1.83
-2	10	6	8.29	8.78	3.50
-2	10	7	1.56*	1.38	4.65
-2	10	8	0.78*	0.21	4.83
-2	10	9	4.35	4.57	4.16
-2	10	10	2.04	2.09	4.55
-2	10	11	10.27	10.15	3.13
-2	10	12	3.97	3.22	4.22
-2	10	13	8.53	8.23	3.46
-2	10	14	1.21*	0.28	4.73
-2	10	15	4.21	4.22	4.18
-2	11	14	3.89	4.13	4.23
-2	11	13	2.66*	2.38	4.44
-2	11	12	3.83	3.47	4.24
-2	11	11	1.16*	0.65	4.74
-2	11	10	1.95*	1.52	4.57
-2	11	9	2.49*	0.57	4.47
-2	11	8	1.18*	0.44	4.74
-2	11	7	5.61	5.54	3.96
-2	11	6	15.92	15.41	2.02
-2	11	5	5.67	5.71	3.85
-2	11	4	4.77	5.09	4.09
-2	11	3	1.68*	0.34	4.63
-2	11	2	7.91	7.13	3.57
-2	11	1	1.14*	1.48	4.74
-2	12	1	6.23	6.26	3.86
-2	12	2	9.06	9.11	3.36
-2	12	3	8.96	8.67	3.38
-2	12	4	8.82	8.64	3.41
-2	12	5	3.78	4.22	4.25
-2	12	6	2.49	3.10	4.47
-2	12	7	5.22	5.53	4.02
-2	12	8	1.41*	1.10	4.68
-2	12	9	7.80	7.62	3.59
-2	12	10	5.28	5.44	4.01
-2	12	11	3.67	4.10	4.27
-2	13	8	2.59	3.10	4.45
-2	13	7	8.66	9.11	3.44
-2	13	6	7.73	7.25	3.60
-2	13	5	9.63	9.59	3.26
-2	13	4	2.18*	0.96	4.63
-2	13	3	19.48	19.84	1.44
-2	13	2	9.64	9.60	3.25
-2	13	1	7.13	6.87	3.71
-1	14	1	9.31	9.66	3.32
-1	14	3	9.24	9.05	3.33
-1	14	2	1.30*	1.01	4.71
-1	14	1	1.17*	1.00	4.74
-1	13	1	11.95	11.99	2.80
-1	13	2	4.96	4.78	4.06
-1	13	3	9.71	10.27	3.24
-1	13	4	11.50	11.29	2.89
-1	13	5	9.60	9.85	3.26
-1	13	6	7.86	8.02	3.58
-1	13	7	6.41	6.47	3.83
-1	13	8	4.35	4.04	4.16
-1	13	9	4.78	4.84	4.09
-1	12	12	4.71	4.66	4.10
-1	12	11	6.89	7.53	3.75
-1	12	10	1.14*	2.44	4.74
-1	12	9	6.24	6.21	3.85
-1	12	8	6.33	6.47	3.84
-1	12	7	6.44	6.51	3.82
-1	12	6	1.53*	0.49	4.66
-1	12	5	6.13	6.31	3.87
-1	12	4	3.37	3.94	4.32
-1	12	3	3.59	3.46	4.28
-1	12	2	17.87	17.65	1.68
-1	12	1	8.88	8.97	3.40
-1	11	1	5.00	4.62	4.05
-1	11	2	5.42	5.39	3.99
-1	11	3	2.29	2.33	4.51
-1	11	4	11.84	11.60	2.82
-1	11	5	3.59	3.69	4.28
-1	11	6	2.92	2.42	4.39
-1	11	7	4.33	4.45	4.16
-1	11	8	3.78	3.46	4.25
-1	11	9	4.71	4.80	4.10
-1	11	10	5.35	4.84	4.00
-1	11	11	1.17*	0.20	4.74
-1	11	12	3.55	3.58	4.29
-1	11	13	4.25	4.32	4.17
-1	11	14	1.24*	0.89	4.72
-1	10	15	1.60*	0.51	4.64
-1	10	14	5.37	5.64	3.99
-1	10	13	2.34*	1.09	4.50
-1	10	12	1.45*	0.59	4.68
-1	10	11	9.01	8.83	3.37
-1	10	10	6.10	5.84	3.88
-1	10	9	16.23	16.42	1.96
-1	10	8	0.95*	1.62	4.79
-1	10	7	8.63	8.98	3.44
-1	10	6	1.02*	1.54	4.77
-1	10	5	3.28	3.07	4.33
-1	10	4	5.73	6.01	3.94
-1	10	3	12.64	12.51	2.66
-1	10	2	5.71	6.42	3.94
-1	10	1	17.21	17.51	1.79
-1	9	1	14.91	14.03	2.21
-1	9	2	8.15	7.99	3.53
-1	9	3	6.84	7.14	3.76
-1	9	4	23.41	23.36	0.98
-1	9	5	6.31	6.29	3.84
-1	9	6	3.46	3.77	4.30
-1	9	7	18.59	18.48	1.57
-1	9	8	15.93	16.30	2.02
-1	9	9	8.87	9.17	3.40
-1	9	10	2.11*	1.36	4.54
-1	9	11	2.75	3.20	4.42
-1	9	12	5.29	5.47	4.01
-1	9	13	4.62	4.77	4.11
-1	9	14	9.61	9.37	3.26
-1	9	15	1.90*	1.89	4.58
-1	9	16	4.80	4.75	4.08
-1	9	17	2.41*	0.86	4.49
-1	8	18	8.84	8.17	3.40
-1	8	17	1.76*	2.28	4.61
-1	8	16	5.14	4.85	4.03
-1	8	15	4.45	3.58	4.14
-1	8	14	10.28	9.84	3.13

h	k	l	Fo	Fc	weight
-1	8	13	10.39	10.82	3.11
-1	8	12	1.08*	0.37	4.76
-1	8	11	1.87*	0.54	4.57
-1	8	10	10.86	10.96	3.02
-1	8	9	17.25	17.89	1.79
-1	8	8	14.04	14.01	2.38
-1	8	7	13.27	13.00	2.53
-1	8	6	6.53	5.40	3.81
-1	8	5	34.38	33.62	0.36
-1	8	4	0.87*	0.57	4.81
-1	8	3	13.89	13.22	2.39
-1	8	2	7.70	8.08	3.61
-1	8	1	5.91	4.97	3.91
-1	7	1	29.91	27.83	0.53
-1	7	2	2.81	3.26	4.41
-1	7	3	3.57	0.16	4.28
-1	7	4	36.00	34.65	0.32
-1	7	5	6.61	6.10	3.79
-1	7	6	2.95	2.78	4.39
-1	7	7	6.95	7.49	3.74
-1	7	8	18.36	17.94	1.60
-1	7	9	2.88	2.60	4.40
-1	7	10	21.21	21.29	1.21
-1	7	11	2.57	2.13	4.46
-1	7	12	1.72*	0.72	4.62
-1	7	13	7.89	8.38	3.57
-1	7	14	13.81	14.02	2.42
-1	7	15	1.18*	2.31	4.73
-1	7	16	6.63	6.23	3.79
-1	7	17	1.21*	1.82	4.73
-1	7	18	6.89	7.09	3.75
-1	7	19	1.26*	0.47	4.72
-1	6	20	6.82	6.08	3.76
-1	6	19	1.97*	2.74	4.57
-1	6	18	2.49*	1.98	4.47
-1	6	17	12.06	12.14	2.78
-1	6	16	1.15*	1.48	4.74
-1	6	15	10.88	11.16	3.01
-1	6	14	1.44*	2.40	4.68
-1	6	13	6.18	6.24	3.86
-1	6	12	4.05	4.78	4.20
-1	6	11	10.04	9.95	3.18
-1	6	10	3.34	3.39	4.32
-1	6	9	28.67	28.75	0.79
-1	6	8	6.13	5.91	3.87
-1	6	7	0.83*	0.24	4.82
-1	6	6	4.42	4.79	4.14
-1	6	5	13.29	12.73	2.53
-1	6	4	14.43	15.12	2.30
-1	6	3	57.35	54.64	0.08
-1	6	2	26.71	25.81	0.71
-1	6	1	23.81	22.18	0.94
-1	5	1	15.71	13.20	2.06
-1	5	2	6.76	8.08	3.77
-1	5	3	10.37	9.39	3.11
-1	5	4	66.50	62.48	0.05
-1	5	5	7.90	7.13	3.57
-1	5	6	5.70	5.64	3.94
-1	5	7	22.77	22.23	1.04
-1	5	8	10.32	10.59	3.12
-1	5	9	15.52	15.54	2.09
-1	5	10	17.17	17.65	1.80
-1	5	11	5.50	5.94	3.97
-1	5	12	10.18	10.38	3.15
-1	5	13	4.15	4.77	4.19
-1	5	14	10.00	10.54	3.19
-1	5	15	2.43	2.54	4.48
-1	5	16	2.08*	0.96	4.55
-1	5	17	0.47*	0.91	4.91
-1	5	18	7.98	8.10	3.56
-1	5	19	4.39	3.92	4.15
-1	5	20	5.49	5.26	3.97
-1	4	21	5.43	5.44	3.98
-1	4	20	1.68*	1.22	4.63
-1	4	19	1.09*	2.09	4.75
-1	4	18	3.63	3.28	4.27
-1	4	17	3.27	3.27	4.33
-1	4	16	14.29	14.06	2.33
-1	4	15	7.58	7.19	3.63
-1	4	14	3.85	3.83	4.24
-1	4	13	17.60	17.87	1.73
-1	4	12	11.12	11.23	2.96
-1	4	11	4.42	3.36	4.14
-1	4	10	19.53	19.02	1.43
-1	4	9	22.33	21.13	1.09
-1	4	8	12.00	11.62	2.79
-1	4	7	62.47	61.72	0.06
-1	4	6	24.49	24.06	0.88
-1	4	5	22.05	21.27	1.12
-1	4	4	17.56	16.27	1.73
-1	4	3	23.49	22.24	0.97
-1	4	2	16.19	16.65	1.97
-1	4	1	24.20	22.08	0.91
-1	3	1	17.71	16.88	1.71
-1	3	2	5.60	5.01	3.96
-1	3	3	26.56	25.56	0.72
-1	3	4	5.11	5.38	4.04
-1	3	5	15.33	15.32	2.13
-1	3	6	32.93	31.42	0.41
-1	3	7	25.30	23.14	0.81
-1	3	8	20.85	21.45	1.26
-1	3	9	20.16	18.90	1.35
-1	3	10	4.54	4.41	4.13
-1	3	11	6.80	7.09	3.76
-1	3	12	12.78	12.81	2.63
-1	3	13	7.98	8.34	3.56
-1	3	14	13.69	14.02	2.45
-1	3	15	10.83	11.25	3.02
-1	3	16	12.21	11.75	2.74
-1	3	17	3.43	3.28	4.31
-1	3	18	1.35*	2.16	4.70
-1	3	19	3.09	3.26	4.36
-1	3	20	4.03	4.03	4.21
-1	3	21	9.31	8.80	3.32
-1	2	22	2.09	2.16	4.55
-1	2	21	1.21*	0.69	4.73
-1	2	20	7.73	7.89	3.60
-1	2	19	1.34*	1.56	4.70
-1	2	18	3.94	3.99	4.22
-1	2	17	4.36	4.60	4.15
-1	2	16	17.23	17.31	1.79
-1	2	15	2.19*	2.41	4.53
-1	2	14	19.74	21.44	1.40
-1	2	13	2.61	2.98	4.45
-1	2	12	21.71	21.46	1.16
-1	2	11	2.52	2.36	4.46
-1	2	10	37.67	37.60	0.28
-1	2	9	9.62	8.71	3.26
-1	2	8	6.05	6.05	3.88
-1	2	7	37.74	36.84	0.28
-1	2	6	42.76	44.83	0.19
-1	2	5	46.42	45.38	0.15
-1	2	4	9.46	10.45	3.29
-1	2	3	14.11	13.39	2.36
-1	2	2	64.89	63.06	0.05
-1	2	1	64.42	61.71	0.06
-1	1	1	22.05	22.71*	1.12
-1	1	2	20.36	20.32	1.32
-1	1	3	53.76	54.42	0.10
-1	1	4	20.29	20.05	1.33
-1	1	5	64.57	68.42	0.06
