THE CRYSTAL STRUCTURE OF HEXAMETHYLCYCLOTRIPHOSPHAZENE - IODINE (1:1 ADDUCT) AND THE STRUCTURAL REDETERMINATION OF SODIUM FORMATE

by

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Abstract

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This thesis consists of the structures of two compounds as determined by single crystal x-ray diffraction. The first structure is that of a phosphazene - iodine complex: hexamethylcyclotriphosphazene - iodine (1:1 adduct) and the second structure is the redetermination of sodium formate.

Crystals of hexamethylcyclotriphosphazene - iodine (1:1 adduct) are triclinic, a = 10.707(13), b = 8.873(5), c = 8.871(6)Å, α = 96.65(6), β = 103.91(12), γ = 97.81(12)°, Z = 2, space-group $P\bar{1}$. The structure was determined with Mo-K_α diffractometer data by Patterson and Fourier synthesis, and was refined by full-matrix least-squares calculations to R = 0.053 for 1934 observed reflexions. The iodine molecule is weakly bonded to a nitrogen atom on the phosphazene ring, N - I = 2.417(7), I - I = 2.823(1)Å, N - I - I = 177.8(2)°. The six-membered phosphazene ring is slightly, but significantly, non-planar, the conformation being that of a chair. The molecule has pseudo-m symmetry. Two distinct P - N bonds are present; the longer ones, mean P - N = 1.64Å, involve the nitrogen that is weakly bonded to the iodine molecule, while the other four P - N bonds are equivalent, mean P - N = 1.598Å. All the P - C bonds are equivalent, mean P - C = 1.789Å. The mean endocyclic N - P - N and P - N - P angles are 114.7 and 124.0° respectively, while the mean exocyclic C - P - C angle is 104°.

Crystals of sodium formate are monoclinic, $a = 6.2590(6)$, $b = 6.7573(16)$, $c = 6.1716(5)$ Å, $\beta = 116.140(6)°$, $Z = 4$, space-group $C2/c$. The structure was determined by direct methods, and was refined by electron density and full-matrix least-squares procedures to $R = 0.022$ for 250 reflexions. Sodium formate is planar and has C_{2v} symmetry. Partial charges were refined on the formate ion. The partial charges found on each atom are as follows: O -0.23(1)e, C +0.16(3)e, H -0.49(10)e, and Na +0.79(14)e. The sodium ion has six oxygen neighbours at an average distance of 2.45Å and there are weak Na...O interactions. There is a C - H...Na hydrogen bond which forms continuous rows of sodium formate ions. The C - O bond distance is 1.246(1)Å and the O - C - O angle is 126.3(2)°.

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Acknowledgements

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GENERAL INTRODUCTION

The historical background and established principles of x-ray crystallography are dealt with in a number of standard texts (1-5). The crystallographic symbols and nomenclature appearing throughout this thesis have their conventional meanings described in the "International Tables for X-ray Crystallography" (6). This thesis consists of two parts. Both parts consist of the crystallographic study of a compound and include introductory material relevant to that compound as well as details of the structure determination and a discussion of the results.

For each crystal structure the least-squares refinement was based on the minimization of $\Sigma w(F_o - F_c)^2$ where F_o and F_c are the observed and calculated structure factors and w is the assigned weighting factor. The anisotropic thermal parameters employed in the refinement are U_{ij} in the expression:

$$f = f^o \exp[-2\pi^2 (U_{11}\, h^2a^{*2} + U_{22}\, k^2b^{*2} + U_{33}\, l^2c^{*2} + U_{12}\, hka^*b^* + U_{13}\, hla^*c^* + U_{23}\, klb^*c^*)]$$

where f^o is the tabulated scattering factor and f is that corrected for thermal motion. The isotropic thermal parameters have the form:

$$f = f^o \exp[-B(\sin\theta/\lambda)^2]$$

where B is related to the mean-square displacement, U^2, of the atom from its mean position by the expression:

$$B = 8\pi^2U^2.$$

PART 1

CRYSTAL STRUCTURE OF

HEXAMETHYLCYCLOTRIPHOSPHAZENE-IODINE (1:1 ADDUCT)

INTRODUCTION

In recent years the cyclophosphazenes have been extensively studied, the primary concern being the bonding. The bonding systems in these rings are now well established (7-9). Detailed structural information is available for several cyclophosphazene derivatives in which the bonding in the ring has been disturbed by protonation (10-12), or by complexing with a transition metal (13-15). The structure of hexamethylcyclotriphosphazene - iodine is the first structural study done in which the cyclophosphazene ring has been perturbed by the formation of a charge transfer complex. The crystal structure of the parent compound has not been determined because of badly developed crystals.

EXPERIMENTAL

Crystals of $N_3P_3Me_6.I_2$ crystallized as purple fragments, generally elongated along b. Unit-cell and space-group data were taken from various rotation, Weissenberg and precession photographs; accurate lattice parameters were determined by a least-squares procedure applied to 2θ values for twenty-five general reflexions measured on a spectrogoniometer.

Crystal Data:

$C_6H_{18}I_2N_3P_3$ f.w. = 478.96

Triclinic, a = 10.707(13), b = 8.873(5), c = 8.871(6)Å, α = 96.65(6), β = 103.91(12), γ = 97.81(12)°, U = 800.8Å^3, Z = 2, D_c = 1.99, F(000) = 452, λ(Mo-Kα) 0.71069Å, μ(Mo-Kα) 42.6cm^{-1}. Space-group $P\bar{1}$ (C_i^1) or P1 (C_1^1).

Intensities were measured on a Datex-automated General Electric XRD 6 diffractometer, with a scintillation counter, Mo-Kα radiation (zirconium filter and pulse height analyser), and a θ-2θ scan at 2° min^{-1} over a range of (1.80 + 0.86tanθ) degrees in 2θ, with 20s background counts being measured at each end of the scan. Data were measured to 2θ = 45° (minimum interplanar spacing 0.93 Å). Reflexions which had a net count of less than 3σ above background, where σ(I) is defined by $\sigma^2(I) = S + B + (0.05)S^2$, where S and B are the scan and background counts respectively, were taken as unobserved. Of 2259 reflexions with 2θ ≤ 45°, 325 (14.4%) were classified as

unobserved. A check reflexion was monitored every 50 reflexions and all the reflexions were appropriately scaled. Lorentz and polarization corrections were applied, and the structure amplitudes were derived. The crystal used had length ca. 0.45mm and cross-section of ca. 0.3 x 0.2mm. No absorption correction was made.

STRUCTURE ANALYSIS

The data were scaled by Wilson's method (16), and the |E| - statistics (17) (Table 1) suggested the centric space-group $P\bar{1}$. This space-group was subsequently shown correct during structure analysis.

The two iodine atom positions were determined from a three - dimensional Patterson function. Initial isotropic thermal parameters were set at 4.25 Å^2. The positicnal and isotropic thermal parameters and an overall scale factor were refined by full-matrix least-squares methods. The weights w in the minimization were such that $w = 0$ for the unobserved reflexions and $w = [A + B|F_o| + C|F_o|^2 + D|F_o|^3]^{-1}$ for the observed reflexions. The coefficients A, B, C, and D were adjusted to achieve best constancy of local averages of $\Sigma w(F_o - F_c)^2$ over the full range of $|F_o|$, the final values being -0.553, 0.391, -0.017, and 0.0002 respectively. Scattering factors were taken from reference 18.

Isotropic refinement of the two iodine atoms converged at R = 0.35. A three dimensional difference synthesis clearly revealed all the other 12 non-hydrogen atoms. Structure factors were calculated with the iodine atoms being corrected for anomalous scattering and the R factor was 0.135. After several cycles of anisotropic refinement R was reduced to 0.056. A difference synthesis at this point failed to reveal the hydrogen atoms and calculated hydrogens were used for the structure factor calculations, but these were not refined. These hydrogen atoms were arranged in staggered tetrahedral

Table 1

|E| - STATISTICS FOR $N_3P_3Me_6.I_2$

		THEORETICAL	
	OBSERVED	CENTRO	NON-CENTRO
Mean|E|	0.8145	0.7980	0.8860
Mean$\|E\|^2$	0.9948	1.0000	1.0000
Mean$\|E^2-1\|$	0.9193	0.9680	0.7360
|E| > 3 (%)	0.04	0.30	0.01
|E| > 2 (%)	3.98	5.00	1.80
|E| > 1 (%)	33.29	32.00	37.00

configurations, 1.00Å away from the carbon atoms to which they were bonded. The hydrogen atoms were all given isotropic thermal parameters of 5.0Å^2. This produced a final R of 0.053. Measured and calculated structure factors are given in Appendix 1.

The final positional parameters and their standard deviations for the non-hydrogen atoms, as well as the positions of the calculated hydrogens, are given in Table 2. The hydrogen atoms are numbered according to the carbon atoms to which they are bonded. The final anisotropic temperature factors for the heavy atoms are given in Table 3.

Table 2

FINAL POSITIONAL PARAMETERS (FRACTIONAL X 10^4)

WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

Atom	x	y	z
I(1)	5665(1)	-2030(1)	7128(1)
I(2)	3567(1)	-4508(1)	6515(1)
P(1)	7575(2)	1576(2)	8881(2)
P(2)	9911(2)	2785(2)	8182(2)
P(3)	8502(2)	-0098(2)	6508(2)
N(1)	7515(7)	0023(8)	7630(8)
N(2)	8907(7)	2773(8)	9251(8)
N(3)	9746(7)	1248(8)	6966(8)
C(1)	7390(10)	0960(11)	10672(10)
C(2)	6184(11)	2476(13)	8146(15)
C(3)	11532(8)	3145(12)	9441(11)
C(4)	9864(10)	4395(11)	7147(11)
C(5)	9045(8)	-1908(9)	6567(10)
C(6)	7605(9)	-0202(13)	4507(10)
H(1)'	8110	0387	11088
H(1)''	7426	1876	11461
H(1)'''	6528	0266	10470
H(2)'	6211	2774	7102
H(2)''	5362	1734	8033
H(2)'''	6208	3414	8903
H(3)'	11658	2285	10067
H(3)''	12175	3220	8791
H(3)'''	11666	4137	10170
H(4)'	8987	4289	6390
H(4)''	10026	5367	7914
H(4)'''	10554	4437	6560
H(5)'	9531	-1968	7666
H(5)''	8273	-2759	6213
H(5)'''	9634	-2017	5854
H(6)'	7229	0761	4376
H(6)''	8201	-0317	3805
H(6)'''	6882	-1111	4221

Table 3

FINAL THERMAL PARAMETERS AND

THEIR ESTIMATED STANDARD DEVIATIONS

ANISOTROPIC THERMAL PARAMETERS (U_{ij} X 100 Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I(1)	3.55(4)	4.41(4)	4.53(4)	-0.16(3)	0.58(2)	0.27(3)
I(2)	5.19(5)	5.99(5)	10.04(6)	-1.90(4)	1.98(4)	-1.40(4)
P(1)	3.6(1)	3.4(1)	3.7(1)	0.3(1)	0.9(1)	-0.4(1)
P(2)	3.3(1)	2.5(1)	3.9(1)	0.0(1)	0.5(1)	0.1(1)
P(3)	3.6(1)	2.8(1)	3.1(1)	0.3(1)	0.7(1)	0.0(1)
N(1)	4.1(4)	2.9(4)	4.6(4)	-1.0(3)	1.8(3)	-1.1(3)
N(2)	5.0(4)	3.4(4)	4.7(4)	-0.1(3)	1.9(3)	-1.4(3)
N(3)	4.3(4)	3.8(4)	4.9(4)	-0.1(3)	2.5(3)	-0.6(3)
C(1)	6.5(6)	5.5(6)	4.3(5)	-0.1(5)	2.2(4)	-0.4(4)
C(2)	5.7(7)	6.2(7)	10.1(9)	1.8(6)	0.3(6)	0.2(6)
C(3)	3.6(5)	6.5(6)	4.8(5)	-0.1(5)	-0.3(4)	0.4(5)
C(4)	6.1(6)	4.7(6)	5.6(6)	0.7(5)	0.5(5)	1.9(5)
C(5)	4.0(5)	2.5(4)	6.0(5)	0.0(4)	1.0(4)	0.1(4)
C(6)	5.5(6)	7.6(7)	3.2(4)	0.8(5)	-0.1(4)	0.8(5)

RESULTS AND DISCUSSION

The iodine molecule is weakly bonded to a nitrogen atom on the phosphazene ring in a linear arrangement. A general view of the adduct is shown in Figure 1. Individual bond lengths along with standard deviations are given in Table 4 and the valency angles with standard deviations are given in Table 5. A weighted least-squares plane was calculated for the phosphazene ring. This was done by the use of the orthogonal coordinates, X, Y, Z, which were derived as follows:

$$\begin{vmatrix} X \\ Y \\ Z \end{vmatrix} = \begin{vmatrix} a & b\cos\gamma & c\cos\beta \\ 0 & b\sin\gamma & c(\cos\alpha-\cos\beta.\cos\gamma)/\sin\gamma \\ 0 & 0 & V/ab\sin\gamma \end{vmatrix} \begin{vmatrix} x \\ y \\ z \end{vmatrix}$$

where V is the cell volume as defined in reference 6. The equation of the plane and distances of the atoms from the plane are given in Table 6.

The phosphazene ring is slightly, but significantly, non-planar, all atoms lying between -0.141 and 0.005Å away from the weighted mean plane. The standard deviations of the phosphorus atoms are less than those of the nitrogen atoms and consequently they are given more weight than the nitrogen atoms. That is why the phosphorus atoms are closer to the mean plane (see Table 6). All the nitrogen atoms are below the plane while all the phosphorus atoms are above. This produces a chair conformation because the phosphorus and nitrogen atoms alternate around the ring. Of $(NPX_2)_3$ molecules whose structures have been reported, the fluoride

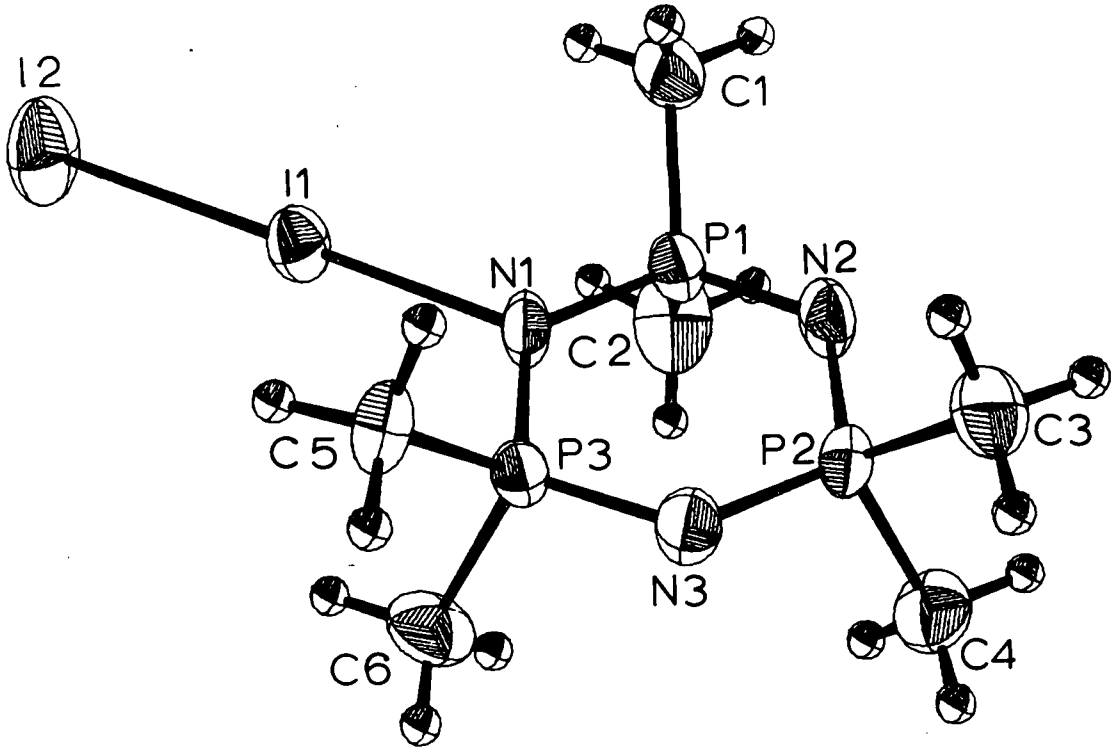


Figure 1

A general view of the adduct.

Table 4

INDIVIDUAL BOND LENGTHS (Å) WITH

STANDARD DEVIATIONS IN PARENTHESES.

Atoms	Bond Length (Å)	Atoms	Bond Length (Å)
I(1) - I(2)	2.823(1)	N(3) - P(3)	1.600(7)
I(1) - N(1)	2.417(7)	P(1) - C(1)	1.785(9)
N(1) - P(1)	1.650(7)	P(1) - C(2)	1.805(11)
N(1) - P(3)	1.623(7)	P(2) - C(3)	1.787(8)
N(2) - P(1)	1.597(7)	P(2) - C(4)	1.786(9)
N(2) - P(2)	1.596(7)	P(3) - C(5)	1.783(8)
N(3) - P(2)	1.599(7)	P(3) - C(6)	1.789(8)

Table 5

VALENCY ANGLES (DEG.) WITH STANDARD DEVIATIONS IN PARENTHESES

Atoms	Angle	Atoms	Angle
I(2) - I(1) - N(1)	177.8(2)	C(2) - P(1) - N(1)	111.1(5)
I(1) - N(1) - P(1)	118.5(3)	C(2) - P(1) - N(2)	108.8(5)
I(1) - N(1) - P(3)	117.3(3)	C(3) - P(2) - N(2)	108.4(4)
		C(3) - P(2) - N(3)	108.5(4)
N(1) - P(1) - N(2)	113.9(3)	C(4) - P(2) - N(2)	110.7(4)
N(2) - P(2) - N(3)	115.7(3)	C(4) - P(2) - N(3)	109.3(4)
N(3) - P(3) - N(1)	114.6(3)	C(5) - P(3) - N(3)	109.1(4)
		C(5) - P(3) - N(1)	108.4(4)
P(1) - N(2) - P(2)	123.4(4)	C(6) - P(3) - N(3)	111.0(4)
P(2) - N(3) - P(3)	124.2(4)	C(6) - P(3) - N(1)	109.1(4)
P(3) - N(1) - P(1)	124.5(4)		
		C(1) - P(1) - C(2)	106.5(5)
C(1) - P(1) - N(1)	107.5(4)	C(3) - P(2) - C(4)	103.5(5)
C(1) - P(1) - N(2)	108.7(4)	C(5) - P(3) - C(6)	104.0(5)

Table 6

WEIGHTED LEAST-SQUARES PLANE FOR THE PHOSPHAZENE RING (X, Y AND Z IN Å) AND DEVIATIONS, D, OF THE ATOMS IN THE RING FROM THE PLANE.

$-0.4377X + 0.5764Y - 0.6901Z = -7.7582$

Atom	D	D/σ
N(1)	-0.103	3.50
N(2)	-0.141	4.57
N(3)	-0.084	2.82
P(1)	0.024	1.92
P(2)	0.005	0.80
P(3)	0.007	0.84

(19) has a planar ring, the dimethylamino derivative (20) is slightly non-planar in the boat conformation while the chloro- (21-23), bromo- (24), and the phenyl (25) derivatives are slightly non-planar in the chair conformation. Of the two perturbed cyclotriphosphazene rings, $N_3P_3Cl_2(NHPr^i)_4H^+$ (11) is slightly boat-shaped and $N_3P_3(NMe_2)_6H^+$ (12) has been shown to have two nearly planar structures, one in a distorted boat and the other in a chair conformation. These small deviations from non-planarity have been associated with inter- and intra-molecular steric effects (21,24,25).

Two distinct P - N bond lengths are present. The longer ones are associated with N(1), the nitrogen bonded to the iodine molecule. These two bond lengths are 1.650(7) and 1.623(7) with an average length of 1.64(2)Å. The number in parentheses after average lengths is the root-mean-square deviation. The four other P - N bond lengths are equivalent with an average value of 1.598(2)Å. This value agrees very well with the P - N bond length in $N_4P_4Me_8$, P - N = 1.596(5)Å (26). The nitrogen atom, N(1), donates electrons into an anti-bonding orbital of the iodine molecule (27). This decreases the amount of electron charge that could be used for π - bonding in the ring and consequently the two P - N bonds, P(1) - N(1) and P(3) - N(1), are longer than the other P - N bonds, which have normal π - bonding present in unperturbed cyclotriphosphazenes (8). The perturbed nitrogen will be called N_P. In one structure of $N_3P_3(NMe_2)_6H^+$, the P - N_P bond distance is 1.668(2)Å, while in the other structure it is 1.69(1)Å (12). The mean P - N bond length in

$N_3P_3(NMe_2)_6$ is 1.588(3)Å (20). The P - N bond distance is increased by 0.08 and 0.11Å respectively upon perturbation for the two structures of $N_3P_3(NMe_2)_6H^+$. In our case the P - N_p distance increases by 0.04Å upon perturbation. This is compatible with the fact that H^+ is a stronger acceptor than I_2.

The N(1) - I(1) bond length is 2.417(7)Å. The sum of the covalent radii for nitrogen and iodine is 2.03Å (28). This shows that a weak bond is present. Values for N - I bond lengths in other charge transfer complexes are: 2.26 for pyridine.ICl (29), 2.31 for γ - picoline.I_2 (30), 2.30 for trimethylamine.ICl (31) and 2.27Å for trimethylamine.I_2 (32). It is more difficult for a nitrogen atom in the cyclotriphosphazene to donate electrons to the iodine molecule than it is in the other compounds above because of the use of the nitrogen electrons in π - bonding in the phosphazene ring and consequently the N - I bond distance is greater in the phosphazene.

The iodine - iodine bond length is 2.823(1)Å. This compares favourably with I - I bond lenghts of 2.83 in γ - picoline.I_2 (30) and 2.84Å in trimethylamine.I_2 (32). The I - I distance in the free halogen is 2.67Å (28). This agrees with the molecular orbital theory that the nitrogen atom donates some electronic charge into an anti-bonding orbital on the iodine molecule (27) and coseguently increases the I - I bond length. N(1), I(1), and I(2) are almost linear, the valence angle being 177.8(2)°. This agrees with

other halogen - nitrogen complexes (29-32).

The P - C bonds are all equivalent and have an average value of 1.789(8) Å. This is in good agreement with the value of 1.805(8) Å for $N_4P_4Me_8$ (26).

The mean endocyclic phosphorus angle is 114.7(8)°. The individual values vary from 113.9(3) to 115.7(3)°. The mean value is a little less than that given for $(NPX_2)_3$ molecules (19-25). These values range from 116.6(20) for the bromo derivative (24) to 120.0(4)° for the chloro derivative (21). However, the mean N - P - N angle is not as small as it is in $N_3P_3(NMe_2)_6H^+$ (12). The mean angles for the two structures are 110.0(2) and 112.0(2)° respectively for the chair and distorted boat conformations. This shows that the amount of π - bonding in the phosphazene ring decreases with increasing perturbation and consequently the angle at the phosphorus atom decreases and aproaches that of a tetrahedron (109.5°) (8).

The mean endocyclic nitrogen angle is 124.0(8)°. The angles at N(2) and N(3) are the same but the angle at N(1) is a little smaller. This would be expected because of the increased N - P bond distances associated with this angle. Values for P - N - P angles for $(NPX_2)_3$ molecules vary from 119.7(10)° for the chloro derivative (21) to 123.0(4)° for the dimethylamino derivative (20). The mean endocyclic nitrogen angle is somewhat greater than for the $(NPX_2)_3$ molecules. This is consistent with the smaller phosphorus angle in that the lower the π - bonding, the greater the

nitrogen angle (8).

The mean exocyclic C - P - C angle is 104(2)°. This is consistent with an angle of 104.1(2)° for $N_4P_4Me_8$ (26).

The unit-cell viewed down b is shown in Figure 2. All the inter-molecular distances correspond to normal van der Waals interactions; the shortest distances being 3.58 and 3.67Å for N(3)...C(6) and N(2)...C(4) respectively.

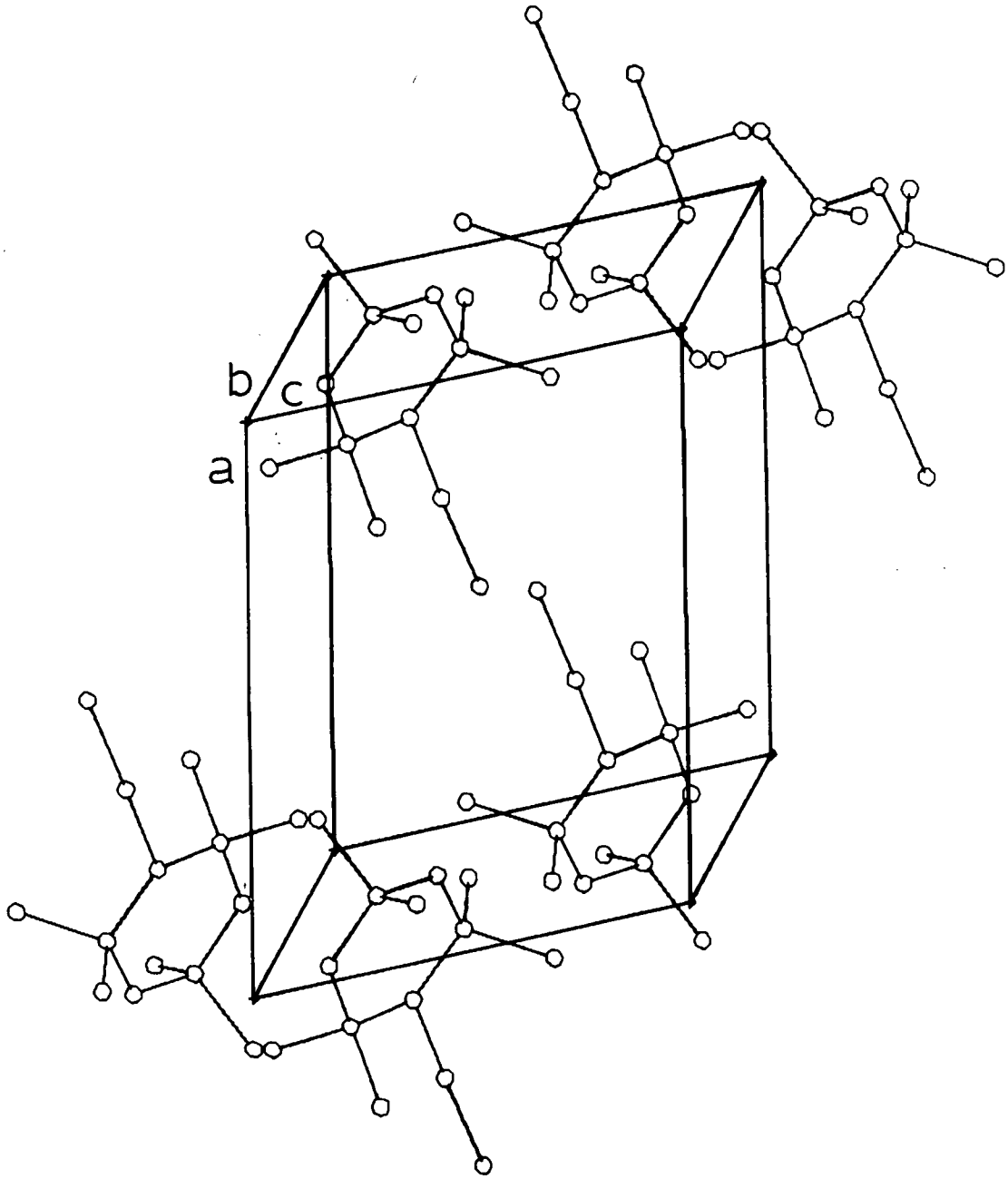


Figure 2

The unit-cell as viewed down b. Hydrogen atoms have been removed for clarity.

PART 2

CRYSTAL AND MOLECULAR STRUCTURE OF SODIUM FORMATE

(A REDETERMINATION)

INTRODUCTION

The structure of sodium formate was originally determined in 1940 by W. H. Zachariasen (33). He found that crystals of sodium formate were monoclinic, space-group C2/c, with an axial system of a = 6.19, b = 6.72, c = 6.49Å and β = 121°42'. There was nothing unusual reported about the structure and complete resonance between the two structures (Figure 3) was reported. No inter-molecular interactions were given and the hydrogen atom was not found but rather a calculated hydrogen position was used. The agreement between the observed and calculated structure factors was not very satisfactory. Accurate hydrogen positions were required as a basis for an E.S.R. and Endor study because hydrogen bonding was thought to exist in sodium formate (34). The structure of sodium formate was therefore redetermined.

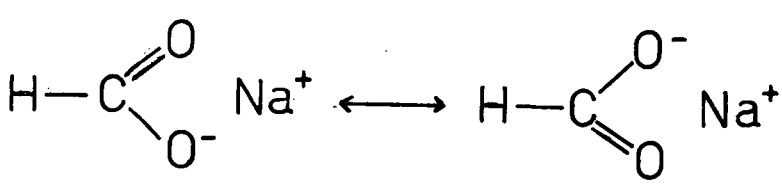


Figure 3

The two conventional resonance structures of sodium formate.

EXPERIMENTAL

Zachariasen had reported that crystals of sodium formate were elongated along c. A crystal of sodium formate was mounted on a goniometer, using this c axis as a guide, and the set of axes used by Zachariasen was found. The systematic absences found by precession and Weissenberg photographs could not be made to fit the space-group C2/c. Upon further investigation a different set of axes was located that did meet the required symmetry conditions for C2/c and Cc. It was found that the c axis used by Zachariasen was not the c axis at all, but the 1 0 1 direction. Accurate lattice parameters were obtained by a least-squares refinement of sixteen 2θ values measured on a spectrogoniometer.

Crystal Data:

$CHNaO_2$ f.w. = 68.01

Monoclinic, a = 6.2590(6), b = 6.7573(16), c = 6.1716(5) Å, β = 116.140(6)°, U = 234.32(6) Å^3, Z = 4 D_c = 1.9278(6), F(000) = 136, λ(Cu-Kα) 1.54178 Å, μ(Cu-Kα) 30.85 cm^{-1}. Absent spectra: hkℓ, h+k=2n, h0ℓ, ℓ=2n define the space-group as C2/c (C_{2h}^6, No. 15) or Cc (C_s^4, No. 9). Since Z = 4, the correct space-group cannot be determined by photographic means as the compound can possess the required symmetry for C2/c; a two-fold rotation axis.

Intensities were measured on a Datex-automated General

Electric XRD 6 diffractometer, with a scintillation counter, Cu-K_α radiation (nickel filter and pulse height analyser), and a θ-2θ scan at 2° min^{-1} over a range of $(1.80 + 0.86\tan\theta)$ degrees in 2θ, with 20s background counts being measured at each end of the scan. Data were measured to $2\theta = 145^\circ$ (minimum interplanar spacing 0.81 Å). A check reflexion was monitored every 20 reflexions and all the reflexions were appropriately scaled. Two sets of data were collected and averaged. The averaged data set contained 253 reflexions of which 2 had intensities less than 3σ above background, where $\sigma(I)$ is defined by $\sigma^2(I) = S + B + (0.05)S^2$, where S and B are the scan and background counts respectively, and only 1 reflexion had an intensity less than 2σ. All the data were used in the structure analysis. Lorentz and polarization corrections were applied and the structure amplitudes were derived. The crystal used had dimensions 0.32 x 0.34 x 0.28mm^3. No absorption correction was applied.

STRUCTURE ANALYSIS

The |E| - statistics are compared with theoretical values (17) for centrosymmetric and noncentrosymmetric structures in Table 7. As can be seen, the |E| - statistics are ambiguous and give no indication about the symmetry of the space-group and therefore it was decided to assume no molecular symmetry. Therefore the structure was solved in the space-group Cc. The structure was solved using the symbolic addition procedure for non-centrosymmetric crystals (35), with 90 reflexions with $|E| \geq 1.00$. The choice of the origin determining pair of reflexions in space-group Cc (type 2P00) (36) is restrictive, requiring that:

$$\begin{vmatrix} H_1 + K_1 & L_1 \\ H_2 + K_2 & L_2 \end{vmatrix} = \pm 1 \qquad (1)$$

where H_n, K_n, L_n, are referred to a primitive cell; if h_n, k_n, l_n refer to the centred cell then:

$$\begin{vmatrix} 0.5 & 0.5 & 0 \\ 0.5 & -0.5 & 0 \\ 0 & 0 & -1 \end{vmatrix} \begin{vmatrix} h_n \\ k_n \\ l_n \end{vmatrix} = \begin{vmatrix} H_n \\ K_n \\ L_n \end{vmatrix} \qquad (2)$$

or $$Th = H$$

Substitution of relation (2) into (1) gives

$$\begin{vmatrix} h_1 & l_1 \\ h_2 & l_2 \end{vmatrix} = \pm 1 \qquad (3)$$

and origin specification and the phase-determining procedure can then proceed by use of the conventional indices for the centred cell. Origin determining reflexions were chosen by use of equation (3) and their phases were arbitrarily fixed

Table 7

|E| - STATISTICS FOR SODIUM FORMATE

		THEORETICAL	
	OBSERVED	CENTRO	NON-CENTRO
Mean|E|	0.8902	0.7980	0.8860
Mean|E|^2	1.1467	1.0000	1.0000
Mean|E^2-1|	0.9823	0.9680	0.7360
|E| > 3 (%)	0.0	0.30	0.01
|E| > 2 (%)	4.72	5.00	1.80
|E| > 1 (%)	38.63	32.00	37.00

at ϕ = 0 millicycles. Three reflexions were assigned symbol phases, a, b, c and the value for the phase of a was constrained to lie between 0 and π; although both enantiomorphs are present in the space-group Cc, this restriction, in this case, defines axial direction. The three symbol phases along with the origin determining phases comprise the basic starting group given in Table 8.