-1	1	6	41.87	42.58	0.20
-1	1	7	66.09	65.80	0.05
-1	1	8	22.44	21.30	1.08
-1	1	9	49.18	48.85	0.13
-1	1	10	4.70	4.98	4.10
-1	1	11	41.17	43.35	0.22
-1	1	12	4.65	4.93	4.11
-1	1	13	0.96*	0.43	4.78
-1	1	14	1.59*	1.16	4.65
-1	1	15	14.74	14.28	2.24
-1	1	16	11.88	12.49	2.81
-1	1	17	2.78	3.76	4.42
-1	1	18	4.73	4.98	4.10
-1	1	19	4.24	4.19	4.17
-1	1	20	3.67	3.40	4.27
-1	1	21	2.56*	0.08	4.46
-1	1	22	3.61	3.30	4.28
-1	0	22	7.09	6.93	3.71
-1	0	20	10.19	9.69	3.15
-1	0	18	1.20*	1.23	4.73
-1	0	16	27.13	27.61	0.68
-1	0	14	7.88	8.29	3.58
-1	0	12	22.23	22.79	1.10
-1	0	10	7.36	8.15	3.67
-1	0	8	48.87	47.98	0.13
-1	0	6	13.88	14.64	2.41
-1	0	4	53.75	56.32	0.10
0	0	2	55.16	58.14	0.09
0	0	4	90.99	96.42	0.02
0	0	6	34.78	37.46	0.35
0	0	8	36.05	37.79	0.32
0	0	10	22.35	23.69	1.09
0	0	12	12.10	12.08	2.77
0	0	14	39.42	41.07	0.24
0	0	16	10.31	11.16	3.12
0	0	18	8.12	8.33	3.53
0	0	20	8.28	8.01	3.51
0	1	21	2.43*	1.73	4.48
0	1	20	0.70*	1.11	4.85
0	1	19	2.31*	0.70	4.50
0	1	18	0.53*	0.26	4.89
0	1	17	1.08*	0.82	4.76
0	1	16	4.33	4.70	4.16
0	1	15	11.28	12.05	2.93
0	1	14	22.01	23.30	1.12
0	1	13	22.99	24.04	1.02
0	1	12	7.53	9.66	3.64
0	1	11	40.31	40.73	0.23
0	1	10	6.06	6.49	3.88
0	1	9	25.08	25.84	0.83
0	1	8	15.04	13.95	2.18
0	1	7	13.48	12.90	2.49
0	1	6	20.32	20.90	1.33
0	1	5	30.40	32.18	0.51
0	1	4	11.24	10.76	2.94
0	1	3	28.48	28.14	0.60
0	1	2	82.10	82.83	0.03
0	1	1	21.21	20.58	1.22
0	2	0	72.52	70.52	0.04
0	2	1	105.61	101.84	0.01
0	2	2	2.79	2.22	4.42
0	2	3	50.44	48.25	0.12
0	2	4	106.94	107.43	0.01
0	2	5	7.94	9.13	3.57
0	2	6	8.98	8.20	3.38
0	2	7	11.73	10.88	2.84
0	2	8	1.20*	0.41	4.73
0	2	9	0.88*	0.13	4.80
0	2	10	33.70	34.45	0.38
0	2	11	10.04	10.36	3.18
0	2	12	2.59	2.72	4.45
0	2	13	5.13	5.56	4.03
0	2	14	24.24	25.18	0.90
0	2	15	8.91	9.70	3.39
0	2	16	16.92	17.50	1.84
0	2	17	1.18*	0.43	4.73
0	2	18	12.50	12.54	2.68
0	2	19	1.18*	2.09	4.73
0	2	20	2.62	2.40	4.45
0	2	21	5.70	5.90	3.94
0	3	21	1.23*	0.48	4.72
0	3	20	1.19*	0.99	4.73
0	3	19	6.52	6.08	3.81
0	3	18	1.12*	1.36	4.75
0	3	17	5.06	5.20	4.04
0	3	16	8.15	8.98	3.53
0	3	15	6.31	6.43	3.84
0	3	14	10.34	10.59	3.12
0	3	13	22.08	23.03	1.11
0	3	12	20.91	21.94	1.25
0	3	11	14.81	14.64	2.23

h	k	l	Fo	Fc	weight
0	3	10	19.28	17.96	1.47
0	3	9	6.53	5.56	3.81
0	3	8	0.91*	1.20	4.80
0	3	7	19.74	18.11	1.40
0	3	6	3.35	2.83	4.32
0	3	5	7.12	6.44	3.71
0	3	4	3.67	3.34	4.27
0	3	3	55.07	51.65	0.09
0	3	2	34.06	32.34	0.37
0	3	1	81.96	78.08	0.03
0	4	0	20.14	20.41	1.35
0	4	1	49.28	46.55	0.13
0	4	2	33.97	31.37	0.37
0	4	3	33.93	32.16	0.38
0	4	4	47.45	41.80	0.14
0	4	5	39.64	38.60	0.24
0	4	6	8.29	7.75	3.50
0	4	7	19.71	18.45	1.41
0	4	8	19.32	19.53	1.46
0	4	9	11.18	10.76	2.85
0	4	10	7.17	6.50	3.70
0	4	11	18.09	17.72	1.65
0	4	12	13.70	14.12	2.44
0	4	13	17.22	17.49	1.79
0	4	14	23.07	22.84	1.01
0	4	15	4.87	5.00	4.07
0	4	16	10.69	11.06	3.05
0	4	17	3.91	4.26	4.23
0	4	18	2.13*	2.39	4.54
0	4	19	2.26*	1.78	4.51
0	4	20	1.17*	0.24	4.74
0	4	21	2.36*	2.54	4.49
0	5	20	8.61	8.39	3.45
0	5	19	1.18*	2.08	4.73
0	5	18	3.22	3.45	4.34
0	5	17	4.12	3.76	4.19
0	5	16	8.11	8.48	3.54
0	5	15	6.91	6.88	3.91
0	5	14	1.72*	1.41	4.62
0	5	13	12.86	12.64	2.61
0	5	12	25.44	25.89	0.80
0	5	11	10.27	10.40	3.13
0	5	10	9.06	9.86	3.36
0	5	9	14.39	13.26	2.31
0	5	8	22.10	22.08	1.11
0	5	7	33.93	32.53	0.38
0	5	6	14.40	14.04	2.31
0	5	5	8.21	7.73	3.52
0	5	4	20.14	19.44	1.35
0	5	3	34.42	33.64	0.36
0	5	2	95.53	90.45	0.02
0	5	1	4.00	2.50	4.21
0	6	0	4.88	4.73	4.07
0	6	1	39.49	38.34	0.24
0	6	2	17.21	15.74	1.79
0	6	3	5.40	4.47	3.99
0	6	4	12.19	12.00	2.75
0	6	5	13.32	11.25	2.52
0	6	6	11.74	11.01	2.84
0	6	7	6.84	7.29	3.75
0	6	8	3.72	3.39	4.26
0	6	9	24.66	24.35	0.87
0	6	10	3.64	3.02	4.27
0	6	11	1.31*	0.26	4.71
0	6	12	10.70	10.36	3.05
0	6	13	23.66	24.77	0.95
0	6	14	5.01	4.49	4.05
0	6	15	8.30	8.37	3.50
0	6	16	1.16*	2.14	4.74
0	6	17	2.10	2.42	4.54
0	6	18	8.80	8.41	3.41
0	6	19	2.09*	1.99	4.55
0	7	19	5.40	5.25	3.99
0	7	18	6.20	6.18	3.86
0	7	17	1.20*	0.69	4.73
0	7	16	11.45	11.43	2.90
0	7	15	4.68	4.90	4.10
0	7	14	1.90*	1.04	4.58
0	7	13	1.42*	1.71	4.68
0	7	12	22.19	21.90	1.10
0	7	11	5.74	5.70	3.93
0	7	10	3.27	3.29	4.33
0	7	9	3.42	3.91	4.31
0	7	8	17.68	17.38	1.71
0	7	7	4.78	4.69	4.09
0	7	6	32.09	31.97	0.44
0	7	5	4.23	3.04	4.17
0	7	4	1.25*	0.16	4.72
0	7	3	18.77	16.62	1.54
0	7	2	60.78	59.73	0.07
0	7	1	28.08	26.14	0.63
0	8	0	26.97	25.75	0.69
0	8	1	12.17	11.19	2.75
0	8	2	3.67	3.27	4.27
0	8	3	13.46	13.16	2.49
0	8	4	16.89	16.53	1.85
0	8	5	2.86	3.01	4.40
0	8	6	0.98*	0.07	4.78
0	8	7	21.86	21.47	1.14
0	8	8	6.99	6.64	3.73
0	8	9	9.33	8.83	3.31
0	8	10	7.09	6.88	3.71
0	8	11	16.77	17.20	1.87
0	8	12	3.11	3.20	4.36
0	8	13	5.24	5.20	4.01
0	8	14	1.20*	2.16	4.73
0	8	15	6.19	6.24	3.86
0	8	16	5.67	5.25	3.95
0	8	17	5.40	5.75	3.99
0	8	18	4.15	4.01	4.19
0	9	16	5.65	5.58	3.95
0	9	15	3.25	3.50	4.34
0	9	14	2.67	2.10	4.46
0	9	13	2.11*	0.68	4.54
0	9	12	14.24	13.92	2.34
0	9	11	1.70*	1.47	4.62
0	9	10	0.94*	1.51	4.79
0	9	9	5.69	6.16	3.94
0	9	8	1.97*	1.54	4.57
0	9	7	10.74	10.22	3.04
0	9	6	20.89	21.35	1.25
0	9	5	6.33	6.15	3.84
0	9	4	3.02	2.96	4.38
0	9	3	23.94	23.92	0.93
0	9	2	26.29	26.70	0.74
0	9	1	18.55	17.92	1.58
0	10	0	14.14	14.50	2.36
0	10	1	17.98	18.38	1.66
0	10	2	4.17	3.87	4.19
0	10	3	3.01	2.61	4.38
0	10	4	9.46	10.63	3.29
0	10	5	1.04*	1.21	4.77
0	10	6	6.06	6.33	3.88
0	10	7	16.59	16.50	1.90
0	10	8	8.08	8.01	3.54
0	10	9	1.86*	0.11	4.59
0	10	10	7.03	7.05	3.72
0	10	11	8.58	8.28	3.45
0	10	12	3.79	4.48	4.25
0	10	13	1.18*	1.41	4.73
0	10	14	2.36*	1.99	4.49
0	10	15	11.34	11.01	2.92
0	11	13	1.56*	1.89	4.65
0	11	12	6.63	6.58	3.78
0	11	11	3.81	3.93	4.24
0	11	10	1.18*	0.61	4.74
0	11	9	1.14*	0.10	4.74
0	11	8	4.71	4.86	4.10
0	11	7	6.26	6.33	3.85
0	11	6	2.82	2.21	4.41
0	11	5	4.94	4.98	4.06
0	11	4	2.79	2.66	4.42
0	11	3	3.58	3.41	4.28
0	11	2	1.04*	1.65	4.77
0	11	1	2.00*	2.44	4.56
0	12	0	23.61	23.50	0.96
0	12	1	1.69*	0.53	4.62
0	12	2	6.96	7.39	3.74
0	12	3	2.87	2.52	4.40
0	12	4	9.55	9.50	3.27
0	12	5	3.50	3.58	4.29
0	12	6	8.40	8.68	3.48
0	12	7	9.25	8.98	3.33
0	12	8	4.93	4.95	4.06
0	12	9	7.29	7.21	3.68
0	12	10	1.23*	1.19	4.72
0	12	11	1.48*	0.63	4.67
0	13	8	6.85	6.81	3.75
0	13	7	4.40	4.75	4.15
0	13	6	4.49	4.68	4.13
0	13	5	4.42	4.91	4.15
0	13	4	7.70	7.67	3.61
0	13	3	6.23	6.53	3.86
0	13	2	13.84	13.92	2.48
0	13	1	8.22	8.33	3.52
0	14	0	1.27*	1.09	4.71
0	14	1	6.09	6.05	3.88
0	14	2	5.55	5.54	3.97
0	14	3	2.36*	1.76	4.49