Eight starting sets were generated by allowing symbol a to have initial values of 125 and 375mc and symbols b and c to have initial values of ±250mc. These sets were used as input to a computer program which determines phases using the tangent formula (37,38)

$$\tan[\phi(h)] \simeq \frac{\Sigma_k |E(k).E(h-k)| . \sin[\phi(k) + \phi(h-k)]}{\Sigma_k |E(k).E(h-k)| . \cos[\phi(k) + \phi(h-k)]} \simeq B/A$$

where h and k are the Miller indices and A and B are the two conventional parts of the structure factor. For each starting set fifteen cycles of tangent refinement were performed as follows: the largest 30 E values were included in the first five cycles, between cycles 5 and 10 the largest 60 values were included and all 90 reflexions were included for the final 5 cycles. A phase assignment was rejected in any cycle if (1) the consistency index,

$$t = \sqrt{A^2 + B^2} / \Sigma_k |E(k)| . |E(h-k)| \qquad (0 < t < 1)$$

was < 0.25, (2) the parameter (35,39)

$$\alpha = |E(h)| \sqrt{A^2 + B^2}$$

was < 1.0 and (3) there was a phase change $\Delta\phi(h)$ > 250mc from the previous cycle. After each cycle overall values were

Table 8

BASIC STARTING SET OF REFLEXIONS FOR CHO_2Na

h	k	l	|E|	phase (mc)	
4	2	-1	1.70	0	origin determining
7	3	-2	1.62	0	origin determining
3	7	-2	2.08	a	
1	7	-4	2.08	b	
4	2	1	1.96	c	

computed for t, α, and the agreement factors, Q and Rk, where Q is defined by: (38)

$$Q = \Sigma_h |E(h) - t(h)E(h)| / \Sigma_h |E(h)|$$

and Rk by: (35)

$$Rk = \Sigma_h ||E(h)|obs - |E(h)|calc| / \Sigma_h |E(h)|obs$$

the method of obtaining |E(h)|calc is given in reference 35.

The values of overall t, α, Q, Rk, and N, the number of phases determined, on the final cycle for each of the non-centrosymmetric sets are given in Table 9. For a consistent set of phases one would expect α and t to be high and Q and Rk to be low. As can be seen from Table 9, there is no clear solution, and from experience, results like this, ones in which there is no separation between the sets, are regarded quite dubiously. Therefore, another eight sets were generated with initial values for all symbols of 0 and 500mc, corresponding to the centrosymmetric case. The results from these sets are shown in Table 10. These results are much better than those of the non-centrosymmetric case and set 6 appears to be the correct solution. An |E| - map based on the 90 phased reflexions of set 6 gave positions for all five atoms, including the hydrogen. The structure was then refined in the centrosymmetric space-group C2/c.

Three cycles of full-matrix least-squares refinement of the positional and isotropic thermal parameters of the atoms gave R = 0.080. This was followed by two cycles of anisotropic refinement of the non-hydrogen atoms which reduced R to 0.071. At this stage three reflexions were given

Table 9

RESULTS FOR THE EIGHT NON-CENTROSYMMETRIC STARTING SETS IN THE PHASE DETERMINATION PROCEDURE

Set	a(mc)	b(mc)	c(mc)	t	α	Q	Rk	N
1	125	250	250	86	101	0.13	0.19	90
2	125	250	-250	83	99	0.16	0.17	90
3	125	-250	250	87	102	0.12	0.18	90
4	125	-250	-250	84	99	0.15	0.17	90
5	375	250	250	84	99	0.15	0.19	90
6	375	250	-250	95	111	0.05	0.19	90
7	375	-250	250	86	101	0.13	0.19	90
8	375	-250	-250	86	101	0.13	0.18	90

Table 10

RESULTS FOR THE EIGHT CENTROSYMMETRIC STARTING SETS IN THE PHASE DETERMINATION PROCEDURE

Set	a(mc)	b(mc)	c(mc)	t	∝	Q	Rk	N
1	0	0	0	79	80	0.22	0.38	80
2	0	0	500	65	56	0.33	0.44	73
3	0	500	0	75	81	0.22	0.34	82
4	0	500	500	84	97	0.14	0.27	87
5	500	0	0	79	80	0.19	0.34	82
6	500	0	500	98	114	0.02	0.20	90
7	500	500	0	75	74	0.25	0.39	79
8	500	500	500	68	62	0.30	0.42	77

zero weight in further refinement due to suspected extinction or counter errors (Table 11). Three cycles of anisotropic refinement brought R to 0.028.

The partial atomic charges were estimated by the method given in reference 40. A "double atom" was placed at the position of each atom, with total scattering power given by $(f_c + pf_v)$ where f_c and f_v are the core and valence scattering factors respectively. The occupancy of the valence shell was found by varying the multiplier p. The core and valence electrons were constrained to lie at the same position with one overall temperature factor for each "double atom". The core scattering for the hydrogen atom is zero. The multipliers p, along with all other variables, were refined for the HCO_2 part of the compound for three cycles. This reduced R to 0.023. The total net charge on the HCO_2 part was -0.79e. The charge on the sodium was therefore set at +0.79e and the scattering factor for Na was modified slightly to give the scattering factor for $Na^{+0.79}$. Two final cycles of anisotropic refinement brought R to 0.022.

The structure was then refined in the non-centrosymmetric space-group Cc. In this case R went to 0.024. With a higher R factor in the non-centrosymmetric case as compared to the centrosymmetric one, it is clear that the centrosymmetric space-group (C2/c) is the correct one.

The scattering factors for H, C, and O were taken from reference 41 and those for Na were modified from reference 18. The final weights used were $w = (0.0313 + 0.0137|F_o| -$

Table 11

REFLEXIONS GIVEN ZERO WEIGHT IN REFINEMENT

Reflexion	|Fobs|	|Fcalc|	$(F_o - F_c)/\sigma(F_o)$
1 1 0	22.72	32.16	7.06
0 2 0	48.91	60.88	11.96
0 0 2	63.31	78.49	15.18

$0.0027|F_o|^2 + 0.0001|F_o|^3)^{-1}$ which gave constant average values of $\Sigma w(F_o - F_c)^2$ over ranges of $|F_o|$.

On the final cycle of refinement no parameter shift was greater than 0.05σ and a final difference map gave peaks no greater than $0.20 e/\mathring{A}^3$. The final positional and thermal parameters appear in Tables 12 and 13 respectively. Observed and calculated structure factors are given in Appendix 2.

Table 12

FINAL POSITIONAL PARAMETERS (FRACTIONAL X 10^4)

WITH ESTIMATED STANDARD DEVIATIONS IN PARENTHESES

Atom	x	y	z
Na(1)	5000	6380(1)	2500
O(1)	3643(2)	3034(2)	3204(2)
C(1)	5000	2201(2)	2500
H(1)	5000	0732(30)	2500

Table 13

FINAL THERMAL PARAMETERS AND

THEIR ESTIMATED STANDARD DEVIATIONS

(A) ANISOTROPIC THERMAL PARAMETERS (U_{ij} X 100 Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	1.74(3)	2.38(4)	1.79(3)	0.00	0.76(2)	0.00
O(1)	1.84(5)	3.16(6)	2.18(5)	-0.21(3)	1.01(4)	-0.41(3)
C(1)	2.67(7)	2.08(7)	2.13(7)	0.00	0.90(5)	0.00

(b) ISOTROPIC THERMAL PARAMETER (Å^2)

Atom	B
H(1)	6.1(8)

RESULTS AND DISCUSSION

This x-ray analysis has confirmed the basic structure of sodium formate as found by Zachariasen (33). The molecule is planar and possesses a two-fold rotation axis through the middle, giving it C_{2v} symmetry. The bond distances and angles appear in Table 14. The C - O distance of 1.246(1)Å and the O - C - O angle of 126.29(16)° are somewhat different from those given by Zachariasen, 1.27Å and 124° respectively. Table 15 gives a list of some formate ion geometries for different salts. The agreement between the present structure and those of the more recent ones, notably references 43 and 46, is very good. The differences in symmetry, ie. loss of the two-fold rotation axis, are due to different packing arrangements, and in the NH_4^+ case is due to the presence of hydrogen bonding.

The entire ion is planar and the equation of the plane is:

$$-0.3510X + 0.0Y - 0.9364Z = -2.1568$$

where X, Y, and Z are the orthogonal coordinates derived as follows:

$$\begin{vmatrix} X \\ Y \\ Z \end{vmatrix} = \begin{vmatrix} a & 0 & c\cos\beta \\ 0 & b & 0 \\ 0 & 0 & c\sin\beta \end{vmatrix} \begin{vmatrix} x \\ y \\ z \end{vmatrix}$$

The sodium atom has six oxygen neighbours at an average distance of 2.45Å. This is greater than the sum of the covalent radius of oxygen (0.66Å) and the ionic radius of sodium (0.95Å), 1.61Å, but is less than the sum of the van

Table 14

BOND LENGTHS (Å) WITH STANDARD DEVIATIONS IN PARENTHESES

Atoms	Bond Length (Å)
C - O	1.246(1)
C - H	0.993(20)

VALENCY ANGLES (DEG.) WITH STANDARD DEVIATIONS IN PARENTHESES

Atoms	Angle (deg.)
O - C - H	116.85(8)
O - C - O	126.29(16)

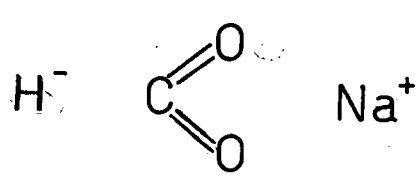
Table 15

FORMATE ION GEOMETRIES IN DIFFERENT SALTS

Cation	C - O Distance(Å)	O - C - O Angle(deg.)	Ref.
Ca^{++}	1.25(avg.)	125, 124	42
Sr^{++}	1.243(avg.)	126.4, 127.5	43
Ba^{++}	1.25(avg.)	127, 128	44
Pb^{++}	1.26(avg.)	127(avg.)	44
Gd^{+++}	1.27, 1.33	121(avg.)	45
NH_4^+	1.237, 1.246	126.3	46

der Waals radius for oxygen (1.40Å) and the metallic radius of sodium (1.572Å), 2.972Å. Therefore there is a weak interaction between the sodium and its six oxygen neighbours. All radii were taken from reference 28. See Figure 4 for a view of the packing in the unit-cell. Individual Na...O distances are given in Table 16. The average Na...O distance compares well with Na...O distances in similar type structures. See Table 17 for some average Na...O distances.

The charges of all the atoms were refined. These charges appear in Table 18. If the structure of sodium formate could be entirely described by the two resonance forms in Figure 3, one would expect the charges on the oxygens to be -0.5e. The refined charge is -0.23(1)e. There is some interaction between the sodium and the oxygens which would account for a small decrease in the oxygen negative charge, but this interaction is small and would not be expected to reduce the charge by 0.27e. Therefore, there appear to be other resonance forms involved. The charge on the hydrogen atom is -0.49(10)e. This indicates a major resonance form of the type:



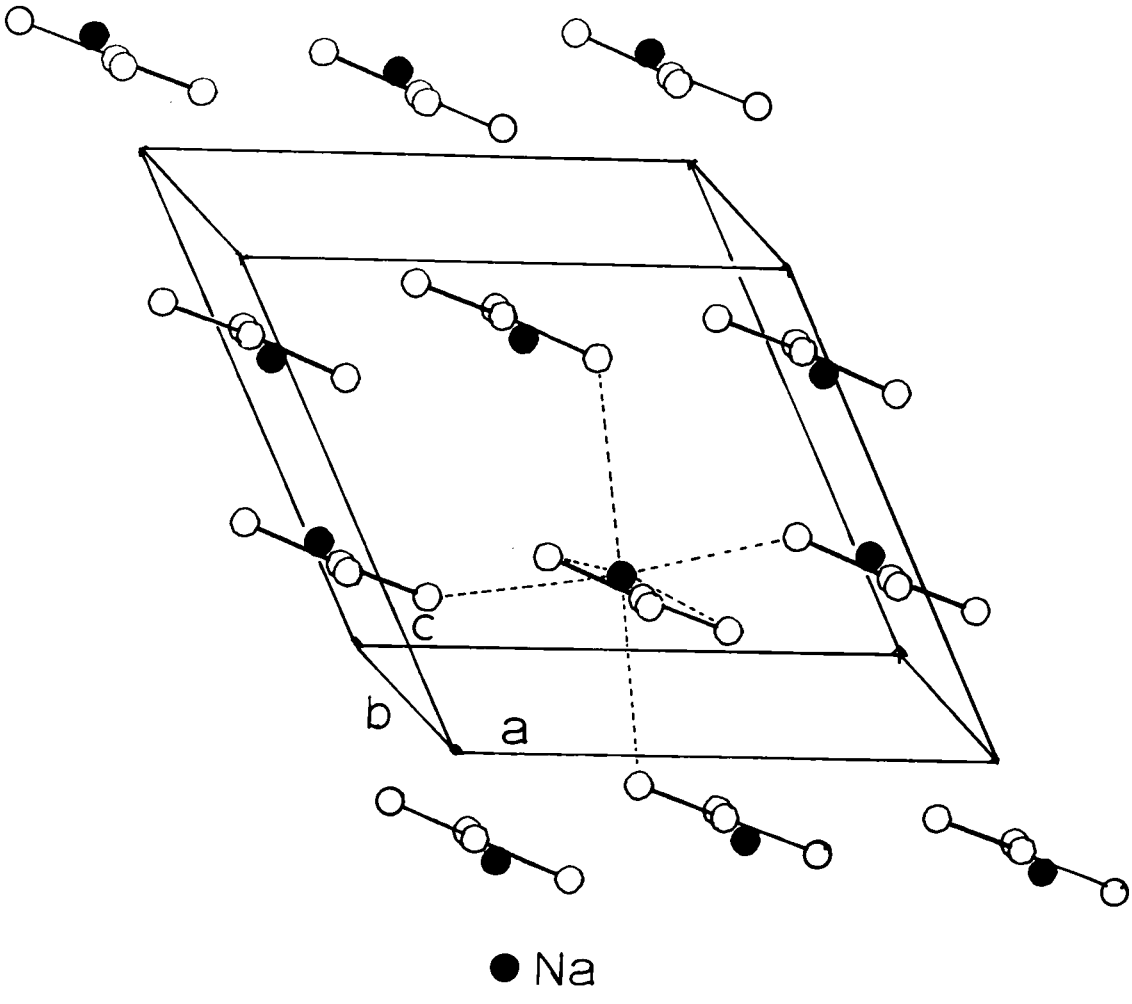


Figure 4

The unit-cell as viewed down b. Dotted lines show weak sodium - oxygen bonds.

Table 16

SODIUM - OXYGEN CONTACT DISTANCES

Atoms	Distance (Å)
Na...O(x,y,z)	2.4008(9)
Na...O(-x,y,0.5-z)	2.4008(9)
Na...O(0.5-x,0.5-y,-z)	2.4337(9)
Na...O(0.5+x,0.5-y,0.5+z)	2.4337(9)
Na...O(0.5+x,0.5+y,z)	2.5194(11)
Na...O(0.5-x,0.5+y,0.5-z)	2.5194(11)

Table 17

AVERAGE Na...O DISTANCES FOR SOME SODIUM COMPOUNDS

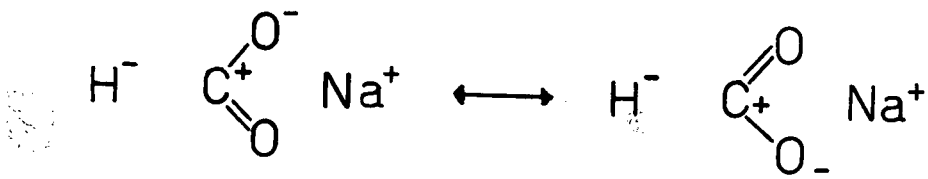
Compound	Avg. Na...O distance (Å)	Ref.
Sodium 2-Oxovalerate	2.46	47
Sodium α-Ketobutyrate	2.5	48
Sodium Pyruvate	2.50	49
Sodium Oxalate	2.48	50

Table 18

REFINED ATOMIC CHARGES

Atom	Charge(e)
Na(1)	+0.79(14)
O(1)	-0.23(1)
C(1)	+0.16(3)
H(1)	-0.49(10)

The positive charge on the carbon (0.16e) is probably the result of some minor resonance forms of the following type:



The distance between a sodium atom of one molecule and the hydrogen atom of the next molecule along the y-axis is 2.94(2) Å. The sum of the ionic radius of sodium and the van der Waals radius of hydrogen (1.2Å) is 2.15Å. The hydrogen atom has almost half an electron charge on it and therefore it is not very appropriate to use the van der Waals radius. The true radius to be used would be somewhere between the van der Waals radius and the ionic radius (2.08Å). The ionic radius would give a distance of 3.03Å for Na...H interaction. Although this distance is not much more than the measured distance, it might be possible that there is some Na...H interaction. This interaction was found to exist and can be seen in the final difference map (Figure 5). This difference map is viewed perpendicular to the formate plane along the y-axis. There is much electron density between the scdium and the hydrogen atoms. Electron density between the oxygens and

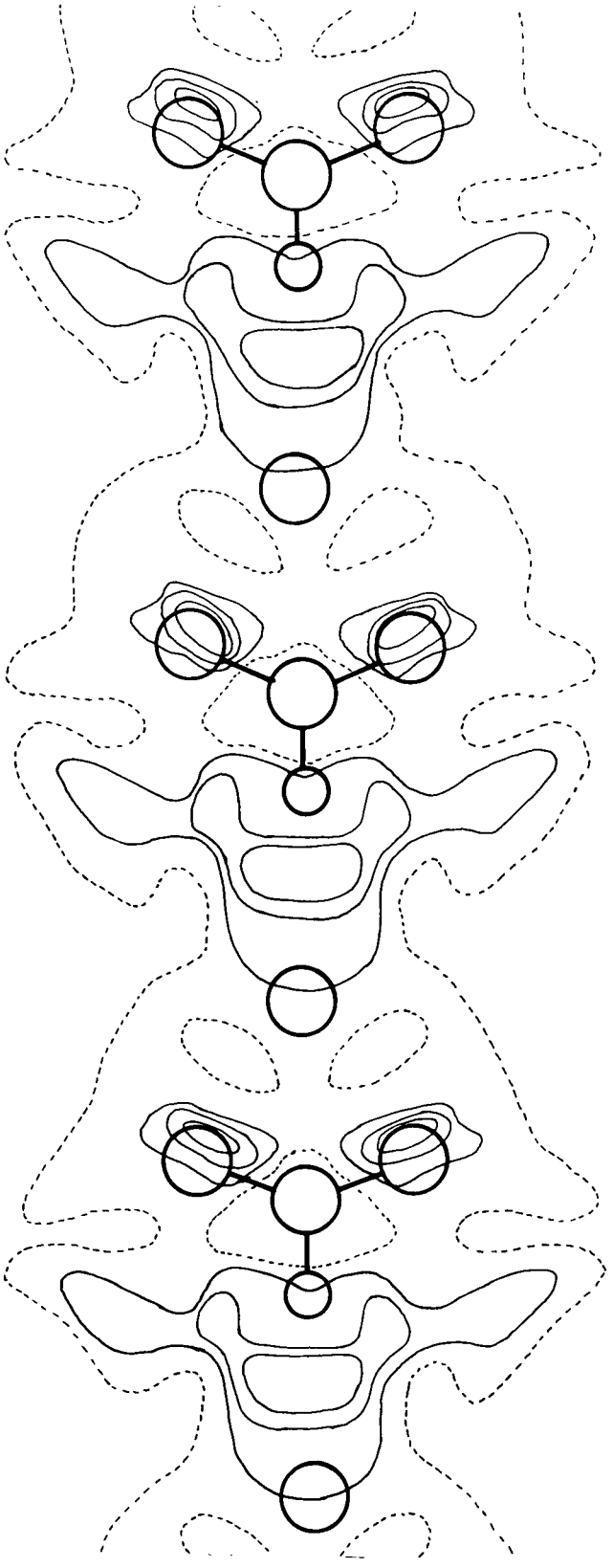


Figure 5

Final difference map. Dotted lines indicate regions of electron density. Contours are drawn at 0.05e/Å^3.

the sodium can also be seen as well as the lone pair electrons on the oxygens. The standard deviation of the electron density was calculated by the method given in reference 51 and was found to be $0.021e/\mathring{A}^3$. Therefore all the peaks found on the difference map are significantly present.

The difference map shows that the crystal structure of sodium formate consists of sodium formate ions hydrogen bonded together into rows. There is much delocalization of electrons throughout the crystal, and the rows interact with each other through weak Na - O bonds.

APPENDIX 1

STRUCTURE FACTORS FOR

HEXAMETHYLCYCLOTRIPHOSPHAZENE - IODINE (1:1 ADDUCT)

h	k	l	Fo	Fc
0	0	1	59.28	50.03
0	0	2	162.84	139.08
0	0	3	134.97	119.37
0	0	5	63.39	63.85
0	0	6	20.13	21.30
0	1	0	5.36	3.77
0	1	1	28.33	26.12
0	1	2	137.47	113.08
0	1	3	25.98	27.35
0	1	4	32.68	31.80
0	1	5	34.56	32.89
0	1	6	10.53	12.51
0	2	0	14.70	14.08
0	2	1	99.48	82.36
0	2	2	17.19	18.26
0	2	3	92.94	86.36
0	2	4	65.68	62.88
0	2	6	36.45	35.29
0	3	0	100.36	88.17
0	3	1	16.35	11.97
0	3	2	60.08	58.71
0	3	3	120.16	110.04
0	3	4	18.53	18.70
0	3	5	97.25	92.64
0	3	6	44.16	44.51
0	4	0	85.28	76.43
0	4	1	90.40	79.92
0	4	2	128.45	117.64
0	4	4	48.51	47.96
0	4	5	8.80	7.27
0	5	0	63.11	59.32
0	5	1	83.35	78.22
0	5	3	23.95	24.10
0	5	4	19.48	19.50
0	6	0	15.72	15.98
0	6	1	37.01	37.61
0	6	2	26.17	24.82
0	6	3	41.73	42.17
0	7	0	23.25	21.94
0	7	1	42.00	38.98
1	0	1	22.61	23.11
1	0	2	15.08	13.53
1	0	3	24.76	31.15
1	0	4	29.75	28.03
1	0	5	31.18	29.97
1	0	6	36.70	35.30
1	1	0	60.55	58.27
1	1	2	66.24	65.46
1	1	3	27.79	29.06
1	1	4	73.74	70.08
1	1	5	67.45	66.68
1	1	6	18.05	17.15
1	2	0	22.47	24.62
1	2	1	143.81	114.89
1	2	2	44.93	40.78
1	2	3	47.77	46.99
1	2	4	92.26	86.44
1	2	5	28.37	26.20
1	2	6	76.15	75.55
1	3	0	192.29	164.97
1	3	2	72.85	64.65
1	3	3	124.59	112.00
1	3	4	11.08	10.92
1	3	5	35.85	34.63
1	4	0	52.73	52.48
1	4	1	55.82	51.25
1	4	2	87.08	76.51
1	4	3	6.63	5.86
1	4	4	27.72	27.35
1	4	5	8.88	7.55
1	5	0	28.96	29.08
1	5	1	34.38	31.79
1	5	2	25.12	24.44
1	5	3	34.90	34.58
1	5	4	50.44	49.15
1	6	0	63.46	59.85
1	6	1	17.01	16.86
1	6	2	41.99	37.33
1	7	0	50.91	47.63
2	0	0	26.41	27.52
2	0	1	53.49	46.43
2	0	2	12.94	9.78
2	0	3	49.72	46.56
2	0	4	36.91	34.50
2	0	5	45.72	44.90
2	0	6	38.34	34.98
2	1	1	13.22	12.68
2	1	2	101.44	90.09
2	1	3	56.03	53.73
2	1	4	21.12	21.20
2	1	5	73.57	67.96
2	1	6	27.65	25.55
2	2	0	18.39	19.26
2	2	1	193.67	166.59
2	2	2	116.63	104.43
2	2	3	53.79	50.08
2	2	4	87.34	81.37
2	2	5	17.65	17.30
2	3	0	137.36	120.04
2	3	1	97.44	85.99
2	3	2	27.95	25.82
2	3	3	77.74	73.14
2	3	4	8.29	6.68
2	3	5	27.52	26.42
2	4	0	31.74	32.02
2	4	1	34.31	31.79
2	4	2	43.99	42.28
2	4	3	36.61	35.83
2	4	4	37.10	36.86
2	5	0	36.01	35.07
2	5	1	79.52	73.36
2	5	2	6.18	7.93
2	5	3	23.28	20.84
2	6	0	43.70	41.01

h	k	l	Fo	Fc
2	6	1	80.87	76.32
2	6	2	16.81	16.02
3	0	0	55.91	53.44
3	0	1	103.46	85.36
3	0	3	53.60	55.60
3	0	4	59.28	58.08
3	0	6	48.81	48.80
3	1	0	198.49	175.05
3	1	1	49.43	46.53
3	1	2	167.30	144.22
3	1	3	129.82	119.79
3	1	4	18.91	20.97
3	1	5	60.03	59.14
3	2	0	38.25	34.88
3	2	1	116.18	100.75
3	2	2	63.24	62.26
3	2	3	16.63	17.11
3	2	4	67.47	65.67
3	3	0	12.71	14.36
3	3	1	36.41	35.68
3	3	2	36.55	33.84
3	3	3	50.22	48.26
3	3	4	52.85	50.19
3	4	0	47.60	46.62
3	4	1	25.28	20.27
3	4	2	76.05	68.85
3	4	3	9.86	8.95
3	5	1	53.85	49.63
3	5	2	105.13	97.79
3	5	3	11.98	10.50
3	6	0	94.92	90.25
3	6	1	59.77	55.83
4	0	0	44.15	42.15
4	0	1	159.90	142.58
4	0	2	51.82	47.52
4	0	3	117.25	107.02
4	0	4	78.32	73.82
4	1	0	185.30	158.59
4	1	1	18.99	18.73
4	1	2	63.02	59.35
4	1	3	47.46	45.45
4	1	4	16.71	16.19
4	1	5	46.74	48.35
4	2	0	31.97	31.20
4	2	1	12.42	13.02
4	2	2	19.59	18.20
4	2	3	31.55	30.71
4	2	4	45.75	44.49
4	3	1	57.33	55.47
4	3	2	21.80	21.22
4	3	3	48.89	46.09
4	3	4	22.38	21.68
4	4	0	97.96	91.58
4	4	1	19.55	20.19
4	4	2	54.63	52.18
4	4	3	99.06	93.96
4	5	0	15.95	14.91
4	5	1	80.24	74.82
4	5	2	61.32	57.93
5	0	0	73.66	67.97
5	0	1	127.99	117.22
5	0	2	7.78	5.77
5	0	3	35.73	34.22
5	0	4	37.42	37.11
5	1	0	56.98	54.51
5	1	1	61.37	61.73
5	1	2	15.05	14.05
5	1	3	6.70	5.61
5	1	4	29.13	28.45
5	2	2	50.51	50.17
5	2	3	7.43	9.04
5	2	4	32.09	30.61
5	3	0	28.83	29.37
5	3	1	106.03	98.46
5	3	2	50.99	49.96
5	3	3	36.42	35.37
5	4	0	105.88	99.60
5	4	1	26.63	24.92
5	4	2	59.82	56.58
5	5	0	39.07	39.63
6	0	1	40.26	39.23
6	0	2	41.56	41.64
6	0	4	6.50	5.38
6	1	0	6.59	0.80
6	1	1	20.71	21.97
6	1	2	14.92	15.38
6	1	3	41.63	40.23
6	2	0	63.12	61.60
6	2	1	17.49	14.81
6	2	2	96.05	90.74
6	2	3	54.09	52.85
6	3	0	47.58	44.43
6	3	1	84.51	81.06
6	3	2	32.13	32.20
6	4	0	44.61	44.81
6	4	1	41.94	41.76
7	0	0	29.24	28.35
7	0	2	19.18	18.84
7	1	0	41.43	42.75
7	1	1	66.76	64.88
7	2	0	84.10	82.65
7	2	1	33.39	34.00
7	3	0	15.28	16.58
8	0	0	15.35	14.63
8	0	1	27.52	28.08
8	1	0	36.50	35.27
0	0	-1	56.94	50.03
0	0	-2	158.54	139.08
0	0	-3	134.16	119.37
0	0	-4	26.57	25.86
0	0	-5	62.76	63.85
0	0	-6	20.69	21.30
0	1	-1	102.32	86.16
0	1	-2	140.10	120.24
0	1	-3	104.31	92.47
0	1	-4	103.17	97.09

h	k	l	Fo	Fc
0	1	-5	8.50	9.45
0	1	-6	52.39	51.22
0	1	-7	15.96	14.29
0	2	-1	69.71	63.68
0	2	-2	58.53	52.34
0	2	-4	38.23	38.84
0	2	-5	70.36	66.31
0	2	-6	6.86	7.38
0	2	-7	33.25	31.56
0	3	-1	41.96	39.77
0	3	-2	78.23	63.13
0	3	-4	21.63	20.90
0	3	-5	15.83	16.54
0	3	-6	53.58	52.87
0	3	-7	19.09	18.76
0	4	-1	158.28	135.90
0	4	-2	27.96	29.22
0	4	-3	60.19	55.69
0	4	-4	43.09	41.67
0	4	-5	11.38	9.67
0	4	-6	28.56	27.55
0	5	-2	99.62	93.30
0	5	-3	69.93	65.81
0	5	-4	53.99	51.57
0	5	-5	59.26	58.37
0	6	-1	38.31	36.91
0	6	-2	13.34	12.05
0	6	-3	28.07	26.29
0	6	-4	15.30	13.26
0	7	-1	47.48	45.12
0	7	-2	26.87	25.30
0	7	-3	24.19	23.93
1	0	-1	90.95	93.31
1	0	-2	123.88	118.00
1	0	-3	123.49	113.25
1	0	-4	12.86	13.22
1	0	-5	62.54	60.56
1	0	-6	24.39	24.60
1	0	-7	42.86	43.41
1	1	-1	34.76	40.40
1	1	-2	18.24	18.06
1	1	-3	63.12	71.95
1	1	-4	97.86	91.03
1	1	-5	40.49	38.06
1	1	-6	65.89	64.68
1	1	-7	54.01	52.67
1	2	-1	25.73	31.28
1	2	-2	22.08	24.10
1	2	-3	6.68	8.66
1	2	-5	65.27	61.27
1	2	-6	17.37	17.05
1	2	-7	34.56	32.80
1	3	-1	22.36	20.93
1	3	-2	82.97	87.51
1	3	-3	63.49	64.65
1	3	-4	10.84	8.47
1	3	-5	41.79	42.30
1	3	-6	30.60	30.01
1	3	-7	21.31	20.58
1	4	-1	108.00	116.75
1	4	-2	58.96	58.66
1	4	-3	92.47	89.79
1	4	-4	91.32	85.33
1	4	-5	20.74	21.39
1	4	-6	27.41	25.77
1	5	-1	20.89	22.29
1	5	-2	35.65	36.98
1	5	-3	7.06	6.14
1	5	-4	18.88	17.18
1	5	-5	44.72	42.87
1	5	-6	7.72	7.65
1	6	-1	36.05	40.82
1	6	-2	22.20	23.39
1	6	-3	11.26	13.36
1	6	-5	19.52	19.12
1	7	-1	28.21	30.18
1	7	-3	29.88	28.26
2	0	-1	16.19	20.37
2	0	-2	163.51	158.71
2	0	-3	95.60	93.93
2	0	-4	64.98	63.42
2	0	-5	86.84	89.04
2	0	-6	63.76	61.50
2	0	-7	39.14	40.02
2	1	-1	46.11	48.52
2	1	-2	15.67	18.72
2	1	-3	28.34	30.41
2	1	-4	57.08	58.49
2	1	-5	12.14	12.33
2	1	-6	45.04	44.35
2	1	-7	18.96	18.84
2	2	-1	171.69	166.50
2	2	-2	71.64	76.73
2	2	-4	48.76	50.41
2	2	-5	46.50	45.54
2	2	-6	30.93	32.74
2	2	-7	7.27	4.35
2	3	-1	39.47	46.33
2	3	-2	117.95	125.35
2	3	-3	113.32	114.43
2	3	-4	61.83	60.60
2	3	-5	48.53	49.14
2	3	-6	8.48	8.43
2	3	-7	11.82	13.68
2	4	-1	30.69	34.14
2	4	-2	22.82	23.93
2	4	-3	39.37	42.39
2	4	-4	55.75	58.44
2	4	-5	11.33	10.15
2	4	-6	58.67	57.13
2	5	-1	25.68	28.69
2	5	-2	10.45	10.44
2	5	-3	12.30	15.14
2	5	-4	25.42	26.67
2	5	-5	35.81	36.70
2	6	-2	44.87	48.63