1	14	2	6.99	7.20	3.73
1	14	1	6.90	6.74	3.75
1	14	0	6.74	7.19	3.77
1	13	0	11.65	11.53	2.86
1	13	1	7.05	7.10	3.72
1	13	2	1.22*	1.82	4.73
1	13	3	5.05	5.27	4.05
1	13	4	5.16	5.45	4.03
1	13	5	2.70	2.59	4.43
1	13	6	7.41	7.56	3.66
1	13	7	4.47	4.70	4.14
1	13	8	0.99*	0.29	4.78
1	12	11	2.42*	0.17	4.48
1	12	10	3.16	3.65	4.35
1	12	9	9.88	10.38	3.21
1	12	8	3.20	3.06	4.35
1	12	7	0.93*	0.31	4.79
1	12	6	7.17	7.17	3.70
1	12	5	16.97	17.02	1.83
1	12	4	3.83	3.62	4.24
1	12	3	2.92	2.16	4.39
1	12	2	13.59	13.52	2.47
1	12	1	5.59	5.59	3.96
1	12	0	1.13*	0.08	4.75
1	11	0	3.38	3.82	4.31
1	11	1	3.65	3.15	4.27
1	11	2	6.48	6.62	3.82
1	11	3	5.15	5.58	4.03
1	11	4	3.24	2.76	4.34
1	11	5	2.29*	3.26	4.51
1	11	6	3.71	3.29	4.26
1	11	7	7.41	7.35	3.66
1	11	8	2.79	3.03	4.42
1	11	9	4.40	4.44	4.15
1	11	10	13.27	13.11	2.53
1	11	11	1.67*	0.85	4.63
1	11	12	1.90	1.95	4.58
1	11	13	9.07	9.10	3.36
1	10	15	2.05*	1.77	4.55
1	10	14	2.50*	0.94	4.47
1	10	13	10.22	9.75	3.14
1	10	12	2.35	2.35	4.50
1	10	11	2.74	2.40	4.42
1	10	10	1.13*	0.32	4.75
1	10	9	12.29	12.29	2.73
1	10	8	3.54	3.39	4.29
1	10	7	0.75*	0.79	4.83
1	10	6	17.85	18.65	1.69
1	10	5	18.17	18.13	1.64
1	10	4	9.10	9.31	3.36
1	10	3	1.79*	1.51	4.60
1	10	2	11.46	12.62	2.90
1	10	1	3.97	4.00	4.22

h	k	l	Fo	Fc	weight
1	10	0	1.92	1.93	4.58
1	9	0	21.02	21.06	1.24
1	9	1	21.16	20.88	1.22
1	9	2	12.29	11.29	2.73
1	9	3	6.39	5.85	3.83
1	9	4	40.26	40.14	0.23
1	9	5	26.01	26.31	0.76
1	9	6	14.58	14.46	2.27
1	9	7	10.77	11.08	3.03
1	9	8	4.14	3.82	4.19
1	9	9	1.89*	1.76	4.58
1	9	10	16.27	16.54	1.95
1	9	11	1.14*	0.28	4.74
1	9	12	1.60*	0.51	4.64
1	9	13	3.12	2.33	4.36
1	9	14	6.99	7.09	3.73
1	9	15	6.13	5.87	3.87
1	9	16	1.17*	1.97	4.74
1	8	17	1.24*	0.83	4.72
1	8	16	3.75	3.90	4.25
1	8	15	13.36	13.00	2.51
1	8	14	3.25	3.13	4.34
1	8	13	1.15*	1.27	4.74
1	8	12	6.50	6.86	3.81
1	8	11	2.74	3.05	4.42
1	8	10	9.70	10.26	3.24
1	8	9	23.68	24.29	0.85
1	8	8	1.68*	0.99	4.63
1	8	7	25.55	25.67	0.80
1	8	6	19.31	19.74	1.46
1	8	5	9.96	9.25	3.19
1	8	4	1.60*	1.72	4.64
1	8	3	3.63	4.47	4.27
1	8	2	15.22	14.87	2.15
1	8	1	15.78	14.75	2.04
1	8	0	2.42	2.51	4.48
1	7	0	41.67	38.04	0.21
1	7	1	27.67	26.88	0.65
1	7	2	26.49	24.78	0.73
1	7	3	15.24	16.10	2.14
1	7	4	28.57	28.60	0.60
1	7	5	0.36*	0.84	4.94
1	7	6	15.22	14.83	2.15
1	7	7	6.62	6.98	3.79
1	7	8	7.76	7.40	3.60
1	7	9	26.90	27.81	0.70
1	7	10	24.14	23.98	0.91
1	7	11	5.57	5.61	3.96
1	7	12	4.11	3.65	4.19
1	7	13	1.41*	0.71	4.68
1	7	14	5.28	5.44	4.01
1	7	15	3.33	3.53	4.32
1	7	16	5.09	5.04	4.04
1	7	17	1.20*	0.63	4.73
1	7	18	1.16*	2.29	4.74
1	6	19	1.38*	1.75	4.69
1	6	16	4.03	3.74	4.21
1	6	17	4.50	4.65	4.13
1	6	16	10.38	10.11	3.11
1	6	15	11.49	11.89	2.89
1	6	14	3.83	3.34	4.24
1	6	13	0.68*	0.84	4.85
1	6	12	0.59*	0.27	4.88
1	6	11	48.11	48.11	0.13
1	6	10	16.56	17.52	1.90
1	6	9	10.74	9.52	3.04
1	6	8	11.17	10.96	2.95
1	6	7	24.24	24.28	0.37
1	6	6	14.07	14.12	2.37
1	6	5	26.63	25.93	0.72
1	6	4	4.49	3.88	4.13
1	6	3	34.26	32.74	0.37
1	6	2	8.71	8.26	3.43
1	6	1	35.13	33.03	0.34
1	6	0	23.61	21.11	0.96
1	5	0	50.21	48.29	0.12
1	5	1	5.81	4.06	3.92
1	5	2	20.43	19.45	1.31
1	5	3	10.34	9.81	3.12
1	5	4	14.81	13.45	2.21
1	5	5	29.33	26.95	0.56
1	5	6	20.82	20.56	1.26
1	5	7	40.14	39.10	0.23
1	5	8	13.28	11.50	2.53
1	5	9	31.56	30.90	0.46
1	5	10	11.34	12.21	2.92
1	5	11	16.94	16.91	1.84
1	5	12	12.15	12.48	2.76
1	5	13	9.18	10.17	3.34
1	5	14	5.05	4.72	4.04
1	5	15	2.42	2.59	4.48
1	5	16	10.19	10.32	3.15
1	5	17	1.73*	1.32	4.62
1	5	18	6.31	6.30	3.84
1	5	19	1.20*	0.42	4.73
1	5	20	2.67*	2.00	4.44
1	4	20	4.12	3.87	4.19
1	4	19	1.18*	1.80	4.73
1	4	18	3.91	3.63	4.23
1	4	17	1.11*	0.05	4.75
1	4	16	12.23	12.56	2.74
1	4	15	10.06	10.63	3.17
1	4	14	1.07*	0.32	4.76
1	4	13	1.05*	1.42	4.76
1	4	12	28.22	27.78	0.62
1	4	11	4.68	5.19	4.10
1	4	10	19.31	18.69	1.46
1	4	9	21.54	21.08	1.18
1	4	8	17.10	17.50	1.81
1	4	7	5.72	6.31	3.94
1	4	6	21.32	21.49	1.20
1	4	5	8.15	7.83	3.53
1	4	4	16.84	16.93	1.85
1	4	3	11.48	10.64	2.89
1	4	2	4.54	3.73	4.13
1	4	1	70.00	67.15	0.04
1	4	0	46.27	40.89	0.15
1	3	0	99.59	95.64	0.01
1	3	1	24.59	23.22	0.87
1	3	2	24.86	24.24	0.85
1	3	3	39.91	38.99	0.24
1	3	4	26.93	26.17	0.70
1	3	5	9.41	9.11	3.30
1	3	6	12.48	11.38	2.69
1	3	7	8.61	7.83	3.45
1	3	8	24.66	22.11	0.87
1	3	9	24.25	22.42	0.90
1	3	10	18.82	18.31	1.54
1	3	11	17.57	18.30	1.73
1	3	12	15.05	14.54	2.18
1	3	13	10.91	12.01	3.01
1	3	14	12.41	12.94	2.70
1	3	15	3.72	3.42	4.26
1	3	16	2.86	3.28	4.40
1	3	17	9.56	8.79	3.27
1	3	18	1.98	2.53	4.57
1	3	19	1.64*	0.67	4.63
1	3	20	2.02*	1.14	4.56
1	2	21	2.38	2.62	4.49
1	2	21	0.52*	0.02	4.89
1	2	20	2.38*	2.72	4.49
1	2	19	2.45*	1.96	4.48
1	2	18	7.21	7.06	3.69
1	2	17	1.11*	1.92	4.75
1	2	16	13.63	14.14	2.46
1	2	15	6.69	7.28	3.78
1	2	14	26.03	26.55	0.76
1	2	13	11.23	11.34	2.94
1	2	12	14.12	15.22	2.36
1	2	11	14.53	15.32	2.28
1	2	10	10.38	10.89	3.11
1	2	9	1.36*	0.83	4.70
1	2	8	33.31	36.22	0.40
1	2	7	2.79	2.75	4.42
1	2	6	5.43	4.14	3.98
1	2	5	13.93	13.11	2.40
1	2	4	32.61	33.12	0.42
1	2	3	43.53	42.07	0.18
1	2	2	39.60	39.03	0.24
1	2	1	11.96	10.80	2.80
1	2	0	53.42	52.40	0.10
1	1	0	107.89	111.42	0.01
1	1	1	74.83	75.94	0.04
1	1	2	21.84	22.23	1.14
1	1	3	53.08	54.84	0.10
1	1	4	20.69	20.43	1.28
1	1	5	81.73	83.44	0.03
1	1	6	5.00	4.60	4.05
1	1	7	8.30	10.17	3.50
1	1	8	24.17	24.53	0.91
1	1	9	63.26	62.00	0.06
1	1	10	5.62	6.08	3.95
1	1	11	12.93	14.26	2.60
1	1	12	11.69	11.95	2.85
1	1	13	28.81	28.86	0.59
1	1	14	11.55	12.13	2.88
1	1	15	7.22	7.46	3.69
1	1	16	14.38	15.10	2.31
1	1	17	7.12	7.46	3.71
1	1	18	2.04*	2.70	4.55
1	1	19	5.97	6.07	3.90
1	1	20	1.20*	1.44	4.73
1	1	21	1.21*	0.13	4.73
1	0	20	2.63	2.76	4.44
1	0	18	6.60	6.34	3.80
1	0	16	3.81	4.09	4.24
1	0	14	6.23	7.22	3.86
1	0	12	10.32	12.22	3.02
1	0	10	8.80	7.69	3.41
1	0	8	0.77*	3.04	4.83
1	0	6	33.96	35.30	0.37
1	0	4	82.83	87.15	0.03
1	0	2	154.48	172.00	0.00
1	0	0	10.68	11.11	3.05
2	0	0	117.32	125.64	0.01
2	0	2	85.88	91.64	0.02
2	0	4	25.93	25.44	0.77
2	0	6	17.97	17.02	1.67
2	0	8	28.03	28.58	0.63
2	0	10	0.84*	2.29	4.81
2	0	12	16.11	16.57	1.98
2	0	14	2.21*	3.44	4.52
2	0	16	2.61	2.78	4.45
2	0	18	3.47	2.81	4.30
2	0	20	1.19*	0.58	4.73
2	1	20	5.37	5.29	3.99
2	1	19	2.25*	0.24	4.51
2	1	18	6.98	6.50	3.73
2	1	17	5.63	5.45	3.95
2	1	16	2.72	3.64	4.43
2	1	15	12.68	12.72	2.65
2	1	14	6.51	6.88	3.81
2	1	13	0.99*	1.29	4.78
2	1	12	11.49	11.57	2.89
2	1	11	38.22	38.35	0.27
2	1	10	6.07	5.38	3.88
2	1	9	10.58	9.62	3.07