h	k	l	Fo	Fc
2	6	-3	28.86	30.28
2	6	-4	20.17	20.45
2	7	-1	74.72	80.15
2	7	-2	9.79	10.30
3	0	-1	36.10	33.62
3	0	-2	56.95	59.89
3	0	-3	34.76	42.68
3	0	-4	9.19	9.06
3	0	-5	56.98	59.05
3	0	-6	10.53	9.41
3	1	-1	77.75	75.34
3	1	-2	23.23	22.74
3	1	-3	50.89	60.51
3	1	-4	58.21	61.58
3	1	-5	42.54	43.36
3	1	-7	9.05	9.70
3	2	-1	171.08	161.28
3	2	-2	104.47	112.92
3	2	-3	71.30	75.58
3	2	-4	70.73	76.67
3	2	-5	15.12	14.34
3	2	-6	15.66	15.73
3	2	-7	13.29	13.08
3	3	-1	14.22	14.92
3	3	-2	52.94	59.20
3	3	-3	56.55	62.39
3	3	-4	23.82	23.38
3	3	-5	79.07	79.06
3	3	-6	19.59	19.99
3	3	-7	44.37	45.22
3	4	-3	28.57	31.35
3	4	-4	32.58	34.13
3	4	-5	15.33	15.69
3	4	-6	47.71	47.36
3	5	-1	73.97	73.50
3	5	-2	45.36	49.92
3	5	-3	24.48	27.05
3	5	-4	30.56	32.33
3	5	-5	10.26	9.37
3	6	-2	60.61	67.60
3	6	-3	60.82	67.34
3	6	-4	23.58	24.74
4	0	-1	39.51	39.58
4	0	-2	71.42	77.58
4	0	-3	54.34	52.03
4	0	-4	21.18	22.32
4	0	-5	6.94	5.94
4	0	-7	23.65	24.69
4	1	-1	85.67	87.67
4	1	-2	64.29	70.02
4	1	-3	95.49	100.86
4	1	-5	40.31	40.92
4	1	-6	18.23	18.35
4	1	-7	16.37	17.11
4	2	-1	62.28	62.57
4	2	-2	38.34	41.03
4	2	-3	66.88	73.46
4	2	-4	92.97	97.72
4	2	-5	12.08	11.60
4	2	-6	66.51	66.87
4	2	-7	44.51	45.24
4	3	-1	22.94	21.23
4	3	-2	27.49	29.81
4	3	-3	23.39	26.97
4	3	-4	20.29	21.88
4	3	-5	65.42	69.63
4	3	-6	7.09	6.20
4	4	-1	46.18	48.29
4	4	-2	41.12	44.37
4	4	-3	39.20	42.57
4	4	-4	23.07	25.27
4	4	-5	39.14	39.97
4	5	-1	91.44	89.49
4	5	-2	63.89	68.41
4	5	-3	38.04	40.72
4	5	-4	41.22	43.41
4	6	-1	21.34	22.32
4	6	-2	34.89	36.45
4	6	-3	10.70	11.33
5	0	-1	112.49	106.85
5	0	-2	107.44	106.66
5	0	-3	21.70	20.84
5	0	-4	70.14	74.88
5	0	-5	22.31	25.71
5	0	-6	20.49	22.32
5	0	-7	16.90	15.77
5	1	-1	18.55	16.12
5	1	-2	96.32	97.22
5	1	-3	96.46	103.82
5	1	-5	77.61	78.34
5	1	-6	59.35	61.02
5	1	-7	37.22	36.13
5	2	-1	19.75	20.24
5	2	-2	29.75	29.66
5	2	-3	23.50	25.03
5	2	-4	74.77	79.58
5	2	-5	8.93	6.40
5	2	-6	32.71	32.49
5	3	-1	54.86	54.02
5	3	-2	60.83	62.42
5	3	-3	20.76	22.07
5	3	-4	43.95	46.84
5	3	-6	29.34	30.90
5	4	-1	58.03	53.07
5	4	-2	61.43	64.00
5	4	-3	54.34	57.19
5	5	-1	43.55	43.39
5	5	-2	10.72	11.51
5	5	-3	30.51	32.87
5	5	-4	67.78	71.34
6	0	-1	82.16	81.48
6	0	-2	84.21	83.44
6	0	-3	16.18	17.28
6	0	-4	85.88	88.76
6	0	-5	64.57	63.31
6	0	-6	43.63	45.30

h	k	l	Fo	Fc	h	k	l	Fo	Fc
6	1	-1	31.44	30.47	-1	1	1	151.71	159.42
6	1	-2	29.88	29.56	-1	1	2	124.72	118.09
6	1	-3	67.35	69.17	-1	1	3	14.76	18.40
6	1	-4	6.39	6.45	-1	1	4	89.98	84.93
6	1	-5	43.08	44.09	-1	1	5	28.87	27.95
6	1	-6	35.53	37.31	-1	2	0	48.36	44.96
6	2	-1	65.30	64.11	-1	2	1	140.41	131.26
6	2	-2	18.10	16.54	-1	2	2	49.81	48.06
6	2	-3	49.11	52.46	-1	2	3	21.04	21.56
6	2	-4	17.31	16.04	-1	2	4	37.40	36.56
6	2	-5	20.85	21.19	-1	2	5	5.95	5.14
6	2	-6	24.70	23.38	-1	2	6	16.49	15.63
6	3	-1	81.79	81.17	-1	3	0	27.90	32.25
6	3	-2	64.89	66.20	-1	3	1	8.14	2.87
6	3	-4	9.77	9.61	-1	3	2	104.97	98.40
6	3	-5	36.44	36.31	-1	3	3	24.35	27.78
6	4	-1	7.86	5.49	-1	3	4	16.74	17.09
6	4	-2	44.79	46.14	-1	3	5	56.38	55.27
6	4	-3	76.43	79.97	-1	3	6	56.74	54.36
6	4	-4	28.29	28.49	-1	4	0	15.66	13.96
7	0	-1	21.13	19.73	-1	4	1	53.29	60.22
7	0	-2	60.72	61.91	-1	4	2	95.56	94.44
7	0	-3	19.69	19.42	-1	4	4	109.02	100.46
7	0	-4	49.95	50.72	-1	4	5	36.99	36.89
7	0	-5	20.54	24.57	-1	5	0	84.88	80.64
7	0	-6	12.48	14.05	-1	5	1	86.50	94.44
7	1	-1	24.03	24.57	-1	5	2	20.74	20.65
7	1	-2	53.72	53.51	-1	5	3	51.26	51.66
7	1	-3	26.17	28.41	-1	5	4	14.46	14.06
7	1	-4	14.21	13.90	-1	6	0	61.08	60.56
7	1	-5	27.53	29.75	-1	6	2	24.14	25.24
7	2	-1	59.60	59.35	-1	6	3	21.27	21.75
7	2	-2	21.46	23.12	-1	7	0	35.86	35.67
7	2	-3	17.61	16.30	-1	7	1	16.90	20.36
7	2	-4	32.28	32.78	-2	0	0	25.84	27.52
7	2	-5	16.33	13.98	-2	0	1	15.87	20.37
7	3	-1	56.17	54.85	-2	0	2	162.41	158.71
7	3	-2	65.69	66.78	-2	0	3	94.19	93.93
7	3	-3	41.51	42.82	-2	0	4	65.44	63.42
7	3	-4	78.20	81.46	-2	0	5	87.04	89.04
8	0	-1	52.35	50.73	-2	0	6	63.44	61.50
8	0	-2	24.53	23.63	-2	0	7	38.85	40.02
8	0	-4	26.00	27.24	-2	1	0	47.29	45.70
8	1	-1	44.86	46.06	-2	1	1	123.97	124.76
8	1	-2	25.50	27.02	-2	1	2	93.71	99.95
8	1	-3	20.73	20.26	-2	1	3	42.02	40.36
8	1	-4	18.96	18.17	-2	1	4	108.45	108.30
8	2	-1	52.86	51.61	-2	1	5	33.95	34.30
8	2	-2	45.83	46.20	-2	1	6	70.86	69.90
8	2	-3	91.38	91.81	-2	1	7	11.31	11.12
-1	0	1	92.29	93.31	-2	2	0	217.39	177.43
-1	0	2	124.41	118.00	-2	2	1	120.19	117.79
-1	0	3	123.36	113.25	-2	2	2	11.98	8.52
-1	0	4	13.00	13.22	-2	2	3	83.89	85.85
-1	0	5	62.14	60.56	-2	2	4	29.29	31.67
-1	0	6	24.86	24.60	-2	2	5	8.41	7.15
-1	0	7	42.80	43.41	-2	3	0	49.25	56.84
-1	1	0	25.34	25.51	-2	3	1	49.78	51.96

h	k	l	Fo	Fc	h	k	l	Fo	Fc
-2	3	2	31.04	34.23	-3	5	3	52.61	56.94
-2	3	3	26.45	27.47	-3	5	4	30.45	32.38
-2	3	5	21.41	22.34	-3	6	0	24.88	22.04
-2	3	6	24.95	25.38	-3	6	1	13.65	14.60
-2	4	0	12.23	12.54	-3	6	2	85.25	94.24
-2	4	1	91.74	96.56	-3	6	3	20.25	23.16
-2	4	2	28.61	31.32	-3	7	0	39.96	39.84
-2	4	3	21.47	22.99	-3	7	1	41.64	43.96
-2	4	4	65.49	67.54	-4	0	0	43.26	42.15
-2	4	5	47.75	49.17	-4	0	1	40.13	39.58
-2	5	0	57.78	55.40	-4	0	2	72.41	77.58
-2	5	1	40.59	42.43	-4	0	3	54.59	52.03
-2	5	2	17.24	17.66	-4	0	4	20.64	22.32
-2	5	3	102.67	104.89	-4	0	5	6.84	5.94
-2	5	4	23.52	26.96	-4	0	7	24.05	24.69
-2	6	0	72.55	69.81	-4	1	0	20.96	22.30
-2	6	1	33.34	35.80	-4	1	1	38.43	42.55
-2	6	2	47.19	52.27	-4	1	2	23.27	27.22
-2	7	0	7.47	8.36	-4	1	3	12.59	10.15
-2	7	1	22.11	22.97	-4	1	4	57.50	61.38
-3	0	0	55.95	53.44	-4	1	5	8.41	6.66
-3	0	1	36.39	33.62	-4	1	6	9.72	9.02
-3	0	2	57.79	59.89	-4	1	7	32.23	31.76
-3	0	3	35.55	42.68	-4	2	0	60.28	59.99
-3	0	4	9.79	9.06	-4	2	1	49.07	46.97
-3	0	5	57.60	59.05	-4	2	2	81.68	83.92
-3	0	6	12.12	9.41	-4	2	3	85.91	89.65
-3	0	7	7.54	5.01	-4	2	4	38.62	39.15
-3	1	0	28.10	26.03	-4	2	5	62.46	64.49
-3	1	1	142.61	131.79	-4	2	6	90.24	92.02
-3	1	2	61.04	67.80	-4	3	0	31.35	32.77
-3	1	3	63.10	70.20	-4	3	1	63.44	63.21
-3	1	4	84.00	87.05	-4	3	2	99.16	103.58
-3	1	5	55.77	58.61	-4	3	3	7.45	0.88
-3	1	6	58.26	57.92	-4	3	4	92.49	97.23
-3	1	7	79.71	77.58	-4	3	5	8.99	8.05
-3	2	0	162.74	134.14	-4	3	6	23.06	24.12
-3	2	1	74.23	70.90	-4	4	0	23.80	25.72
-3	2	2	53.48	57.09	-4	4	1	94.07	94.61
-3	2	3	140.26	143.52	-4	4	2	6.71	6.74
-3	2	4	20.35	21.52	-4	4	3	8.34	7.76
-3	2	5	84.25	85.08	-4	4	4	18.66	17.77
-3	2	6	7.19	8.67	-4	4	5	9.47	9.24
-3	3	0	95.95	85.90	-4	5	0	44.39	43.23
-3	3	1	19.14	19.91	-4	5	1	11.14	11.94
-3	3	3	24.79	28.15	-4	5	4	9.02	9.65
-3	3	4	8.02	10.39	-4	6	0	17.05	17.16
-3	3	5	20.22	20.23	-4	6	1	25.01	24.66
-3	3	6	10.45	10.33	-4	6	2	40.90	42.88
-3	4	0	53.12	49.18	-4	6	3	14.74	15.80
-3	4	1	51.62	52.17	-4	7	0	11.70	15.41
-3	4	2	11.54	14.19	-4	7	1	64.29	64.67
-3	4	3	8.03	6.76	-5	0	0	73.75	67.97
-3	4	4	20.25	22.70	-5	0	1	112.46	106.85
-3	4	5	15.06	15.96	-5	0	2	106.74	106.66
-3	5	0	76.37	72.80	-5	0	3	22.19	20.84
-3	5	1	34.34	35.01	-5	0	4	69.98	74.88
-3	5	2	25.64	27.88	-5	0	5	22.51	25.71

h	k	l	Fo	Fc
-5	0	6	21.88	22.32
-5	0	7	16.07	15.77
-5	1	0	42.76	44.75
-5	1	1	74.25	75.07
-5	1	2	34.07	33.48
-5	1	3	18.80	20.48
-5	1	4	17.66	17.33
-5	1	5	10.25	8.48
-5	1	6	16.54	17.29
-5	2	0	42.57	40.13
-5	2	1	35.98	36.95
-5	2	2	6.70	1.39
-5	2	3	45.00	47.84
-5	2	4	16.00	13.61
-5	2	5	31.20	31.30
-5	2	6	28.28	28.92
-5	3	0	31.17	30.95
-5	3	1	89.04	84.97
-5	3	2	76.73	78.28
-5	3	3	19.94	23.39
-5	3	4	62.23	64.27
-5	3	5	87.96	93.26
-5	3	6	30.76	31.29
-5	4	0	56.03	56.22
-5	4	1	74.39	71.86
-5	4	2	11.34	11.64
-5	4	3	102.22	107.07
-5	4	4	12.06	13.48
-5	4	5	34.55	36.08
-5	5	0	56.10	54.66
-5	5	1	13.44	14.60
-5	5	2	8.01	7.77
-5	6	0	14.36	13.54
-5	6	1	7.56	7.18
-5	6	2	7.73	7.84
-5	6	3	13.31	14.48
-6	0	1	82.39	81.48
-6	0	2	83.56	83.44
-6	0	3	17.70	17.28
-6	0	4	85.93	88.76
-6	0	5	64.46	63.31
-6	0	6	44.37	45.30
-6	1	0	120.49	113.43
-6	1	1	83.61	83.13
-6	1	2	27.00	27.60
-6	1	3	70.77	75.05
-6	1	4	22.11	26.56
-6	1	5	30.17	31.47
-6	1	6	14.46	12.58
-6	2	0	57.96	56.74
-6	2	1	16.81	16.32
-6	2	2	45.24	48.60
-6	2	3	18.39	20.85
-6	2	4	8.30	8.94
-6	2	5	14.00	14.59
-6	2	6	15.84	15.32
-6	3	0	38.11	37.10
-6	3	2	29.57	29.21
-6	3	3	12.70	15.16
-6	3	4	25.54	27.21
-6	3	5	16.18	15.74
-6	4	0	59.49	59.30
-6	4	1	46.22	46.51
-6	4	2	16.11	17.37
-6	4	3	61.44	64.42
-6	4	4	70.85	74.46
-6	4	5	32.24	32.49
-6	5	0	60.15	59.62
-6	5	1	16.41	17.22
-6	5	2	91.34	93.91
-6	5	3	9.19	8.33
-6	6	0	18.40	18.31
-6	6	1	11.54	10.71
-7	0	0	28.00	28.35
-7	0	1	20.28	19.73
-7	0	2	61.14	61.91
-7	0	3	19.10	19.42
-7	0	4	48.56	50.72
-7	0	5	20.27	24.57
-7	0	6	14.39	14.05
-7	1	0	76.74	74.13
-7	1	1	49.24	47.19
-7	1	3	86.71	91.06
-7	1	4	51.82	52.78
-7	1	5	48.40	50.92
-7	2	0	50.36	50.65
-7	2	1	28.38	27.99
-7	2	2	64.39	68.03
-7	2	3	8.82	8.52
-7	2	4	36.45	37.98
-7	2	5	16.26	13.69
-7	3	1	36.94	40.73
-7	3	2	10.95	11.64
-7	3	4	14.76	17.08
-7	3	5	11.69	11.99
-7	4	0	11.09	11.61
-7	4	1	20.85	19.37
-7	4	2	12.23	12.64
-7	4	3	16.48	16.65
-7	4	4	6.99	6.10
-7	5	0	24.41	23.85
-7	5	1	6.29	4.32
-7	5	2	47.39	48.34
-8	0	0	16.71	14.63
-8	0	1	50.90	50.73
-8	0	2	23.08	23.63
-8	0	3	22.19	24.11
-8	0	4	25.80	27.24
-8	1	1	51.15	52.79
-8	1	2	31.66	32.96
-8	1	3	41.90	44.60
-8	1	4	12.16	12.68
-8	2	0	29.20	29.81
-8	2	1	28.76	29.62
-8	2	2	74.20	75.63
-8	2	3	39.11	41.58

h	k	l	Fo	Fc
-8	2	4	61.56	63.92
-8	3	0	32.47	33.57
-8	3	1	60.42	63.38
-8	3	2	9.31	10.37
-8	3	3	35.76	36.73
-8	4	0	19.18	18.72
-1	0	-1	21.93	23.11
-1	0	-2	15.07	13.53
-1	0	-3	22.99	31.15
-1	0	-4	30.60	28.03
-1	0	-5	31.12	29.97
-1	0	-6	36.52	35.30
-1	1	-2	73.63	66.44
-1	1	-3	119.91	101.28
-1	1	-4	96.92	91.74
-1	1	-5	29.51	27.34
-1	1	-6	39.45	40.82
-1	1	-7	17.05	16.74
-1	2	-1	16.97	16.48
-1	2	-2	140.83	111.54
-1	2	-3	131.33	112.16
-1	2	-4	52.51	52.59
-1	2	-5	69.64	67.21
-1	2	-6	12.90	10.40
-1	2	-7	34.44	36.26
-1	3	-1	12.53	14.40
-1	3	-2	53.82	44.85
-1	3	-3	33.51	32.22
-1	3	-4	16.32	17.78
-1	3	-5	36.76	35.73
-1	3	-6	45.36	44.15
-1	4	-1	63.45	59.77
-1	4	-2	29.59	27.33
-1	4	-3	31.60	29.89
-1	4	-4	6.23	6.18
-1	4	-5	27.14	27.55
-1	4	-6	19.42	20.62
-1	5	-1	63.61	55.09
-1	5	-2	96.78	86.49
-1	5	-3	23.91	24.10
-1	5	-4	54.21	52.96
-1	5	-5	25.29	25.02
-1	6	-1	56.27	53.46
-1	6	-2	6.93	3.73
-1	6	-3	63.79	59.80
-1	6	-4	52.17	52.52
-1	6	-5	24.04	23.35
-1	7	-1	9.98	8.26
-1	7	-2	36.34	36.00
-2	0	-1	53.46	46.43
-2	0	-2	12.72	9.78
-2	0	-3	48.67	46.56
-2	0	-4	36.46	34.50
-2	0	-5	44.08	44.90
-2	0	-6	37.03	34.98
-2	1	-1	80.98	66.03
-2	1	-2	47.03	43.86
-2	1	-4	30.99	30.96
-2	1	-5	36.43	35.90
-2	1	-6	19.16	21.01
-2	2	-1	12.40	9.53
-2	2	-2	199.15	170.64
-2	2	-3	50.96	50.66
-2	2	-4	55.50	53.36
-2	2	-5	43.31	43.65
-2	2	-6	21.15	23.46
-2	3	-1	53.27	54.11
-2	3	-2	45.47	39.20
-2	3	-3	69.44	65.75
-2	3	-4	108.37	99.36
-2	3	-5	25.41	24.34
-2	3	-6	45.36	44.76
-2	4	-1	8.21	6.87
-2	4	-2	23.94	22.74
-2	4	-3	25.36	23.36
-2	4	-4	15.25	15.36
-2	4	-5	17.65	15.47
-2	4	-6	14.18	13.34
-2	5	-1	33.10	29.42
-2	5	-2	47.22	43.49
-2	5	-3	14.56	14.72
-2	5	-4	10.75	11.09
-2	5	-5	7.20	7.55
-2	6	-1	67.65	61.72
-2	6	-2	20.47	19.38
-2	6	-3	49.13	45.70
-2	6	-4	18.89	17.12
-2	7	-1	30.41	29.18
-2	7	-2	49.72	47.09
-3	0	-1	105.33	85.36
-3	0	-3	53.30	55.60
-3	0	-4	59.64	58.08
-3	0	-6	48.45	48.80
-3	1	-1	33.27	28.42
-3	1	-2	38.89	29.39
-3	1	-3	17.03	15.93
-3	1	-4	42.33	38.83
-3	1	-5	37.93	37.55
-3	1	-6	18.92	18.08
-3	2	-1	33.55	22.67
-3	2	-2	37.51	37.80
-3	2	-3	26.86	27.65
-3	2	-4	6.03	5.79
-3	2	-5	38.88	39.58
-3	2	-6	29.47	29.56
-3	3	-1	177.96	145.77
-3	3	-2	9.45	8.25
-3	3	-3	152.68	132.87
-3	3	-4	34.80	33.67
-3	3	-5	24.64	25.56
-3	3	-6	21.89	23.66
-3	4	-1	43.17	40.12
-3	4	-2	53.15	51.55
-3	4	-3	50.42	46.90
-3	4	-4	23.07	22.10
-3	4	-5	74.56	71.92

h	k	l	Fo	Fc
-3	5	-1	25.27	23.10
-3	5	-2	28.63	28.19
-3	5	-3	27.87	28.40
-3	5	-5	7.47	5.21
-3	6	-1	36.02	34.43
-3	6	-2	28.33	28.55
-3	6	-3	29.19	26.20
-3	7	-1	48.39	44.14
-3	7	-2	43.13	41.01
-4	0	-1	161.26	142.58
-4	0	-2	51.94	47.52
-4	0	-3	116.81	107.02
-4	0	-4	77.35	73.82
-4	1	-1	38.34	36.56
-4	1	-2	80.70	75.97
-4	1	-3	35.55	32.49
-4	1	-4	34.40	34.03
-4	1	-5	55.34	54.21
-4	2	-1	14.54	14.39
-4	2	-2	20.17	20.16
-4	2	-3	5.32	4.09
-4	2	-4	10.41	9.50
-4	2	-5	22.24	22.53
-4	3	-1	107.31	95.89
-4	3	-2	5.69	4.61
-4	3	-3	17.02	18.82
-4	3	-4	12.29	12.43
-4	3	-5	10.72	10.82
-4	4	-1	47.60	45.15
-4	4	-2	100.45	93.23
-4	4	-3	10.79	10.49
-4	4	-4	89.88	85.21
-4	4	-5	20.00	20.35
-4	5	-1	45.02	43.83
-4	5	-2	37.36	35.27
-4	5	-3	41.47	38.96
-4	5	-4	42.08	40.66
-4	6	-1	46.88	43.99
-4	6	-2	22.40	21.71
-4	6	-3	28.53	27.51
-4	7	-1	17.11	17.73
-5	0	-1	129.45	117.22
-5	0	-2	8.77	5.77
-5	0	-3	34.97	34.22
-5	0	-4	35.91	37.11
-5	1	-2	135.20	121.58
-5	1	-3	52.87	50.64
-5	1	-4	66.51	66.77
-5	1	-5	39.41	38.60
-5	2	-1	27.72	26.47
-5	2	-2	14.48	15.46
-5	2	-3	28.10	26.77
-5	2	-4	39.97	39.76
-5	2	-5	15.65	15.10
-5	3	-1	63.48	58.92
-5	3	-3	15.60	16.10
-5	3	-4	14.48	13.75
-5	4	-1	10.74	9.26
-5	4	-2	43.87	41.78
-5	4	-3	14.36	15.45
-5	4	-4	10.96	11.56
-5	5	-1	37.16	36.10
-5	5	-2	20.15	19.33
-5	5	-3	58.39	56.99
-5	6	-1	29.71	29.82
-5	6	-2	34.58	32.93
-6	0	-1	41.07	39.23
-6	0	-2	40.98	41.64
-6	1	-1	37.65	36.59
-6	1	-2	80.77	76.77
-6	1	-3	6.76	3.09
-6	1	-4	21.93	23.73
-6	2	-1	50.90	50.93
-6	2	-2	6.47	2.68
-6	2	-3	89.60	88.02
-6	2	-4	44.38	44.06
-6	3	-1	38.02	38.34
-6	3	-2	34.89	35.02
-6	3	-4	13.58	12.50
-6	4	-1	21.89	21.50
-6	4	-2	53.62	53.87
-6	5	-1	43.21	42.54
-6	6	-1	22.65	21.49
-7	0	-2	19.32	18.84
-7	1	-2	24.32	25.34
-7	1	-3	13.82	13.89
-7	2	-1	71.41	69.01
-7	2	-2	12.23	12.20
-7	2	-3	44.79	45.24
-7	3	-1	32.74	32.79
-7	3	-2	47.83	48.03
-7	4	-1	25.39	25.02
-7	4	-2	22.39	23.75
-7	5	-1	38.61	37.84
-8	0	-1	28.22	28.08
-8	1	-1	26.04	26.09
-8	2	-1	60.47	61.08
-8	3	-1	24.69	24.38
0	0	8	11.96	11.41
0	0	9	9.46	7.82
0	1	8	20.77	19.92
0	2	7	53.88	51.20
0	3	7	37.65	38.38
0	3	8	18.77	19.60
0	4	7	10.48	11.62
0	5	7	23.77	24.08
0	6	4	16.91	16.63
0	6	5	36.13	35.94
0	6	6	23.90	24.15
0	7	2	49.55	48.94
0	7	4	54.82	52.52
0	7	5	32.64	32.73
0	8	0	28.92	26.33
0	8	1	53.87	52.98
0	8	2	16.62	15.20
0	8	3	26.68	25.36

h	k	l	Fo	Fc
0	9	0	22.02	20.77
1	0	7	16.16	14.80
1	1	7	24.31	25.14
1	1	8	45.91	46.02
1	2	7	28.85	29.57
1	2	8	23.08	24.68
1	4	6	11.17	11.72
1	5	5	19.73	19.58
1	5	6	28.96	28.71
1	6	3	61.66	59.34
1	6	5	56.44	55.22
1	7	1	28.98	26.17
1	7	2	70.37	67.64
1	7	3	8.81	7.03
1	7	4	21.77	20.65
1	8	0	34.78	34.19
1	8	1	29.82	27.02
1	8	2	15.02	15.35
1	8	3	10.91	11.75
1	9	0	10.61	8.63
2	0	7	21.47	22.15
2	0	8	15.89	16.52
2	1	7	45.52	47.84
2	1	8	14.66	13.48
2	2	6	22.56	22.74
2	3	7	16.79	15.34
2	4	5	41.20	40.04
2	4	6	23.19	21.42
2	4	7	22.01	22.96
2	5	4	62.42	59.80
2	5	5	20.88	19.98
2	5	6	45.94	45.45
2	6	3	76.61	72.75
2	6	5	12.71	13.21
2	7	0	45.12	44.13
2	7	1	39.31	36.18
2	7	2	30.75	28.60
2	7	3	26.81	26.50
2	7	4	12.51	10.81
2	8	0	11.11	11.26
2	8	1	14.16	12.66
2	8	2	10.56	10.51
3	0	7	23.22	22.30
3	0	8	24.84	26.82
3	1	6	19.35	19.30
3	1	7	14.86	17.12
3	2	6	18.63	18.81
3	3	5	21.64	21.58
3	3	6	30.75	30.25
3	3	7	28.41	27.61
3	4	5	55.12	54.53
3	4	6	26.53	25.53
3	5	4	63.36	62.94
3	5	5	8.21	8.96
3	6	2	39.00	36.18
3	6	3	33.92	32.14
3	6	4	25.23	24.89
3	7	0	12.69	12.10
3	7	1	9.05	7.73
3	7	3	16.20	16.44
3	8	1	35.65	34.41
4	0	6	41.83	43.81
4	0	7	15.57	16.03
4	1	6	18.36	19.37
4	1	7	17.94	19.15
4	2	5	43.01	42.09
4	2	6	9.03	9.17
4	2	7	25.34	24.33
4	3	5	8.22	5.20
4	3	6	38.82	39.99
4	4	5	48.87	50.08
4	5	3	18.25	17.95
4	5	4	30.43	29.37
4	5	5	16.04	15.39
4	6	0	24.44	22.79
4	6	1	19.28	18.37
4	6	4	19.85	20.48
4	7	0	23.32	24.53
4	7	1	11.56	10.73
4	7	2	38.79	38.13
5	0	6	29.24	31.88
5	0	7	18.15	16.07
5	1	5	27.79	26.82
5	1	6	30.39	29.73
5	2	5	19.38	18.91
5	2	6	15.85	13.83
5	3	4	78.97	77.79
5	4	3	54.66	54.04
5	4	5	18.93	19.21
5	5	1	20.41	19.22
5	5	2	14.74	13.94
5	5	3	9.52	8.98
5	6	1	32.16	31.04
5	6	2	9.12	7.62
5	6	3	31.44	31.28
5	7	0	27.12	25.55
5	7	1	11.55	13.49
6	0	5	26.35	26.14
6	0	6	15.42	15.14
6	1	4	16.75	16.44
6	1	5	14.99	16.32
6	1	6	12.75	11.56
6	2	4	15.99	17.82
6	2	5	60.28	60.83
6	3	3	42.66	43.24
6	3	4	40.26	41.46
6	4	2	21.15	21.41
6	4	4	12.32	12.98
6	5	2	32.37	32.27
6	6	0	25.85	24.60
6	6	1	37.94	37.24
6	6	2	23.52	23.03
6	7	0	59.10	57.96
7	0	4	27.65	28.37
7	0	5	21.58	20.71
7	1	3	62.48	63.57

h	k	l	Fo	Fc
7	1	4	41.54	41.41
7	2	2	57.65	58.74
7	2	3	27.03	27.87
7	2	4	25.31	26.54
7	3	1	33.48	33.22
7	3	2	33.47	34.34
7	3	3	13.83	16.25
7	4	0	25.79	24.35
7	4	1	9.61	9.46
7	4	3	31.73	33.32
7	5	0	33.88	33.58
7	5	1	14.65	14.14
7	5	2	33.21	32.84
8	0	2	52.79	53.60
8	0	3	13.78	11.33
8	0	4	35.10	37.45
8	1	2	11.73	10.96
8	1	3	41.60	43.82
8	1	4	16.69	16.51
8	2	0	55.48	55.87
8	2	1	23.00	22.92
8	2	2	16.59	17.11
8	2	3	25.59	27.16
8	3	1	24.62	23.65
8	3	2	12.15	12.03
8	4	0	29.96	29.11
8	4	1	42.64	42.65
8	5	0	49.75	48.67
9	0	0	43.29	43.89
9	0	1	16.29	17.19
9	0	2	55.15	55.80
9	1	0	38.14	37.90
9	1	1	40.34	41.21
9	1	2	16.26	14.93
9	1	3	12.23	12.69
9	2	0	25.95	25.33
9	2	2	19.84	21.82
9	3	0	19.48	17.82
9	3	1	19.61	19.21
9	4	0	33.08	32.75
10	0	0	44.50	42.71
10	0	1	21.50	22.09
10	0	2	22.27	22.13
10	1	0	17.30	17.17
10	1	1	20.42	20.23
10	2	0	23.94	25.06
11	0	0	19.65	17.32
0	0	-8	10.20	11.41
0	1	-8	20.87	21.05
0	2	-8	37.67	36.86
0	2	-9	14.69	14.81
0	3	-8	22.05	22.71
0	3	-9	13.27	12.44
0	4	-7	20.61	21.37
0	4	-8	23.18	21.94
0	5	-7	9.83	11.92
0	6	-6	28.47	28.26
0	7	-4	16.06	14.07
0	7	-6	14.10	12.33
0	7	-7	11.56	12.42
0	8	-1	34.38	31.58
0	8	-2	15.69	14.29
0	8	-3	15.49	14.66
0	8	-4	15.89	15.70
0	8	-5	15.38	14.73
0	8	-6	13.66	13.84
0	9	-1	38.72	38.43
0	9	-2	15.42	13.98
0	9	-3	44.91	41.96
1	0	-9	9.48	8.06
1	1	-8	24.63	24.44
1	1	-9	45.46	45.60
1	2	-8	16.40	15.72
1	2	-9	8.82	8.57
1	3	-9	12.58	14.11
1	4	-9	8.43	8.91
1	5	-7	39.16	38.71
1	6	-6	22.93	25.04
1	6	-8	16.55	17.09
1	7	-4	20.31	17.77
1	7	-5	20.43	20.52
1	7	-6	18.46	17.67
1	8	-1	24.98	27.07
1	8	-2	55.42	57.59
1	8	-3	9.09	8.81
1	8	-4	29.89	29.02
1	8	-5	27.46	26.95
1	9	-1	10.38	10.64
1	9	-3	16.65	18.06
2	0	-8	62.23	60.87
2	0	-9	9.52	9.73
2	1	-9	18.32	18.77
2	2	-8	17.14	17.14
2	3	-8	10.07	10.89
2	3	-9	11.42	11.10
2	4	-7	16.07	17.25
2	4	-8	24.21	23.76
2	4	-9	19.60	20.60
2	5	-7	31.38	30.20
2	5	-8	21.22	19.71
2	6	-5	25.14	25.09
2	6	-7	24.62	23.65
2	7	-3	45.29	47.70
2	7	-4	46.74	47.40
2	7	-5	12.32	12.41
2	7	-6	19.09	18.27
2	7	-7	10.06	10.19
2	8	-2	25.72	29.66
2	8	-4	8.92	10.11
2	8	-5	22.19	22.88
2	9	-3	11.44	11.39
3	0	-8	24.99	24.64
3	0	-9	13.46	14.34
3	1	-8	17.03	16.31
3	1	-9	11.47	12.09
3	2	-8	15.47	13.68