2	1	8	13.70	13.09	2.44
2	1	7	58.52	58.94	0.07
2	1	6	18.31	17.92	1.61
2	1	5	22.29	20.11	1.09
2	1	4	12.36	12.37	2.71
2	1	3	4.73	5.80	4.10
2	1	2	4.61	4.27	4.11
2	1	1	99.48	105.37	0.01
2	1	0	11.80	11.78	2.81
2	2	0	36.01	35.74	0.32
2	2	1	49.27	49.12	0.13
2	2	2	2.02	1.55	4.56
2	2	3	36.98	34.68	0.29
2	2	4	2.54	1.36	4.46
2	2	5	28.82	28.98	0.59

h	k	l	Fo	Fc	weight
2	2	6	18.12	18.47	1.64
2	2	7	22.09	22.06	1.11
2	2	8	9.11	9.41	3.35
2	2	10	2.88	2.16	4.40
2	2	11	11.00	11.38	2.99
2	2	12	19.20	19.49	1.48
2	2	13	1.60*	2.52	4.64
2	2	14	20.29	21.46	1.33
2	2	15	3.64	3.80	4.27
2	2	16	9.91	10.13	3.20
2	2	17	0.98*	2.81	4.78
2	2	18	1.41*	0.38	4.68
2	2	19	2.35*	0.79	4.50
2	2	20	6.57	6.21	3.80
2	3	20	2.09*	1.37	4.54
2	3	19	1.15*	0.97	4.74
2	3	18	2.13*	1.61	4.64
2	3	17	1.77*	2.15	4.61
2	3	16	7.07	7.06	3.72
2	3	15	11.17	11.20	2.95
2	3	14	2.13*	1.49	4.54
2	3	13	1.49*	1.93	4.67
2	3	12	11.31	11.96	2.93
2	3	11	16.51	16.32	1.91
2	3	10	11.14	11.45	2.96
2	3	9	4.10	3.92	4.20
2	3	8	7.23	6.43	3.69
2	3	7	40.67	39.55	0.22
2	3	6	17.95	18.39	1.67
2	3	5	12.99	12.77	2.59
2	3	4	32.06	29.88	0.44
2	3	3	39.53	38.13	0.24
2	3	2	87.95	82.88	0.02
2	3	1	47.10	46.81	0.14
2	3	0	2.21	2.82	4.52
2	4	0	80.02	74.34	0.03
2	4	1	15.93	14.29	2.02
2	4	2	29.07	25.60	0.57
2	4	3	18.82	16.87	1.54
2	4	4	52.19	48.49	0.11
2	4	5	15.38	15.66	2.12
2	4	6	10.28	8.77	3.13
2	4	7	10.90	9.91	3.01
2	4	8	7.68	7.95	3.61
2	4	9	9.79	9.44	3.23
2	4	10	29.09	28.46	0.57
2	4	11	0.98*	0.39	4.78
2	4	12	17.87	18.24	1.68
2	4	13	15.92	15.98	2.02
2	4	14	17.07	17.37	1.82
2	4	15	7.37	7.35	3.67
2	4	16	3.01	3.71	4.38
2	4	17	4.21	3.86	4.18
2	4	18	4.91	5.14	4.07
2	4	19	5.27	4.96	4.01
2	5	19	1.26*	1.60	4.72
2	5	18	2.77*	3.98	4.42
2	5	17	2.99	2.72	4.38
2	5	16	4.49	4.99	4.13
2	5	15	2.53*	3.17	4.46
2	5	14	10.20	10.34	3.15
2	5	13	5.96	6.26	3.90
2	5	12	3.70	4.18	4.26
2	5	11	2.16	2.88	4.53
2	5	10	5.58	4.67	3.96
2	5	9	23.60	23.33	0.96
2	5	8	4.37	4.79	4.15
2	5	7	1.04*	1.76	4.77
2	5	6	28.55	26.50	0.60
2	5	5	23.70	22.95	0.95
2	5	4	7.23	7.92	3.69
2	5	3	2.26	0.22	4.51
2	5	2	16.96	14.88	1.83
2	5	1	11.59	12.69	2.87
2	5	0	25.85	25.95	0.77
2	6	0	28.75	28.22	0.59
2	6	1	10.79	11.14	3.03
2	6	2	11.93	10.71	2.80
2	6	3	48.17	47.19	0.13
2	6	4	21.55	21.24	1.17
2	6	5	7.85	7.34	3.58
2	6	6	16.07	16.29	1.99
2	6	7	17.68	17.50	1.71
2	6	8	9.75	10.60	3.23
2	6	9	53.31	54.79	0.10
2	6	10	2.51	3.14	4.47
2	6	11	5.17	5.31	4.03
2	6	12	4.37	4.71	4.15
2	6	13	18.14	18.74	1.64
2	6	14	10.93	10.87	3.00
2	6	15	5.44	5.72	3.98
2	6	16	7.99	7.59	3.56
2	6	17	2.78	3.50	4.42
2	6	18	5.13	5.31	4.03
2	7	17	1.20*	1.09	4.73
2	7	16	1.32*	1.40	4.70
2	7	15	1.24*	1.56	4.72
2	7	14	7.47	7.46	3.65
2	7	13	2.33*	0.72	4.50
2	7	12	10.26	10.23	3.13
2	7	11	25.40	25.13	0.81
2	7	10	17.10	16.02	1.81
2	7	9	3.28	3.18	4.33
2	7	8	19.06	18.85	1.50
2	7	7	27.32	28.35	0.67
2	7	6	17.46	16.65	1.75
2	7	5	15.70	15.77	2.06
2	7	4	19.53	18.55	1.43
2	7	3	2.72	1.84	4.43
2	7	2	17.32	16.69	1.77
2	7	1	14.31	14.47	2.32
2	7	0	33.01	31.75	0.41
2	8	0	0.95*	0.05	4.79
2	8	1	1.92*	0.19	4.58
2	8	2	16.12	16.28	1.98
2	8	3	0.94*	1.43	4.79
2	8	4	2.10	1.14	4.54
2	8	5	34.97	35.06	0.34
2	8	6	7.04	6.59	3.72
2	8	7	22.74	23.09	1.04
2	8	8	8.14	8.90	3.53
2	8	9	2.62	2.66	4.45
2	8	10	2.34*	3.55	4.50
2	8	11	8.15	8.18	3.53
2	8	12	6.17	6.03	3.87
2	8	13	21.85	21.97	1.14
2	8	14	1.26*	1.15	4.72
2	8	15	1.33*	0.42	4.70
2	8	16	4.60	4.34	4.12
2	9	15	4.63	4.31	4.11
2	9	14	4.33	4.30	4.16
2	9	13	4.54	4.79	4.13
2	9	12	8.60	8.59	3.45
2	9	11	1.33*	0.03	4.70
2	9	10	9.28	9.55	3.32
2	9	9	2.54*	3.38	4.46
2	9	8	22.05	21.93	1.12
2	9	7	9.99	10.14	3.19
2	9	6	12.03	11.82	2.78
2	9	5	5.29	5.48	4.01
2	9	4	9.17	8.60	3.34
2	9	3	15.89	16.55	2.02
2	9	2	40.89	41.03	0.22
2	9	1	3.30	2.61	4.33
2	9	0	21.60	21.75	1.17
2	10	0	4.95	5.43	4.06
2	10	1	5.95	5.85	3.90
2	10	2	1.04*	0.76	4.77
2	10	3	14.24	14.06	2.34
2	10	4	16.31	16.70	1.95
2	10	5	6.96	6.85	3.74
2	10	6	0.77*	0.89	4.83
2	10	7	6.18	6.14	3.86
2	10	8	1.99*	0.83	4.56
2	10	9	18.58	18.11	1.57
2	10	10	2.54*	2.62	4.46
2	10	11	5.10	5.20	4.04
2	10	12	2.40	2.51	4.49
2	10	13	5.86	5.89	3.92
2	10	14	3.90	4.10	4.23
2	11	12	7.73	7.74	3.60
2	11	11	7.54	7.26	3.64
2	11	10	0.80*	0.28	4.90
2	11	9	3.20	3.27	4.34
2	11	8	8.57	8.37	3.45
2	11	7	5.88	5.94	3.91
2	11	6	4.85	4.66	4.08
2	11	5	6.31	5.89	3.84
2	11	4	7.63	7.96	3.62
2	11	3	7.07	7.48	3.72
2	11	2	7.22	6.75	3.69
2	11	1	4.09	3.78	4.20
2	11	0	9.95	10.54	3.19
2	12	0	8.21	8.30	3.52
2	12	1	5.60	5.28	3.96
2	12	2	9.52	9.18	3.28
2	12	3	10.12	10.67	3.16
2	12	4	6.82	7.05	3.76
2	12	5	11.72	11.00	2.84
2	12	6	8.27	8.49	3.51
2	12	7	14.88	15.05	2.21
2	12	8	7.37	7.91	3.67
2	12	9	5.79	6.02	3.93
2	12	10	4.42	4.22	4.14
2	13	7	5.89	6.00	3.91
2	13	6	3.06	2.90	4.37
2	13	5	4.07	3.96	4.20
2	13	4	1.23*	1.72	4.72
2	13	3	1.24*	1.58	4.72
2	13	2	8.39	8.87	3.49
2	13	-1	10.29	10.54	3.13
2	13	0	7.58	7.78	3.63
3	13	0	4.20	4.13	4.18
3	13	1	2.16	2.81	4.53
3	13	2	3.31	3.85	4.33
3	13	3	2.13*	1.11	4.54
3	13	4	1.31*	1.54	4.71
3	13	5	2.74*	2.64	4.43
3	12	9	2.21*	0.31	4.52
3	12	8	10.55	10.73	3.08
3	12	7	15.97	16.13	2.01
3	12	6	10.82	10.45	3.02
3	12	5	11.09	10.90	2.97
3	12	4	6.18	5.75	3.86
3	12	3	18.79	18.69	1.54
3	12	2	4.19	4.54	4.18
3	12	1	1.97	1.51	4.57
3	12	0	18.06	17.53	1.65
3	11	0	4.84	5.68	4.08
3	11	1	6.37	6.05	3.83
3	11	2	13.93	14.41	2.40
3	11	3	1.13*	1.82	4.75
3	11	4	1.14*	1.99	4.74
3	11	5	3.28	3.29	4.33
3	11	6	6.69	6.92	3.78
3	11	7	3.13	3.44	4.36
3	11	8	0.79*	1.30	4.83
3	11	9	8.57	8.70	3.45
3	11	10	5.07	5.31	4.04
3	11	11	1.96*	3.18	4.57
3	10	13	1.20*	1.30	4.73
3	10	12	8.75	8.86	3.42
3	10	11	15.95	16.27	2.01
3	10	10	1.44*	0.06	4.68
3	10	9	0.84*	1.09	4.81
3	10	8	0.95*	0.79	4.79
3	10	7	22.14	22.54	1.11
3	10	6	1.21*	2.17	4.73
3	10	5	5.01	4.82	4.05
3	10	4	6.99	6.72	3.73
3	10	3	19.46	19.06	1.44
3	10	2	9.41	9.78	3.30

h	k	l	Fo	Fc	weight
3	10	1	7.23	6.86	3.69
3	10	0	2.07*	0.41	4.65
3	9	0	17.18	16.82	1.80
3	9	1	20.71	20.88	1.28
3	9	2	9.83	9.32	3.22
3	9	3	1.25*	0.55	4.72
3	9	4	5.16	4.81	4.03
3	9	5	11.74	12.69	2.84
3	9	6	18.14	18.39	1.64
3	9	7	7.99	7.75	3.56
3	9	8	16.91	16.96	1.84
3	9	9	7.67	6.86	3.61
3	9	10	6.03	5.93	3.89
3	9	11	3.09	3.91	4.36
3	9	12	6.43	6.39	3.82
3	9	13	1.25*	2.59	4.72
3	9	14	6.18	6.03	3.86
3	8	16	1.28*	1.11	4.71
3	8	15	5.63	5.70	3.95
3	8	14	6.58	6.17	3.80
3	8	13	3.38	3.52	4.31
3	8	12	4.03	3.97	4.21
3	8	11	12.19	12.32	2.75