h	k	l	Fo	Fc
3	3	-8	32.03	31.44
3	3	-9	8.89	9.04
3	4	-7	20.42	20.44
3	4	-8	9.67	10.72
3	4	-9	19.27	18.36
3	5	-6	30.95	32.65
3	5	-8	16.62	16.17
3	6	-5	27.99	29.35
3	6	-6	13.74	14.55
3	7	-1	28.83	30.94
3	7	-2	7.72	5.99
3	7	-3	21.94	23.72
3	7	-4	20.46	21.72
3	7	-6	30.94	31.02
3	8	-1	12.99	14.91
3	8	-4	24.90	26.96
4	0	-8	19.18	18.49
4	1	-8	13.01	14.47
4	1	-9	9.61	8.85
4	2	-8	17.96	18.32
4	2	-9	27.06	26.66
4	3	-7	21.25	20.56
4	3	-8	27.08	27.19
4	3	-9	10.00	8.16
4	4	-7	23.00	23.06
4	4	-8	12.87	12.19
4	5	-7	15.87	17.00
4	5	-8	9.34	6.15
4	6	-4	16.87	16.42
4	6	-5	46.54	47.83
4	6	-7	30.05	29.48
4	7	-3	36.15	39.83
4	7	-4	10.94	9.95
4	7	-5	19.48	18.14
4	7	-6	20.80	21.80
4	8	-1	15.57	15.99
4	8	-2	18.97	21.58
4	8	-3	17.85	18.66
4	8	-4	13.81	13.24
5	0	-8	8.30	7.20
5	0	-9	18.06	17.78
5	1	-8	35.69	34.72
5	2	-7	37.03	37.68
5	2	-8	9.95	10.18
5	2	-9	30.44	27.84
5	3	-7	17.69	17.00
5	3	-8	10.81	10.98
5	4	-6	25.93	26.51
5	4	-8	9.71	9.65
5	5	-5	12.26	11.48
5	5	-6	44.45	45.14
5	5	-8	11.47	11.20
5	6	-2	45.29	48.44
5	6	-3	7.42	7.12
5	6	-4	24.49	26.97
5	6	-5	32.61	33.96
5	6	-6	14.10	14.33
5	6	-7	27.05	26.81
5	7	-1	26.87	26.58
5	7	-2	22.81	24.27
5	7	-3	21.08	22.17
5	7	-4	16.14	17.60
5	7	-5	9.02	8.41
6	0	-7	42.25	41.28
6	1	-8	37.33	36.04
6	2	-7	10.91	8.45
6	2	-8	16.85	14.56
6	3	-7	11.28	9.22
6	3	-8	17.42	16.02
6	4	-5	59.19	61.18
6	4	-6	10.40	11.13
6	4	-7	21.52	21.36
6	4	-8	23.65	21.65
6	5	-1	36.10	37.46
6	5	-3	36.78	38.08
6	5	-4	33.56	36.46
6	5	-5	8.50	8.02
6	5	-6	37.59	37.36
6	5	-7	25.61	26.30
6	6	-1	28.07	27.52
6	6	-2	32.90	35.15
6	6	-3	14.84	15.58
6	6	-4	10.00	10.18
6	7	-1	11.52	11.74
6	7	-2	30.74	29.57
6	7	-3	35.60	38.03
6	7	-4	7.52	6.14
7	0	-7	45.19	45.38
7	1	-7	18.99	17.13
7	1	-8	18.20	18.39
7	2	-6	10.89	9.82
7	2	-7	15.70	13.92
7	3	-5	8.52	9.79
7	3	-6	33.24	32.75
7	3	-7	29.19	28.88
7	3	-8	8.84	9.14
7	4	-2	47.81	48.39
7	4	-3	28.68	29.25
7	4	-5	46.84	48.02
7	4	-6	25.36	25.09
7	4	-7	13.16	12.84
7	5	-1	36.74	38.24
7	5	-2	12.33	12.30
7	5	-3	14.09	14.38
7	5	-6	14.52	15.55
7	6	-1	43.12	42.89
7	6	-2	38.09	37.20
7	6	-4	15.26	16.02
7	6	-5	14.15	13.37
8	0	-6	19.63	18.20
8	0	-7	22.47	21.84
8	1	-5	16.27	16.67
8	1	-6	17.45	17.24
8	1	-8	15.88	13.36
8	2	-5	43.45	43.20
8	2	-6	39.35	37.97

h	k	l	Fo	Fc
8	2	-7	10.44	9.66
8	2	-8	22.31	19.89
8	3	-1	41.23	40.93
8	3	-2	25.27	25.10
8	3	-3	12.73	12.87
8	3	-4	53.04	54.41
8	3	-5	24.83	25.84
8	3	-6	20.50	19.12
8	3	-7	33.70	32.01
8	4	-1	15.76	13.75
8	4	-2	19.23	18.55
8	4	-4	7.17	6.55
8	4	-5	21.55	22.14
8	5	-1	36.80	35.34
8	5	-2	13.13	12.47
8	5	-3	25.36	24.07
8	5	-4	20.94	20.97
8	5	-5	8.09	7.41
9	0	-1	29.06	29.93
9	0	-3	19.93	19.42
9	0	-4	18.19	17.51
9	0	-5	20.11	19.14
9	0	-7	10.82	9.92
9	1	-1	48.35	47.54
9	1	-2	78.23	77.50
9	1	-4	50.34	49.88
9	1	-5	46.82	44.04
9	1	-6	12.48	10.40
9	1	-7	22.42	20.96
9	2	-1	24.71	24.40
9	2	-2	19.39	18.91
9	2	-3	53.41	52.36
9	2	-4	13.18	15.43
9	2	-5	23.60	22.75
9	2	-6	36.06	34.07
9	3	-1	22.00	22.16
9	3	-3	9.40	7.52
9	3	-4	18.28	18.54
9	3	-6	28.24	26.58
9	4	-1	20.13	19.84
9	4	-2	31.98	31.99
9	4	-3	20.72	19.84
9	4	-4	8.47	5.97
9	4	-5	17.00	15.84
10	0	-1	58.41	57.42
10	0	-3	53.38	51.58
10	0	-4	41.29	40.13
10	0	-5	21.88	20.61
10	0	-6	22.98	20.90
10	1	-1	20.70	20.31
10	1	-2	41.44	39.45
10	1	-4	27.74	27.17
10	1	-5	31.71	29.14
10	2	-2	7.58	6.36
10	2	-3	14.49	13.95
10	2	-5	36.94	34.57
10	3	-1	25.24	25.94
10	3	-2	10.90	10.63
10	3	-3	10.31	8.40
10	3	-4	19.08	18.78
11	0	-1	26.39	25.53
11	0	-2	10.28	5.82
11	0	-3	29.55	28.52
11	0	-4	23.25	21.97
11	1	-1	9.54	9.14
11	1	-2	12.61	13.43
11	1	-4	34.47	31.97
-1	1	8	10.09	8.97
-1	2	7	25.90	25.40
-1	3	7	14.84	14.08
-1	3	8	38.87	37.79
-1	4	6	52.29	53.83
-1	4	7	28.91	27.52
-1	5	6	9.30	7.39
-1	5	7	9.04	7.61
-1	6	6	17.55	17.81
-1	7	2	26.26	26.16
-1	7	3	7.06	6.36
-1	7	4	37.55	38.09
-1	7	5	16.79	16.63
-1	8	0	29.41	28.52
-1	8	1	27.59	31.67
-1	8	3	47.97	48.73
-1	8	4	23.53	23.33
-1	9	0	34.90	33.91
-1	9	1	17.61	18.79
-2	0	8	60.76	60.87
-2	0	9	10.77	9.73
-2	1	8	9.55	10.26
-2	1	9	8.95	10.03
-2	2	8	11.82	10.94
-2	3	7	17.76	18.98
-2	3	8	24.87	24.71
-2	4	6	25.86	25.39
-2	4	7	42.58	41.70
-2	4	8	12.09	13.39
-2	5	5	56.67	58.95
-2	5	6	36.52	38.06
-2	6	4	12.34	13.15
-2	6	5	8.61	7.15
-2	6	6	9.16	10.43
-2	7	2	16.87	19.33
-2	7	5	12.64	13.17
-2	8	0	11.18	10.75
-2	8	1	20.67	21.46
-2	8	3	32.22	33.57
-2	8	4	10.15	9.18
-2	9	0	20.01	18.48
-2	9	1	11.30	11.62
-2	9	2	37.88	42.24
-3	0	8	23.69	24.64
-3	0	9	15.57	14.34
-3	1	8	10.69	11.34
-3	1	9	25.33	26.19
-3	2	7	14.69	14.75
-3	2	8	15.96	15.71

h	k	l	Fo	Fc
-3	3	7	11.19	10.38
-3	3	8	26.86	26.64
-3	4	6	21.93	22.01
-3	4	7	23.90	24.42
-3	4	8	9.63	9.70
-3	5	5	29.39	30.46
-3	5	6	45.04	45.97
-3	5	7	8.98	10.22
-3	6	4	53.62	58.02
-3	6	5	37.45	39.46
-3	7	2	15.05	16.54
-3	7	3	10.30	12.90
-3	7	4	12.50	12.43
-3	7	5	8.69	8.40
-3	8	0	18.81	18.81
-3	8	1	14.20	14.94
-3	8	2	8.70	9.75
-3	8	3	6.94	1.16
-3	8	4	15.21	14.98
-3	9	0	22.55	21.44
-3	9	2	22.18	24.42
-4	0	8	18.33	18.49
-4	1	9	26.39	25.61
-4	2	7	20.67	21.44
-4	2	8	31.51	31.43
-4	2	9	10.31	9.17
-4	3	7	19.21	19.17
-4	4	6	7.27	6.79
-4	4	7	31.02	32.11
-4	5	5	25.74	27.18
-4	5	6	18.75	19.78
-4	5	7	17.31	18.07
-4	6	4	31.39	33.10
-4	6	5	36.46	37.92
-4	7	2	8.96	8.88
-4	7	3	47.28	52.43
-4	7	4	29.70	32.68
-4	7	5	13.03	12.09
-4	8	0	26.60	26.87
-4	8	1	12.84	14.24
-4	8	2	9.00	9.70
-4	8	3	10.09	10.12
-4	9	1	8.41	8.08
-5	0	8	8.02	7.20
-5	0	9	19.10	17.78
-5	1	7	19.78	20.19
-5	1	9	27.59	26.07
-5	2	8	29.44	28.55
-5	3	7	43.37	42.92
-5	3	8	12.41	13.37
-5	4	6	16.19	17.14
-5	4	7	9.71	8.79
-5	4	8	25.67	24.44
-5	5	5	11.09	9.81
-5	5	6	27.27	28.40
-5	6	4	27.06	30.31
-5	6	5	19.32	20.01
-5	6	6	21.04	21.54
-5	7	0	19.13	19.13
-5	7	1	32.46	31.91
-5	7	3	29.43	32.32
-5	7	4	20.24	20.67
-5	8	0	39.81	37.74
-5	8	2	41.80	43.54
-5	8	3	23.49	25.26
-5	9	0	13.32	13.87
-6	0	7	42.85	41.28
-6	1	8	21.28	20.94
-6	2	7	7.45	8.42
-6	2	8	35.56	34.56
-6	3	6	8.50	9.53
-6	3	7	27.88	27.00
-6	4	6	46.24	46.28
-6	4	7	11.07	10.82
-6	5	4	37.17	38.12
-6	5	5	18.91	19.25
-6	5	6	10.51	10.07
-6	5	7	26.55	26.15
-6	6	4	12.07	12.33
-6	6	5	20.40	20.96
-6	7	0	13.09	12.72
-6	7	2	12.65	14.22
-6	7	3	24.48	23.40
-6	7	4	15.31	14.74
-6	7	5	22.18	22.87
-6	8	0	21.20	19.96
-6	8	1	7.85	5.77
-6	8	2	20.97	22.85
-6	8	3	12.57	11.42
-7	0	7	46.65	45.38
-7	1	6	49.79	48.43
-7	1	7	9.71	7.39
-7	1	8	13.42	11.58
-7	2	7	18.47	17.50
-7	3	7	41.40	40.43
-7	4	5	20.62	20.08
-7	4	6	29.54	29.70
-7	5	3	46.55	47.33
-7	5	4	29.28	29.02
-7	5	5	35.20	36.20
-7	5	6	7.79	4.02
-7	6	0	15.21	15.79
-7	6	1	66.10	68.61
-7	6	3	33.95	35.42
-7	6	4	20.44	21.23
-7	7	2	6.90	2.53
-7	7	3	9.10	8.45
-7	7	4	18.53	18.23
-7	8	2	15.79	13.45
-8	0	6	19.63	18.20
-8	0	7	23.48	21.84
-8	1	5	18.38	16.24
-8	1	6	48.72	50.45
-8	1	8	30.25	26.78
-8	2	5	50.99	51.22
-8	2	6	16.78	15.38

h	k	l	Fo	Fc
-8	2	7	20.21	17.51
-8	3	6	18.73	18.04
-8	4	3	9.50	7.84
-8	4	4	13.77	15.92
-8	4	5	7.68	6.81
-8	4	6	39.42	37.18
-8	5	0	19.50	18.44
-8	5	1	8.34	8.50
-8	5	2	19.89	19.19
-8	5	4	26.05	24.33
-8	5	5	27.61	26.72
-8	5	6	10.03	10.94
-8	6	1	27.28	24.82
-8	6	2	29.63	30.05
-8	6	3	25.33	24.68
-8	6	4	29.23	28.76
-8	7	0	47.91	47.34
-8	7	1	10.13	8.43
-8	7	2	34.14	33.59
-8	7	3	14.04	13.60
-9	0	0	41.41	43.89
-9	0	1	27.88	29.93
-9	0	3	20.25	19.42
-9	0	4	18.75	17.51
-9	0	5	18.94	19.14
-9	0	7	11.75	9.92
-9	1	0	41.50	41.75
-9	1	3	16.70	14.79
-9	1	5	24.10	23.83
-9	1	6	20.99	19.08
-9	2	0	36.90	37.47
-9	2	1	20.26	20.44
-9	2	2	30.29	30.42
-9	2	4	12.72	11.44
-9	2	5	42.30	42.34
-9	2	6	10.43	8.01
-9	2	7	29.98	27.28
-9	3	0	28.63	29.61
-9	3	1	50.67	50.83
-9	3	2	25.98	27.70
-9	3	3	60.13	61.75
-9	3	4	43.23	43.24
-9	3	5	19.25	18.44
-9	3	6	15.48	13.89
-9	4	0	44.23	45.86
-9	4	1	12.41	12.32
-9	4	2	33.61	36.16
-9	4	3	10.13	10.31
-9	4	5	22.40	20.69
-9	4	6	9.28	7.27
-9	5	1	7.17	7.18
-9	5	3	14.50	14.90
-9	5	4	8.16	6.63
-9	5	5	29.64	28.07
-9	6	1	17.19	14.66
-9	6	3	20.15	20.00
-9	6	4	16.92	15.29
-10	0	0	43.25	42.71
-10	0	1	57.20	57.42
-10	0	3	52.18	51.58
-10	0	4	41.66	40.13
-10	0	5	21.61	20.61
-10	0	6	22.91	20.90
-10	1	0	15.78	16.22
-10	1	2	22.80	23.28
-10	1	3	10.21	9.55
-10	1	4	15.38	15.73
-10	1	6	7.74	5.96
-10	2	0	7.99	7.87
-10	2	1	14.27	14.61
-10	2	2	9.99	9.40
-10	2	4	24.85	24.97
-10	2	5	18.00	16.47
-10	2	6	9.74	7.88
-10	3	0	8.69	7.74
-10	3	1	20.29	18.44
-10	3	3	15.90	14.12
-10	3	4	26.87	26.44
-10	3	5	12.11	11.52
-10	4	0	28.69	28.43
-10	4	1	16.45	16.32
-10	4	2	43.08	42.95
-10	4	3	31.53	30.20
-10	4	4	19.86	19.84
-10	4	5	14.99	12.65
-10	5	0	13.35	13.10
-10	5	1	31.96	32.95
-10	5	4	15.88	14.87
-11	0	0	16.04	17.32
-11	0	1	26.86	25.53
-11	0	2	7.59	5.82
-11	0	3	28.97	28.52
-11	0	4	22.08	21.97
-11	1	0	40.59	41.68
-11	1	1	11.89	10.41
-11	1	2	47.48	46.81
-11	1	3	29.04	28.16
-11	1	4	28.35	26.48
-11	2	0	11.27	10.97
-11	2	1	24.55	23.35
-11	2	3	17.83	17.25
-11	3	0	11.86	12.67
-11	3	1	13.31	13.16
-11	3	3	19.87	18.68
-11	3	4	15.36	13.75
-1	0	-7	16.25	14.80
-1	0	-8	8.21	8.28
-1	1	-8	11.50	12.36
-1	2	-8	8.60	10.53
-1	2	-9	12.02	13.02
-1	3	-7	9.73	5.47
-1	3	-8	18.64	19.30
-1	4	-7	35.79	35.46
-1	4	-8	17.18	17.23
-1	5	-7	20.63	20.35
-1	5	-8	11.46	12.67