3	8	10	2.24*	2.50	4.52
3	8	9	4.75	4.98	4.09
3	8	8	1.18*	3.27	4.73
3	8	7	10.27	10.69	3.13
3	8	6	2.97	2.87	4.39
3	8	5	18.14	17.37	1.64
3	8	4	22.65	22.88	1.05
3	8	3	42.47	42.75	0.20
3	8	2	23.08	22.45	1.01
3	8	1	1.88*	0.53	4.59
3	8	0	18.03	18.52	1.66
3	7	0	0.89*	0.18	4.80
3	7	1	7.11	7.09	3.71
3	7	2	20.53	19.31	1.30
3	7	3	10.85	10.38	3.02
3	7	4	29.47	29.04	0.55
3	7	5	24.01	23.97	0.92
3	7	6	12.01	11.66	2.79
3	7	7	2.85	2.87	4.41
3	7	8	32.23	31.75	0.43
3	7	9	33.78	34.12	0.38
3	7	10	13.41	13.26	2.50
3	7	11	5.52	4.93	3.97
3	7	12	15.65	14.49	2.07
3	7	13	1.63*	1.74	4.64
3	7	14	2.69	1.85	4.43
3	7	15	6.00	6.08	3.89
3	7	16	5.49	5.33	3.97
3	7	17	1.94*	2.39	4.57
3	6	17	5.03	5.37	4.05
3	6	16	1.84*	0.95	4.59
3	6	15	1.78*	2.02	4.61
3	6	14	6.39	6.22	3.83
3	6	13	8.62	8.64	3.44
3	6	12	1.17*	1.74	4.74
3	6	11	21.77	21.92	1.15
3	6	10	4.65	4.65	4.11
3	6	9	10.09	10.44	3.17
3	6	8	1.33*	0.31	4.70
3	6	7	36.69	37.52	0.30
3	6	6	23.38	23.03	0.98
3	6	5	4.73	4.25	4.10
3	6	4	22.91	22.87	1.03
3	6	3	12.18	12.32	2.75
3	6	2	13.89	14.26	2.41
3	6	1	31.09	30.16	0.48
3	6	0	6.31	7.35	3.84
3	5	0	3.85	3.27	4.24
3	5	1	36.12	33.27	0.31
3	5	2	10.21	9.76	3.14
3	5	3	2.58	2.89	4.45
3	5	4	23.75	21.63	0.95
3	5	5	30.51	30.46	0.50
3	5	6	3.36	3.21	4.32
3	5	7	23.63	22.62	0.96
3	5	8	18.92	16.04	2.02
3	5	9	10.73	10.18	3.04
3	5	10	4.31	4.78	4.16
3	5	11	7.84	8.35	3.58
3	5	12	5.84	5.99	3.92
3	5	13	4.80	4.42	4.08
3	5	14	6.04	5.99	3.89
3	5	15	6.48	6.10	3.81
3	5	16	11.73	11.32	2.84
3	5	17	5.18	5.49	4.02
3	5	18	2.58*	0.98	4.45
3	4	19	1.94*	2.41	4.57
3	4	18	3.31	2.98	4.33
3	4	17	5.62	5.61	3.95
3	4	16	1.37*	1.15	4.69
3	4	15	1.07*	0.19	4.76
3	4	14	4.03	3.17	4.21
3	4	13	10.23	10.47	3.14
3	4	12	3.31	4.06	4.33
3	4	11	10.15	9.98	3.16
3	4	10	9.91	10.16	3.20
3	4	9	3.76	3.76	4.25
3	4	8	15.20	16.01	2.15
3	4	7	2.35	1.04	4.50
3	4	6	10.30	10.39	3.13
3	4	5	1.56*	0.59	4.65
3	4	4	16.80	14.07	1.91
3	4	3	8.39	8.35	3.49
3	4	2	67.02	69.38	0.05
3	4	1	14.37	11.97	2.31
3	4	0	17.05	14.33	1.82
3	3	0	59.20	56.40	0.07
3	3	1	40.63	39.69	0.22
3	3	2	24.23	20.79	0.90
3	3	3	11.07	11.33	2.87
3	3	4	23.72	20.03	0.95
3	3	5	49.13	47.66	0.13
3	3	6	13.08	11.77	2.57
3	3	7	11.68	11.72	2.85
3	3	8	3.88	4.68	4.23
3	3	9	32.24	32.51	0.43
3	3	10	8.50	8.99	3.47
3	3	11	1.88*	2.71	4.59
3	3	12	2.89	3.07	4.40
3	3	13	17.26	16.95	1.78
3	3	14	3.49	3.81	4.30
3	3	15	8.17	7.59	3.53
3	3	16	4.87	4.75	4.07
3	3	17	6.43	6.61	3.82
3	3	18	1.18*	1.04	4.73
3	3	19	7.22	6.66	3.69
3	2	19	1.75*	1.15	4.61
3	2	18	13.37	13.36	2.51
3	2	17	1.36*	1.70	4.69
3	2	16	5.17	4.70	4.03
3	2	15	13.12	13.41	2.56
3	2	14	4.52	4.30	4.13
3	2	13	7.50	7.79	3.64
3	2	12	13.33	14.15	2.52
3	2	11	15.14	15.21	2.16
3	2	10	28.09	27.25	0.63
3	2	9	8.78	9.19	3.41
3	2	8	12.13	10.98	2.76
3	2	7	6.27	6.48	3.85
3	2	6	2.79	2.18	4.42
3	2	5	18.16	17.97	1.64
3	2	4	32.33	32.38	0.43
3	2	3	2.34	1.78	4.50
3	2	2	74.76	74.42	0.04
3	2	1	17.58	15.73	1.73
3	2	0	22.10	20.08	1.11
3	1	0	22.18	21.72	1.10
3	1	1	9.85	11.78	3.21
3	1	2	8.66	8.74	3.44
3	1	3	8.56	8.31	3.46
3	1	4	16.84	17.16	1.86
3	1	5	47.21	48.75	0.14
3	1	6	9.77	8.78	3.23
3	1	7	17.64	16.51	1.72
3	1	8	2.25	2.84	4.52
3	1	9	33.37	34.17	0.39
3	1	10	3.93	3.88	4.22
3	1	11	1.94*	3.17	4.57
3	1	12	10.30	10.42	3.13
3	1	13	6.18	5.86	3.86
3	1	14	1.02*	0.66	4.77
3	1	15	10.02	9.80	3.18
3	1	16	10.78	10.81	3.03
3	1	17	1.27*	0.39	4.72
3	1	18	4.62	4.50	4.11
3	1	19	6.24	6.19	3.85
3	1	20	3.62	3.83	4.27
3	0	20	9.97	9.41	3.19
3	0	18	3.94	3.80	4.22
3	0	16	2.06	0.91	4.55
3	0	14	12.50	12.33	2.69
3	0	12	0.68*	0.35	4.85
3	0	10	12.55	12.60	2.67
3	0	8	0.78*	0.87	4.83
3	0	6	44.78	44.65	0.17
3	0	4	3.02	1.32	4.38
3	0	2	31.19	30.41	0.47
3	0	0	21.41	23.74	1.19
4	0	0	2.44	1.77	4.48
4	0	2	4.87	5.12	4.07
4	0	4	16.44	16.40	1.92
4	0	6	7.39	6.50	3.66
4	0	8	19.01	18.95	1.51
4	0	10	11.72	11.41	2.84
4	0	12	31.12	32.03	0.48
4	0	14	3.61	4.34	4.28
4	0	16	5.69	5.78	3.94
4	0	18	13.68	13.13	2.45
4	1	19	4.39	4.00	4.15
4	1	18	8.53	8.67	3.46
4	1	17	4.89	4.75	4.07
4	1	16	0.34*	1.95	4.94
4	1	15	2.10	2.18	4.54
4	1	14	0.89*	2.00	4.80
4	1	13	10.17	10.17	3.15
4	1	12	1.00*	0.21	4.78
4	1	11	7.62	7.38	3.62
4	1	10	4.13	4.53	4.19
4	1	9	9.21	8.17	3.34
4	1	8	10.87	11.57	3.01
4	1	7	39.16	39.40	0.25
4	1	6	0.84*	0.16	4.81
4	1	5	28.29	27.88	0.61
4	1	4	14.19	14.79	2.35
4	1	3	18.43	19.46	1.59
4	1	2	11.06	11.77	2.98
4	1	1	35.53	36.06	0.33
4	1	0	4.59	4.76	4.12
4	2	0	28.10	27.70	0.63
4	2	1	19.10	19.90	1.49
4	2	2	43.60	43.27	0.18
4	2	3	8.63	8.38	3.44
4	2	4	8.41	8.04	3.48
4	2	5	0.78*	1.35	4.83
4	2	6	15.53	14.76	2.08
4	2	7	4.77	4.60	4.09
4	2	8	38.69	38.89	0.26
4	2	9	17.68	18.09	1.71
4	2	10	2.16*	3.52	4.53
4	2	11	1.15*	0.85	4.74
4	2	12	7.55	7.48	3.63
4	2	13	26.67	26.71	0.71
4	2	14	5.95	5.37	3.90
4	2	15	1.48*	1.68	4.67
4	2	16	14.98	15.33	2.19
4	2	17	1.87*	3.02	4.59
4	2	18	2.50*	0.28	4.47
4	3	18	1.24*	0.97	4.72
4	3	17	5.17	5.06	4.03

h	k	l	Fo	Fc	weight
4	3	16	2.44*	3.21	4.48
4	3	15	10.49	11.02	3.09
4	3	14	3.86	4.02	4.24
4	3	13	7.91	7.70	3.57
4	3	12	5.03	5.29	4.05
4	3	11	28.71	29.33	0.59
4	3	10	1.85*	1.81	4.59
4	3	9	3.24	3.27	4.34
4	3	8	11.23	10.92	2.94
4	3	7	25.72	25.76	0.78
4	3	6	11.94	12.33	2.80
4	3	5	6.18	5.41	3.86
4	3	4	2.66	2.09	4.44
4	3	3	27.70	25.88	0.65
4	3	2	58.60	55.29	0.07
4	3	1	10.93	10.05	3.00
4	3	0	15.55	13.59	2.09
4	4	0	45.61	41.07	0.16
4	4	1	9.39	9.24	3.30
4	4	2	16.65	14.86	1.89
4	4	3	11.29	10.82	2.93
4	4	4	1.38*	0.31	4.69
4	4	5	3.12	4.46	4.36
4	4	6	2.30	1.38	4.50
4	4	7	9.98	9.54	3.19
4	4	8	17.17	16.81	1.80
4	4	9	13.92	14.01	2.40
4	4	10	6.64	6.03	3.78
4	4	11	6.23	6.74	3.86
4	4	12	15.26	15.04	2.14
4	4	13	1.46*	2.12	4.67
4	4	14	5.35	4.80	4.00
4	4	15	4.83	4.97	4.08
4	4	16	1.98*	1.55	4.57
4	4	17	3.22	3.66	4.34
4	4	18	4.58	4.37	4.12
4	5	17	2.47	2.94	4.47
4	5	16	1.19*	0.48	4.73
4	5	15	9.20	9.47	3.34
4	5	14	13.13	12.83	2.56
4	5	13	6.79	6.65	3.76
4	5	12	1.76*	1.92	4.61
4	5	11	0.97*	0.16	4.78
4	5	10	15.93	16.78	2.02
4	5	9	8.58	8.76	3.45
4	5	8	0.84*	2.23	4.81
4	5	7	18.54	19.44	1.58
4	5	6	11.20	11.65	2.95
4	5	5	3.09	2.39	4.36
4	5	4	3.94	4.41	4.22
4	5	3	18.80	17.95	1.54
4	5	2	20.45	20.03	1.31
4	5	1	7.07	6.28	3.72
4	5	0	16.09	15.48	1.99
4	6	0	24.84	25.15	0.85
4	6	1	6.80	5.99	3.76
4	6	2	10.24	9.80	3.14
4	6	3	2.58	2.27	4.45
4	6	4	6.87	7.59	3.75
4	6	5	36.36	35.33	0.31
4	6	6	10.55	10.25	3.08
4	6	7	12.24	12.18	2.74*
4	6	8	2.24	3.28	4.52
4	6	9	20.61	21.35	1.29
4	6	10	9.84	9.56	3.21
4	6	11	14.26	14.60	2.33
4	6	12	5.97	6.49	3.90
4	6	13	1.67*	2.31	4.63
4	6	14	5.46	4.77	3.98
4	6	15	4.47	4.52	4.14
4	6	16	4.47	4.43	4.14
4	7	16	1.23*	1.05	4.72
4	7	15	5.34	5.03	4.00
4	7	14	11.06	10.95	2.97
4	7	13	5.73	5.48	3.94
4	7	12	4.50	4.08	4.13
4	7	11	7.68	7.70	3.61
4	7	10	18.62	18.56	1.57
4	7	9	10.10	9.76	3.17
4	7	8	1.17*	0.33	4.74
4	7	7	22.79	22.24	1.04
4	7	6	39.02	38.89	0.25
4	7	5	3.48	3.70	4.30
4	7	4	0.79*	1.50	4.83
4	7	3	11.74	11.63	2.84
4	7	2	14.15	15.34	2.36
4	7	1	6.58	5.87	3.80
4	7	0	29.25	28.63	0.56
4	8	0	36.82	37.60	0.30
4	8	1	43.97	43.33	0.18
4	8	2	13.95	14.90	2.39
4	8	3	2.22*	0.31	4.52
4	8	4	11.22	11.71	2.94
4	8	5	6.97	7.16	3.73
4	8	6	7.06	7.44	3.72
4	8	7	12.46	12.86	2.69
4	8	8	2.10	2.66	4.54
4	8	9	6.93	7.19	3.74
4	8	10	7.09	7.33	3.71
4	8	11	6.98	7.51	3.73
4	8	12	5.51	5.25	3.97
4	8	13	1.20*	1.71	4.73
4	8	14	1.79*	1.73	4.61
4	8	15	8.87	8.87	3.40
4	9	13	5.27	5.20	4.01
4	9	12	13.67	13.27	2.45
4	9	11	10.72	10.67	3.04
4	9	10	10.81	11.15	3.02
4	9	9	1.94*	1.28	4.57
4	9	8	5.51	5.84	3.97
4	9	7	3.96	3.42	4.22
4	9	6	16.12	16.38	1.98
4	9	5	1.80*	1.78	4.60
4	9	4	2.27*	2.78	4.51
4	9	3	5.41	5.91	3.99
4	9	2	1.79*	1.57	4.60
4	9	1	1.24*	2.13	4.72
4	9	0	19.71	20.76	1.41
4	10	0	12.01	11.61	2.79
4	10	1	14.54	14.25	2.28
4	10	2	6.05	5.17	3.89
4	10	3	2.54	2.85	4.46
4	10	4	1.03*	0.95	4.77
4	10	5	15.70	15.17	2.06
4	10	6	1.15*	0.14	4.74
4	10	7	4.59	4.69	4.12
4	10	8	1.21*	0.45	4.73
4	10	9	13.61	13.93	2.46
4	10	10	8.75	8.93	3.42
4	10	11	8.12	7.88	3.54
4	10	12	2.05*	1.50	4.55
4	11	10	2.09	2.45	4.54
4	11	9	4.98	4.70	4.06
4	11	8	1.24*	1.78	4.72
4	11	7	9.22	9.36	3.33
4	11	6	3.28	3.66	4.33
4	11	5	5.46	5.42	3.98
4	11	4	5.12	5.24	4.03
4	11	3	1.16*	1.02	4.74
4	11	2	9.61	10.35	3.26
4	11	1	2.17*	1.93	4.53
4	11	0	12.05	11.81	2.78
4	12	0	3.57	3.35	4.28
4	12	1	18.70	19.03	1.55
4	12	2	2.79*	2.15	4.42
4	12	3	7.10	7.34	3.71
4	12	4	10.62	10.47	3.06
4	12	5	15.42	15.40	2.11
4	12	6	8.01	7.90	3.55
4	12	7	1.05*	0.51	4.76
4	13	3	1.68*	2.08	4.63
4	13	2	1.25*	1.11	4.72
4	13	1	1.29*	1.90	4.71
4	13	0	7.06	7.34	3.72
5	12	5	1.28*	0.64	4.71
5	12	4	2.62*	1.89	4.45
5	12	3	14.75	14.71	2.24
5	12	2	7.74	7.40	3.60
5	12	1	0.96*	2.18	4.78
5	12	0	2.60*	0.87	4.45
5	11	0	10.94	11.77	3.00
5	11	1	2.04*	2.36	4.55
5	11	2	1.17*	1.13	4.74
5	11	3	4.85	4.84	4.08
5	11	4	8.21	9.35	3.33
5	11	5	4.27	4.03	4.17
5	11	6	2.14*	0.74	4.54
5	11	7	5.36	5.32	4.00
5	11	8	3.15	3.07	4.35
5	10	10	3.49	3.25	4.30
5	10	9	10.81	11.00	3.03
5	10	8	3.55	3.80	4.29
5	10	7	4.58	4.60	4.12
5	10	6	4.33	4.26	4.16
5	10	5	2.44*	2.95	4.48
5	10	4	1.13*	0.64	4.74
5	10	3	12.06	12.17	2.77
5	10	2	1.10*	0.04	4.75
5	10	1	9.95	10.34	3.19
5	10	0	4.10	3.69	4.20
5	9	0	3.76	3.80	4.25
5	9	1	3.49	2.89	4.30
5	9	2	8.12	8.41	3.54
5	9	3	4.04	4.57	4.21
5	9	4	17.82	17.98	1.69
5	9	5	6.14	6.27	3.87
5	9	6	1.96*	1.32	4.57
5	9	7	4.29	4.02	4.17
5	9	8	8.01	7.84	3.55
5	9	9	11.46	11.57	2.90
5	9	10	10.88	11.09	3.01
5	8	11	1.25*	0.56	4.72
5	8	12	1.83*	1.62	4.60
5	8	13	7.49	7.59	3.64
5	8	12	1.20*	0.97	4.73
5	8	11	4.48	4.37	4.13
5	8	10	1.17*	0.32	4.74
5	8	9	7.34	7.85	3.67
5	8	8	6.12	6.05	3.87
5	8	7	6.36	6.51	3.84
5	8	6	3.18	4.00	4.35
5	8	5	21.91	21.95	1.13
5	8	4	1.05*	1.55	4.76
5	8	3	2.06	1.41	4.55
5	8	2	21.87	22.78	1.14
5	8	1	9.07	9.48	3.36
5	8	0	6.27	6.95	3.85
5	7	0	24.94	26.21	0.84
5	7	1	5.80	6.98	3.91
5	7	2	0.57*	1.02	4.88
5	7	3	6.66	7.88	3.79
5	7	4	32.93	34.25	0.41
5	7	5	10.68	10.07	3.05
5	7	6	4.34	3.73	4.16
5	7	7	1.91*	0.71	4.58
5	7	8	20.37	20.49	1.32
5	7	9	3.21	2.96	4.34
5	7	10	7.46	7.67	3.65
5	7	11	1.13*	1.24	4.75
5	7	12	8.64	8.52	3.44
5	7	13	5.43	5.02	3.98
5	7	14	3.16	2.99	4.35
5	6	15	12.72	12.11	2.64
5	6	14	2.51*	1.69	4.47
5	6	13	0.92*	0.21	4.79
5	6	12	9.36	8.76	3.31
5	6	11	8.84	9.11	3.40
5	6	10	6.92	7.72	3.74
5	6	9	21.53	21.82	1.18
5	6	8	7.36	7.54	3.67
5	6	7	10.80	9.86	3.03
5	6	6	4.42	4.93	4.15

h	k	l	Fo	Fc	weight
5	6	5	12.31	12.80	2.72
5	6	4	12.52	12.13	2.68
5	6	3	25.66	23.80	0.79
5	6	2	10.86	9.75	3.02
5	6	1	20.27	20.54	1.33
5	6	0	1.88*	0.27	4.59
5	5	0	11.46	11.51	2.90
5	5	1	23.74	23.30	0.95
5	5	2	2.81	2.51	4.41
5	5	3	11.62	13.00	2.86
5	5	4	25.82	24.56	0.78
5	5	5	20.58	21.83	1.29
5	5	6	6.15	6.15	3.87
5	5	7	10.73	11.10	3.04
5	5	8	18.99	19.66	1.51
5	5	9	2.04*	2.37	4.56
5	5	10	4.14	3.83	4.19
5	5	11	1.11*	0.31	4.75
5	5	12	14.50	14.59	2.29
5	5	13	1.70*	1.88	4.62
5	5	14	1.16*	1.94	4.74
5	5	15	0.88*	2.16	4.80
5	5	16	1.66*	0.45	4.63
5	4	17	3.26	3.31	4.33
5	4	16	11.75	11.24	2.84
5	4	15	1.20*	1.34	4.73
5	4	14	1.13*	0.80	4.75
5	4	13	4.91	5.42	4.07
5	4	12	8.91	8.49	3.39
5	4	11	5.31	5.51	4.00
5	4	10	13.50	13.75	2.48
5	4	9	1.22*	0.73	4.73
5	4	8	15.88	15.62	2.02
5	4	7	21.42	21.19	1.19
5	4	6	14.39	14.32	2.31
5	4	5	19.40	19.45	1.45
5	4	4	7.91	7.86	3.57
5	4	3	13.12	13.69	2.56
5	4	2	10.48	10.00	3.09
5	4	1	16.83	16.01	1.86
5	4	0	18.65	17.67	1.56
5	3	0	44.81	41.77	0.17
5	3	1	24.02	23.46	0.92
5	3	2	6.55	5.33	3.80
5	3	3	7.83	8.27	3.59
5	3	4	4.22	4.44	4.18
5	3	5	31.43	32.05	0.46
5	3	6	4.52	4.57	4.13
5	3	7	4.68	4.73	4.10
5	3	8	15.94	15.82	2.01
5	3	9	28.81	30.55	0.59
5	3	10	1.05*	1.82	4.76
5	3	11	5.82	5.91	3.92
5	3	12	7.93	7.89	3.57
5	3	13	12.96	13.32	2.59
5	3	14	5.59	5.21	3.96
5	3	15	5.20	5.25	4.02
5	3	16	2.03*	1.23	4.56
5	3	17	6.83	6.23	3.76
5	2	17	6.17	6.03	3.87
5	2	16	6.73	6.02	3.77
5	2	15	4.24	4.68	4.17
5	2	14	6.44	6.80	3.82
5	2	13	0.91*	0.38	4.80
5	2	12	13.25	12.87	2.53
5	2	11	32.96	33.81	0.41
5	2	10	14.10	14.13	2.36
5	2	9	9.90	9.82	3.20
5	2	8	3.52	3.59	4.29
5	2	7	16.71	17.28	1.88
5	2	6	38.46	38.72	0.26
5	2	5	9.06	8.85	3.36
5	2	4	3.11	3.60	4.36
5	2	3	17.83	17.84	1.69
5	2	2	37.92	37.65	0.27
5	2	1	16.11	16.88	1.88
5	2	0	29.80	29.16	0.54
5	1	0	23.37	23.21	0.98
5	1	1	5.27	4.37	4.01
5	1	2	9.69	10.07	3.24
5	1	3	34.79	35.40	0.35
5	1	4	20.22	19.72	1.34
5	1	5	33.79	33.23	0.38
5	1	6	13.51	13.64	2.48
5	1	7	23.32	23.29	0.99
5	1	8	1.65*	1.12	4.63
5	1	9	3.76	3.65	4.25
5	1	10	2.11*	3.22	4.54
5	1	11	10.83	11.32	3.02
5	1	12	2.15*	2.58	4.53
5	1	13	5.57	5.17	3.96
5	1	14	1.07*	0.87	4.76
5	1	15	4.56	4.62	4.12
5	1	16	7.41	7.40	3.66
5	1	17	7.78	8.01	3.59
5	0	18	5.96	5.35	3.90
5	0	16	19.37	18.50	1.46
5	0	14	1.08*	0.12	4.76
5	0	12	2.27*	4.48	4.51
5	0	10	33.58	34.92	0.39
5	0	8	18.86	18.79	1.53
5	0	6	32.93	34.39	0.41
5	0	4	6.26	6.19	3.85
5	0	2	32.19	33.34	0.43
5	0	0	16.65	15.77	1.89
6	0	0	37.09	37.90	0.29
6	0	2	6.90	7.68	3.75
6	0	4	4.96	5.30	4.06
6	0	6	38.31	38.74	0.27
6	0	8	37.24	38.70	0.29
6	0	10	0.75*	0.49	4.83
6	0	12	1.08*	0.23	4.76
6	0	14	16.69	16.10	1.88
6	0	16	6.40	5.75	3.83
6	1	16	1.23*	0.34	4.72
6	1	15	8.16	7.62	3.53
6	1	14	1.16*	1.26	4.74
6	1	13	4.88	5.46	4.07
6	1	12	5.34	5.50	4.00
6	1	11	16.87	16.60	1.85
6	1	10	1.07*	0.70	4.76
6	1	9	17.29	17.58	1.78
6	1	8	5.25	5.51	4.01
6	1	7	7.36	7.60	3.67
6	1	6	8.72	8.74	3.43
6	1	5	33.81	33.78	0.38
6	1	4	16.04	15.52	2.00
6	1	3	19.36	18.65	1.46
6	1	2	31.96	31.94	0.44
6	1	1	25.47	26.93	0.80
6	1	0	10.88	10.44	3.01
6	2	0	25.64	25.40	0.79
6	2	1	5.09	5.08	4.04
6	2	2	0.88*	0.35	4.80
6	2	3	9.34	9.61	3.31
6	2	4	44.29	44.42	0.17
6	2	5	7.61	7.88	3.62
6	2	6	10.89	11.41	2.99
6	2	7	14.53	14.89	2.28
6	2	8	12.15	12.39	2.76
6	2	9	25.96	26.71	0.76
6	2	10	20.78	21.30	1.27
6	2	11	2.48*	1.92	4.47
6	2	12	5.42	6.02	3.99
6	2	13	6.18	6.41	3.86
6	2	14	8.36	8.20	3.49
6	2	15	5.46	5.40	3.98
6	2	16	2.07*	1.93	4.55
6	3	16	7.88	7.53	3.58
6	3	15	5.67	5.11	3.95
6	3	14	2.70	2.91	4.43
6	3	13	3.21	3.37	4.34
6	3	12	8.40	8.31	3.49
6	3	11	14.14	14.91	2.36
6	3	10	5.61	5.76	3.96
6	3	9	7.67	7.81	3.61
6	3	8	9.14	9.07	3.35
6	3	7	16.78	18.02	1.87
6	3	6	20.18	20.77	1.34
6	3	5	7.88	8.59	3.58
6	3	4	5.84	6.59	3.92
6	3	3	8.23	6.66	3.52
6	3	2	2.65	2.78	4.44
6	3	1	12.15	12.24	2.76
6	3	0	5.59	5.41	3.96
6	4	0	16.13	16.54	1.98
6	4	1	14.15	14.28	2.36
6	4	2	7.72	8.16	3.61
6	4	3	24.55	25.97	0.88
6	4	4	5.01	5.23	4.05
6	4	5	16.88	17.29	1.85
6	4	6	21.59	21.63	1.17
6	4	7	15.45	15.31	2.10
6	4	8	15.59	15.88	2.08
6	4	9	7.90	8.30	3.57
6	4	10	13.94	14.12	2.40
6	4	11	6.96	7.54	3.74
6	4	12	2.66	2.78	4.44
6	4	13	5.44	5.37	3.98
6	4	14	14.80	14.33	2.23
6	4	15	2.37*	1.63	4.49
6	5	15	1.26*	0.66	4.72
6	5	14	1.65*	1.82	4.65
6	5	13	2.66	2.66	4.44
6	5	12	6.45	6.19	3.82
6	5	11	1.35*	3.12	4.70
6	5	10	11.66	11.93	2.86
6	5	9	1.81*	1.34	4.60
6	5	8	8.94	9.68	3.20
6	5	7	7.70	7.87	3.61
6	5	6	11.58	11.39	2.87
6	5	5	1.98*	2.08	4.67
6	5	4	10.19	11.03	3.15
6	5	3	8.86	9.44	3.40
6	5	2	15.37	14.77	2.12
6	5	1	11.60	12.54	2.87
6	5	0	2.24	1.73	4.52
6	6	0	2.27	1.56	4.51
6	6	1	17.12	16.46	1.81
6	6	2	0.87*	0.46	4.81
6	6	3	16.16	17.08	1.97
6	6	4	8.13	9.34	3.53
6	6	5	0.70*	0.31	4.85
6	6	6	4.86	5.00	4.12
6	6	7	24.91	25.51	0.85
6	6	8	1.13*	1.30	4.75
6	6	9	3.71	3.84	4.26
6	6	10	7.18	6.62	3.70
6	6	11	1.15*	1.09	4.74
6	6	12	4.59	4.94	4.12
6	6	13	9.74	9.48	3.24
6	6	14	9.11	8.86	3.35
6	7	13	2.24*	1.51	4.52
6	7	12	4.92	5.11	4.07
6	7	11	1.14*	1.34	4.74
6	7	10	5.13	4.86	4.03
6	7	9	0.59*	1.19	4.88
6	7	8	11.69	12.03	2.85
6	7	7	1.96*	3.01	4.57
6	7	6	16.48	16.78	1.92
6	7	5	2.37*	1.96	4.49
6	7	4	9.37	9.16	3.31
6	7	3	3.03	2.89	4.37
6	7	2	22.16	23.25	1.11
6	7	1	10.06	10.98	3.17
6	7	0	5.05	5.48	4.04
6	8	0	12.41	12.66	2.70
6	8	1	5.40	5.37	3.99
6	8	2	1.34*	1.79	4.70
6	8	3	12.97	13.04	2.59
6	8	4	2.60	1.71	4.45
6	8	5	3.61	4.05	4.28

h	k	l	Fo	Fc	weight
6	8	6	0.94*	1.31	4.79
6	8	7	6.94	7.53	3.74
6	8	8	0.49*	1.16	4.90
6	8	9	5.84	5.54	3.92
6	8	10	1.18*	0.49	4.73
6	8	11	5.91	5.99	3.91
6	8	12	1.50*	0.48	4.66
6	9	10	2.41*	2.02	4.48
6	9	9	3.89	3.65	4.23
6	9	8	8.53	8.79	3.46
6	9	7	7.87	8.08	3.58
6	9	6	7.75	7.65	3.60
6	9	5	4.57	3.90	4.12
6	9	4	6.82	7.37	3.76
6	9	3	3.58	4.11	4.28
6	9	2	17.27	16.85	1.78
6	9	1	1.93*	0.04	4.58
6	9	0	8.88	8.77	3.40
6	10	0	1.13*	0.20	4.75
6	10	1	4.64	4.76	4.11
6	10	2	0.33*	1.62	4.84
6	10	3	1.83	1.71	4.58
6	10	4	3.12	3.14	4.36
6	10	5	4.42	4.07	4.15
6	10	6	5.60	5.66	3.96
6	10	7	9.27	9.10	3.32
6	10	8	3.66	3.37	4.27
6	11	6	4.52	4.18	4.13
6	11	5	5.55	5.33	3.97
6	11	4	2.58	2.68	4.45
6	11	3	4.86	5.00	4.08
6	11	2	10.43	10.33	3.10
6	11	1	6.67	6.78	3.78
6	11	0	4.62	4.67	4.11
6	12	0	4.64	4.18	4.11
6	12	1	12.02	11.78	2.78
7	11	0	8.86	8.58	3.38
7	11	1	6.48	6.35	3.81
7	11	2	2.65*	2.61	4.44
7	10	6	5.25	5.16	4.01
7	10	5	10.33	10.58	3.12
7	10	4	5.84	5.66	3.92
7	10	3	10.60	10.39	3.07
7	10	2	5.48	5.38	3.98
7	10	1	2.20*	1.66	4.52
7	10	0	1.18*	0.86	4.73
7	9	0	10.39	9.89	3.11
7	9	1	8.26	7.94	3.51
7	9	2	7.71	8.21	3.61
7	9	3	1.35*	1.77	4.70
7	9	4	8.99	8.73	3.38
7	9	5	2.11*	1.79	4.54
7	9	6	8.42	8.67	3.48
7	9	7	6.60	6.73	3.79
7	9	8	0.84*	1.01	4.81
7	8	10	1.24*	0.26	4.72
7	8	9	3.43	3.40	4.31
7	8	8	0.96*	1.36	4.78
7	8	7	2.38*	2.38	4.49
7	8	6	1.44*	0.09	4.68
7	8	5	8.51	8.78	3.47
7	8	4	4.19	3.61	4.18
7	8	3	1.61*	2.57	4.64
7	8	2	2.73	1.93	4.43
7	8	1	14.17	14.11	2.35
7	8	0	4.22	3.46	4.18
7	7	0	6.33	7.00	3.84
7	7	1	4.68	4.59	4.10
7	7	2	20.60	20.56	1.29
7	7	3	2.66	2.66	4.44
7	7	4	6.19	5.70	4.02
7	7	5	3.21	2.92	4.34
7	7	6	16.12	15.77	1.98
7	7	7	3.44	3.51	4.30
7	7	8	0.93*	1.95	4.79
7	7	9	2.23*	2.57	4.52
7	7	10	9.65	9.61	3.25
7	7	11	2.21*	2.57	4.52
7	6	12	8.57	8.26	3.45
7	6	11	2.68	3.03	4.44
7	6	10	5.09	4.78	4.04
7	6	9	1.15*	0.28	4.74
7	6	8	1.36*	0.20	4.69
7	6	7	2.80	3.02	4.41
7	6	6	1.35*	2.04	4.70
7	6	5	19.77	20.25	1.40
7	6	4	0.77*	1.38	4.83
7	6	3	2.11*	2.34	4.54
7	6	2	1.41*	0.29	4.68
7	6	1	14.95	15.24	2.20
7	6	0	5.05	5.05	4.04
7	5	0	1.96*	1.51	4.57
7	5	1	10.46	10.38	3.10
7	5	2	21.83	22.70	1.14
7	5	3	15.17	14.97	2.16
7	5	4	7.58	7.03	3.63
7	5	5	1.07*	0.32	4.76
7	5	6	14.81	14.82	2.23
7	5	7	7.34	6.96	3.67
7	5	8	1.69*	2.15	4.62
7	5	9	4.75	4.62	4.09
7	5	10	8.43	8.13	3.48
7	5	11	4.85	4.62	4.08
7	5	12	4.59	4.07	4.12
7	5	13	8.02	7.78	3.55
7	4	13	1.37*	1.43	4.69
7	4	12	11.35	11.05	2.92
7	4	11	9.70	9.59	3.24
7	4	10	2.12*	1.61	4.64
7	4	9	9.04	9.46	3.37
7	4	8	6.22	6.25	3.86
7	4	7	9.88	10.63	3.21
7	4	6	14.06	13.91	2.37
7	4	5	20.44	20.06	1.31
7	4	4	4.87	4.31	4.07
7	4	3	3.88	3.89	4.23
7	4	2	6.17	6.08	3.87
7	4	1	17.84	18.81	1.69
7	4	0	25.42	25.58	0.81
7	3	0	16.29	16.44	1.95
7	3	1	20.17	21.31	1.35
7	3	2	2.54	2.68	4.46
7	3	3	23.48	23.92	0.87
7	3	4	12.32	12.26	2.72
7	3	5	1.85*	1.37	4.57
7	3	6	8.25	8.36	3.51
7	3	7	11.00	10.93	2.89
7	3	8	7.74	8.15	3.60
7	3	9	5.74	6.01	3.83
7	3	10	5.20	5.53	4.02
7	3	11	2.38*	3.23	4.48
7	3	12	1.54*	1.31	4.66
7	3	13	4.60	4.18	4.12
7	3	14	2.26*	2.36	4.51
7	2	14	5.93	5.51	3.90
7	2	13	3.80	4.02	4.25
7	2	12	6.91	6.69	3.74
7	2	11	1.13*	2.00	4.75
7	2	10	3.02	3.90	4.38
7	2	9	5.89	5.86	3.91
7	2	8	21.00	20.91	1.24
7	2	7	6.41	6.84	3.83
7	2	6	9.56	9.13	3.27
7	2	5	16.41	16.25	1.93
7	2	4	10.42	10.42	3.10
7	2	3	18.50	19.37	1.58
7	2	2	28.31	27.97	0.61
7	2	1	2.26	2.14	4.51
7	2	0	8.92	9.40	3.39
7	1	0	16.60	17.11	1.90
7	1	1	9.76	9.67	3.23
7	1	2	19.33	19.92	1.46
7	1	3	32.40	32.78	0.43
7	1	4	25.11	25.36	0.83
7	1	5	1.56*	1.94	4.65
7	1	6	5.84	5.48	3.92
7	1	7	11.96	12.34	2.78
7	1	8	1.03*	0.03	4.77
7	1	9	18.35	18.21	1.61
7	1	10	2.95	3.31	4.39
7	1	11	1.14*	0.72	4.74
7	1	12	1.12*	0.60	4.75
7	1	13	8.66	8.62	3.44
7	1	14	1.21*	1.51	4.73
7	1	15	7.29	6.61	3.68
7	0	14	5.84	5.80	3.92
7	0	12	13.25	12.85	2.53
7	0	10	5.42	4.83	3.99
7	0	8	13.18	13.32	2.55
7	0	6	21.57	21.92	1.17
7	0	4	61.72	64.14	0.06
7	0	2	18.87	19.85	1.53
7	0	0	32.01	33.92	0.44
8	0	0	16.98	17.77	1.83
8	0	2	42.70	44.35	0.19
8	0	4	6.83	7.79	3.76
8	0	6	21.64	21.76	1.16
8	0	8	6.32	6.14	3.84
8	0	10	13.12	13.00	2.56
8	0	12	6.54	6.35	3.80
8	1	13	11.15	10.83	2.96
8	1	12	3.74	3.92	4.25
8	1	11	5.87	6.13	3.91
8	1	10	1.15*	0.23	4.74
8	1	9	4.64	4.33	4.11
8	1	8	1.09*	1.02	4.75
8	1	7	14.95	15.09	2.20
8	1	6	3.68	3.67	4.26
8	1	5	5.18	5.24	4.02
8	1	4	9.55	9.47	3.27
8	1	3	3.40	3.33	4.31
8	1	2	15.03	14.83	2.18
8	1	1	25.61	25.66	0.79
8	1	0	5.69	5.95	3.94
8	2	0	6.67	6.91	3.78
8	2	1	14.85	15.12	2.22
8	2	2	3.14	2.61	4.36
8	2	3	8.08	8.79	3.54
8	2	4	1.84	0.86	4.60
8	2	5	2.11*	0.33	4.54
8	2	6	15.10	15.38	2.17
8	2	7	5.26	5.21	4.01
8	2	8	3.00	2.60	4.38
8	2	9	4.47	4.40	4.14
8	2	10	4.75	4.38	4.09
8	2	11	4.51	5.01	4.13
8	2	12	8.82	8.35	3.41
8	3	12	4.35	4.12	4.16
8	3	11	5.13	4.56	4.03
8	3	10	0.61*	2.14	4.87
8	3	9	6.58	6.68	3.80
8	3	8	3.04	3.27	4.37
8	3	7	2.83	2.87	4.41
8	3	6	3.79	3.71	4.25
8	3	5	11.35	11.33	2.92
8	3	4	6.66	6.75	3.78
8	3	3	5.76	6.64	3.93
8	3	2	6.24	5.62	3.85
8	3	1	21.50	21.51	1.18
8	3	0	7.21	7.67	3.69
8	4	0	12.28	11.88	2.73
8	4	1	3.99	3.64	4.21
8	4	2	0.88*	2.08	4.80
8	4	3	7.71	7.55	3.61
8	4	4	2.20	2.47	4.52
8	4	5	13.50	13.94	2.48
8	4	6	4.10	3.41	4.20
8	4	7	9.73	10.00	3.24
8	4	8	1.13*	0.22	4.75
8	4	9	9.01	9.13	3.37
8	4	10	6.31	5.85	3.84
8	4	11	4.04	3.64	4.21

h	k	l	Fo	Fc	weight
8	4	12	0.53*	1.95	4.89
8	5	11	14.60	13.86	2.27
8	5	10	5.30	5.48	4.01
8	5	9	8.97	8.93	3.38
8	5	8	6.46	6.56	3.82
8	5	7	9.59	9.85	3.26
8	5	6	1.17*	0.19	4.74
8	5	5	11.57	11.22	2.87
8	5	4	9.23	9.68	3.33
8	5	3	1.88*	2.18	4.59
8	5	2	1.80*	1.06	4.60
8	5	1	14.41	14.56	2.30
8	5	0	18.24	19.13	1.62
8	6	0	6.50	5.31	3.81
8	6	1	9.70	10.39	3.24
8	6	2	1.13*	1.82	4.74
8	6	3	14.05	13.92	2.37
8	6	4	5.60	5.03	3.96
8	6	5	1.23*	1.68	4.72
8	6	6	1.13*	0.35	4.74
8	6	7	3.07	3.23	4.37
8	6	8	3.93	3.95	4.22
8	6	9	1.25*	2.14	4.72
8	6	10	5.82	4.92	3.92
8	7	9	2.07	1.43	4.55
8	7	8	12.73	12.19	2.64
8	7	7	7.58	7.32	3.63
8	7	6	5.92	6.24	3.91
8	7	5	4.94	4.68	4.06
8	7	4	12.07	11.87	2.77
8	7	3	1.18*	0.71	4.74
8	7	2	0.68*	1.69	4.85
8	7	1	4.31	4.53	4.16
8	7	0	12.45	12.46	2.68
8	8	0	1.03*	0.81	4.77
8	8	1	2.02*	0.12	4.56
8	8	2	2.61	2.05	4.45
8	8	3	9.16	9.03	3.35
8	8	4	2.39	2.31	4.49
8	8	5	1.93	2.29	4.58
8	8	6	3.89	3.58	4.23
8	8	7	5.94	5.51	3.90
8	9	5	4.16	4.34	4.19
8	9	4	8.97	8.84	3.38
8	9	3	6.74	6.63	3.77
8	9	2	4.07	3.78	4.20
8	9	1	4.24	4.19	4.17
8	9	0	6.80	7.01	3.76
8	10	0	4.20	3.68	4.18
8	10	1	6.56	5.97	3.80
8	10	2	1.31*	0.24	4.70
9	9	0	4.21	3.82	4.18
9	8	4	1.28*	0.33	4.71
9	8	3	6.75	6.94	3.77
9	8	2	3.54	3.29	4.29
9	8	1	7.38	6.94	3.66
9	8	0	2.00	2.45	4.56
9	7	0	2.26*	0.85	4.51
9	7	1	2.04*	0.56	4.56
9	7	2	5.48	5.31	3.98
9	7	3	2.45*	2.49	4.48
9	7	4	6.07	6.82	3.73
9	7	5	9.09	8.47	3.36
9	7	6	6.37	5.94	3.83
9	6	7	6.26	5.62	3.85
9	6	6	2.23*	1.85	4.52
9	6	5	1.19*	0.33	4.73
9	6	4	5.41	5.22	3.99
9	6	3	13.04	12.83	2.58
9	6	2	0.78*	1.98	4.83
9	6	1	7.87	7.20	3.58
9	6	0	3.04	3.21	4.37
9	5	0	5.04	5.45	4.05
9	5	1	1.06*	0.42	4.76
9	5	2	3.49	3.92	4.30
9	5	3	10.81	10.62	3.02
9	5	4	1.81*	0.72	4.60
9	5	5	6.01	6.17	3.89
9	5	6	1.18*	0.44	4.74
9	5	7	7.65	7.47	3.62
9	5	8	5.02	4.96	4.05
9	4	9	3.32	2.88	4.32
9	4	8	7.29	6.44	3.68
9	4	7	4.07	3.96	4.20
9	4	6	5.25	4.95	4.01
9	4	5	9.43	9.44	3.29
9	4	4	11.70	11.22	2.85
9	4	3	8.55	8.85	3.46
9	4	2	1.73*	1.44	4.62
9	4	1	2.40	2.20	4.49
9	4	0	3.60	3.15	4.28
9	3	0	1.57*	2.43	4.65
9	3	1	8.31	8.81	3.50
9	3	2	8.26	8.34	3.51
9	3	3	10.19	9.96	3.15
9	3	4	3.73	3.99	4.26
9	3	5	2.72	2.61	4.43
9	3	6	9.96	9.73	3.19
9	3	7	4.49	4.16	4.13
9	3	8	3.76	4.04	4.25
9	3	9	5.29	4.92	4.01
9	3	10	2.64	2.51	4.44
9	2	10	11.17	10.87	2.95
9	2	9	0.96*	1.88	4.78
9	2	8	2.14*	1.71	4.54
9	2	7	2.21*	0.14	4.52
9	2	6	1.13*	0.37	4.75
9	2	5	0.95*	0.59	4.78
9	2	4	8.77	8.99	3.42
9	2	3	5.99	5.81	3.89
9	2	2	8.45	9.04	3.47
9	2	1	1.07*	1.04	4.76
9	2	0	1.05*	0.36	4.76
9	1	0	2.24*	2.10	4.52
9	1	1	11.95	12.76	2.80
9	1	2	1.43*	2.75	4.68
9	1	3	6.44	6.55	3.82
9	1	4	5.80	5.51	3.93
9	1	5	13.06	12.80	2.57
9	1	6	2.26*	0.03	4.51
9	1	7	1.12*	0.32	4.75
9	1	8	1.10*	0.31	4.75
9	1	9	3.64	3.32	4.27
9	1	10	2.39	2.26	4.49
9	0	10	6.45	5.93	3.82
9	0	8	7.78	7.40	3.59
9	0	6	9.38	9.41	3.30
9	0	4	11.78	12.17	2.83
9	0	2	13.70	14.36	2.44
9	0	0	18.56	18.56	1.68
10	0	0	10.94	11.24	3.00
10	0	2	5.81	5.54	3.82
10	0	4	10.70	11.24	3.05
10	0	6	6.06	5.66	3.88
10	0	8	6.73	6.09	3.77
10	1	8	0.92*	0.86	4.79
10	1	7	3.42	3.41	4.31
10	1	6	2.11	2.06	4.64
10	1	5	2.11*	0.44	4.54
10	1	4	1.96*	0.44	4.57
10	1	3	7.65	7.39	3.62
10	1	2	0.70*	0.10	4.85
10	1	1	4.67	4.65	4.10
10	1	0	2.50	3.40	4.47
10	2	0	11.18	11.11	2.85
10	2	1	4.14	3.74	4.19
10	2	2	6.24	5.68	3.85
10	2	3	3.59	3.38	4.28
10	2	4	2.16*	0.13	4.53
10	2	5	2.90	3.10	4.40
10	2	6	5.42	5.93	3.99
10	2	7	1.18*	0.61	4.74
10	3	7	6.24	5.85	3.85
10	3	6	2.56*	1.04	4.46
10	3	5	1.72*	0.62	4.62
10	3	4	10.11	9.31	3.16
10	3	3	3.02	2.50	4.38
10	3	2	3.71	3.51	4.26
10	3	1	7.82	7.37	3.59
10	3	0	2.17*	2.48	4.53
10	4	0	2.36*	1.73	4.49
10	4	1	7.38	7.36	3.66
10	4	2	8.16	8.03	3.53
10	4	3	8.18	7.73	3.52
10	4	4	10.71	9.64	3.05
10	4	5	0.90*	0.32	4.80
10	4	6	7.75	7.50	3.60
10	5	5	3.22	3.22	4.34
10	5	4	2.62*	2.40	4.45
10	5	3	1.67*	2.45	4.63
10	5	2	1.20*	0.38	4.73
10	5	1	10.33	10.29	3.12
10	5	0	5.88	5.83	3.91
10	6	0	2.62*	3.45	4.45
10	6	1	10.87	10.39	3.01
10	6	2	4.78	4.59	4.09
10	6	3	1.22*	0.87	4.72
10	7	1	1.25*	2.00	4.72
10	7	0	4.42	4.24	4.14
11	4	1	4.98	4.63	4.06
11	4	0	7.59	7.22	3.63
11	3	0	2.23*	1.77	4.52
11	3	1	1.23*	0.23	4.72
11	3	2	7.89	7.09	3.58
11	3	3	1.07*	2.09	4.76
11	2	3	0.83*	1.38	4.81
11	2	2	6.04	5.94	3.89
11	2	1	2.61*	1.43	4.45
11	2	0	4.59	4.35	4.12
11	1	0	2.42*	2.35	4.48
11	1	1	7.84	7.60	3.58
11	1	2	1.23*	1.67	4.72
11	1	3	2.38*	0.25	4.49
11	1	4	0.75*	0.78	4.83
11	0	4	4.87	4.31	4.06
11	0	2	10.59	10.32	3.07
11	0	0	1.21*	1.42	4.73

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