h	k	l	Fo	Fc
-1	6	-6	34.98	36.31
-1	7	-4	14.36	15.34
-1	7	-5	13.04	13.60
-1	7	-7	18.02	18.01
-1	8	-1	18.77	17.69
-1	8	-2	32.92	30.20
-1	8	-3	10.32	10.22
-1	8	-4	17.84	17.46
-1	8	-5	11.99	11.41
-1	9	-1	17.80	16.39
-1	9	-2	19.14	19.17
-1	9	-4	8.95	7.23
-2	0	-7	20.51	22.15
-2	0	-8	15.19	16.52
-2	1	-7	33.60	33.44
-2	1	-8	15.80	16.83
-2	2	-7	26.25	27.93
-2	2	-8	11.70	14.01
-2	3	-7	8.87	7.22
-2	3	-8	11.77	12.95
-2	4	-7	25.73	26.36
-2	5	-6	22.53	22.46
-2	5	-7	9.15	7.31
-2	5	-8	20.49	21.08
-2	6	-5	31.42	30.54
-2	6	-6	16.32	17.50
-2	7	-4	37.40	35.67
-2	7	-5	35.58	33.67
-2	7	-6	13.52	13.17
-2	8	-1	20.76	19.48
-2	8	-2	8.93	7.83
-2	8	-3	23.56	22.92
-2	9	-1	24.67	23.17
-2	9	-2	9.01	10.75
-2	9	-3	21.92	20.73
-3	0	-7	23.42	22.30
-3	0	-8	25.51	26.82
-3	1	-7	19.38	19.51
-3	1	-8	16.60	15.16
-3	2	-7	17.80	19.10
-3	2	-8	19.50	19.50
-3	3	-7	14.62	12.54
-3	3	-8	16.96	19.07
-3	4	-7	24.11	26.38
-3	4	-8	9.14	7.06
-3	5	-6	14.85	12.36
-3	6	-5	12.82	14.45
-3	6	-7	12.65	13.58
-3	7	-4	26.21	25.44
-3	7	-5	9.21	10.61
-3	7	-6	11.50	10.71
-3	8	-1	18.39	15.97
-3	8	-2	10.83	10.73
-3	8	-3	36.83	35.83
-3	8	-4	12.04	10.68
-3	8	-5	20.94	20.94
-3	9	-2	16.75	16.41
-4	0	-6	41.88	43.81
-4	0	-7	14.12	16.03
-4	1	-7	24.78	27.54
-4	2	-6	29.49	28.93
-4	3	-6	19.58	22.13
-4	3	-7	20.58	20.92
-4	4	-6	14.72	15.44
-4	4	-7	18.43	20.65
-4	5	-5	13.64	15.05
-4	5	-6	43.47	43.35
-4	6	-4	20.08	18.47
-4	7	-2	18.22	17.90
-4	7	-3	19.34	19.94
-4	7	-4	18.97	17.94
-4	8	-1	30.11	29.93
-4	8	-2	25.68	24.33
-4	8	-3	20.92	20.21
-4	9	-1	11.95	11.51
-4	9	-2	13.01	12.78
-5	0	-6	30.41	31.88
-5	0	-7	15.87	16.07
-5	1	-7	23.04	26.44
-5	2	-6	35.18	35.64
-5	2	-7	12.49	10.07
-5	3	-5	10.79	12.43
-5	3	-6	8.33	8.46
-5	3	-7	17.17	16.99
-5	4	-7	9.04	9.30
-5	5	-5	39.37	40.70
-5	5	-6	9.27	9.72
-5	6	-3	11.20	12.61
-5	6	-4	21.11	21.52
-5	6	-5	29.28	29.93
-5	6	-6	13.13	11.56
-5	7	-1	13.29	11.61
-5	7	-2	29.59	29.54
-5	7	-3	19.63	18.86
-5	7	-4	13.10	12.19
-5	8	-1	17.58	15.08
-5	8	-3	14.48	11.71
-5	8	-4	13.45	15.16
-5	9	-1	14.61	13.57
-6	0	-5	26.40	26.14
-6	0	-6	15.33	15.14
-6	1	-5	18.30	22.82
-6	1	-6	8.19	7.32
-6	2	-5	36.92	39.92
-6	2	-6	26.23	28.90
-6	3	-5	31.37	32.29
-6	4	-4	14.31	15.25
-6	4	-6	13.15	13.52
-6	5	-3	21.44	22.79
-6	5	-5	7.93	7.98
-6	6	-2	28.87	29.73
-6	6	-4	30.55	31.57
-6	7	-1	13.95	13.52
-6	7	-2	18.61	18.80
-6	7	-3	25.32	25.37
-6	8	-1	12.20	10.69

h	k	l	Fo	Fc
-6	8	-2	15.23	14.48
-6	8	-3	21.49	21.88
-7	0	-4	27.54	28.37
-7	0	-5	20.46	20.71
-7	1	-4	9.66	8.21
-7	2	-5	9.27	8.54
-7	3	-4	50.84	53.48
-7	3	-5	25.30	27.71
-7	4	-3	26.39	27.60
-7	4	-5	10.42	10.14
-7	5	-2	16.54	16.13
-7	5	-3	27.81	31.22
-7	5	-4	10.27	8.39
-7	5	-5	13.16	12.69
-7	6	-1	34.27	35.19
-7	6	-2	24.77	25.10
-7	6	-4	17.58	18.27
-7	7	-1	15.51	16.98
-7	7	-2	16.16	13.57
-7	7	-3	16.34	15.98
-7	8	-1	10.56	8.90
-8	0	-2	50.91	53.60
-8	0	-3	12.99	11.33
-8	0	-4	35.25	37.45
-8	1	-2	7.06	5.40
-8	1	-3	19.07	17.46
-8	1	-4	17.03	16.06
-8	1	-5	12.33	13.40
-8	2	-3	15.84	17.33
-8	2	-4	9.95	11.27
-8	2	-5	9.92	12.32
-8	3	-2	39.11	40.22
-8	3	-4	21.48	23.19
-8	4	-1	9.25	8.73
-8	4	-2	12.89	13.63
-8	4	-3	27.60	28.53
-8	4	-4	13.95	15.28
-8	5	-1	14.37	14.17
-8	5	-2	23.14	23.09
-8	5	-3	11.69	10.81
-8	5	-4	16.18	16.61
-8	6	-1	14.42	14.02
-8	6	-2	26.65	25.59
-8	6	-3	9.81	8.62
-8	7	-1	14.45	13.97
-8	7	-2	14.99	14.51
-9	0	-1	14.84	17.19
-9	0	-2	53.69	55.80
-9	1	-2	14.68	15.16
-9	1	-3	34.55	36.73
-9	2	-2	23.72	24.03
-9	2	-4	16.36	15.46
-9	3	-1	22.51	23.11
-9	3	-2	37.17	39.03
-9	4	-1	28.79	29.73
-9	4	-2	10.10	9.99
-9	4	-3	27.61	29.13
-9	5	-1	14.64	13.09
-9	5	-2	9.36	9.33
-9	6	-1	14.66	14.26
-10	0	-1	20.73	22.09
-10	0	-2	19.92	22.13
-10	1	-1	34.85	36.14
-10	2	-1	27.44	27.81
-10	2	-2	7.97	7.45
-10	3	-1	28.21	28.63
-10	4	-1	20.34	20.96
-10	4	-2	10.92	9.83
-10	5	-1	26.21	25.86
8	0	-3	22.96	24.11
-3	3	2	91.85	94.55
-7	0	2	59.92	61.91
0	1	7	13.90	13.98
7	0	3	19.57	18.44
8	1	1	71.76	72.94
-8	3	4	14.37	15.40
-7	0	-3	18.45	18.44
-7	3	-3	8.33	7.53

APPENDIX 2

STRUCTURE FACTORS FOR SODIUM FORMATE

h	k	l	Fo	Fc
-1	-1	7	8.42	8.58
-3	-1	7	4.16	4.10
-5	-1	7	1.02	1.04
-2	-2	7	9.43	9.78
-4	-2	7	4.28	4.36
-3	-3	7	10.94	10.99
-2	0	6	13.78	13.36
-4	0	6	30.09	30.04
-6	0	6	14.20	14.38
-1	-1	6	3.11	3.02
-3	-1	6	9.17	9.18
-5	-1	6	9.57	9.46
-2	-2	6	3.18	3.08
-4	-2	6	15.40	14.98
-6	-2	6	5.12	5.24
-1	-3	6	1.44	1.50
-3	-3	6	11.21	11.09
-5	-3	6	13.18	12.76
-2	-4	6	6.03	5.93
-4	-4	6	3.78	3.51
-3	-5	6	1.83	1.84
-1	-1	5	22.46	22.68
-3	-1	5	5.97	5.91
-5	-1	5	8.06	7.95
-7	-1	5	6.32	6.31
-2	-2	5	25.06	25.56
-4	-2	5	9.12	9.04
-6	-2	5	8.44	8.23
-1	-3	5	3.85	3.74
-3	-3	5	12.23	12.17
-5	-3	5	15.36	15.47
-2	-4	5	15.44	15.11
-4	-4	5	2.31	2.16
-6	-4	5	1.01	0.65
-1	-5	5	12.07	12.04
-3	-5	5	12.31	12.06
-5	-5	5	8.60	8.69
-2	-6	5	0.93	0.96
-2	0	4	7.03	6.82
-4	0	4	34.41	35.96
-6	0	4	27.20	29.00
-1	-1	4	5.36	5.36
-3	-1	4	8.37	8.63
-5	-1	4	13.80	14.26
-7	-1	4	5.50	5.88
-2	-2	4	6.76	7.11
-4	-2	4	14.71	14.95
-6	-2	4	13.65	13.98
-1	-3	4	1.23	1.30
-3	-3	4	5.19	5.56
-5	-3	4	19.40	19.59
-7	-3	4	5.76	6.07
-2	-4	4	13.55	13.38
-4	-4	4	7.26	6.99
-6	-4	4	4.38	4.09
-1	-5	4	18.22	18.03
-3	-5	4	12.36	12.07
-5	-5	4	2.59	2.50
-2	-6	4	1.35	1.25
-4	-6	4	3.74	3.45
-1	-7	4	14.89	14.83
-1	-1	3	28.04	29.52
-3	-1	3	30.35	31.04
-5	-1	3	6.42	6.56
-7	-1	3	1.93	1.79
-2	-2	3	40.71	47.53
-4	-2	3	22.50	22.14
-6	-2	3	5.80	5.87
-1	-3	3	9.35	9.01
-3	-3	3	6.87	7.18
-5	-3	3	16.94	17.53
-7	-3	3	9.99	9.96
-2	-4	3	27.49	27.73
-4	-4	3	7.80	7.64
-6	-4	3	3.82	3.96
-1	-5	3	17.10	17.06
-3	-5	3	16.88	16.79
-5	-5	3	10.78	10.88
-2	-6	3	3.60	3.81
-4	-6	3	4.81	4.83
-1	-7	3	1.76	1.97
-3	-7	3	3.21	3.23
-2	0	2	9.65	10.01
-4	0	2	21.26	21.12
-6	0	2	30.95	32.48
-1	-1	2	14.40	14.47
-3	-1	2	3.02	3.79
-5	-1	2	12.26	12.67
-7	-1	2	8.33	8.37
-2	-2	2	11.18	10.91
-4	-2	2	2.19	2.17
-6	-2	2	16.44	16.02
-1	-3	2	13.88	13.37
-3	-3	2	5.18	5.07
-5	-3	2	15.11	15.05
-7	-3	2	11.86	11.51
-2	-4	2	19.02	18.74
-4	-4	2	11.88	11.98
-6	-4	2	4.20	4.00
-1	-5	2	13.41	13.57
-3	-5	2	22.65	23.01
-5	-5	2	2.80	2.76
-2	-6	2	0.92	0.66
-4	-6	2	1.12	1.04
-1	-7	2	14.41	14.69
-3	-7	2	17.53	17.35
-1	-1	1	4.93	5.07
-3	-1	1	39.42	44.22
-5	-1	1	7.17	7.13
-7	-1	1	6.00	5.97
-2	-2	1	39.18	49.89
-4	-2	1	34.10	34.00
-6	-2	1	7.38	7.31
-1	-3	1	26.62	27.11
-3	-3	1	3.89	3.91
-5	-3	1	11.03	10.93

h	k	l	Fo	Fc
-2	-4	1	22.68	23.54
-4	-4	1	20.09	19.49
-6	-4	1	1.40	1.51
-1	-5	1	19.90	20.18
-3	-5	1	18.31	18.49
-2	-6	1	0.96	0.72
-4	-6	1	1.59	1.66
-1	-7	1	3.00	2.81
-3	-7	1	4.56	4.67
-2	-8	1	0.86	0.88
2	0	0	38.52	44.17
4	0	0	6.17	6.09
6	0	0	20.33	20.25
3	1	0	5.28	5.32
5	1	0	6.37	6.46
2	2	0	10.75	10.44
4	2	0	6.37	6.66
6	2	0	8.68	8.57
1	3	0	35.02	38.74
3	3	0	2.22	2.20
5	3	0	3.72	3.77
0	4	0	10.31	10.64
2	4	0	14.98	14.92
4	4	0	12.97	12.71
6	4	0	4.74	4.72
1	5	0	0.62	0.51
3	5	0	20.75	20.47
5	5	0	10.19	10.14
0	6	0	8.89	9.59
2	6	0	2.49	2.52
4	6	0	1.63	1.00
1	7	0	9.41	9.83
3	7	0	16.55	16.10
0	8	0	0.91	0.33
2	8	0	6.50	6.55
1	1	1	29.57	31.44
3	1	1	23.60	22.19
5	1	1	15.02	14.84
0	2	1	15.16	14.36
2	2	1	26.15	25.09
4	2	1	29.46	28.60
6	2	1	9.89	9.94
1	3	1	35.10	36.29
3	3	1	9.88	9.53
5	3	1	4.14	4.20
0	4	1	10.70	10.69
2	4	1	4.62	4.40
4	4	1	19.25	18.45
1	5	1	18.32	18.26
3	5	1	15.96	15.72
5	5	1	9.47	9.51
0	6	1	16.97	17.70
2	6	1	9.09	9.05
4	6	1	3.06	3.05
1	7	1	6.25	6.37
3	7	1	2.20	2.18
0	8	1	3.12	3.34
2	0	2	50.79	53.54
4	0	2	7.70	7.71
1	1	2	27.77	27.12
3	1	2	9.95	9.59
5	1	2	2.58	2.55
0	2	2	33.19	32.41
2	2	2	25.31	23.31
4	2	2	1.73	1.84
1	3	2	35.53	36.65
3	3	2	8.67	8.49
5	3	2	1.65	1.72
0	4	2	11.88	11.91
2	4	2	7.83	7.94
4	4	2	8.17	8.06
1	5	2	4.50	4.64
3	5	2	8.40	8.25
0	6	2	7.39	6.98
2	6	2	5.03	4.92
1	7	2	6.54	6.67
1	1	3	12.47	11.97
3	1	3	1.24	1.19
0	2	3	24.52	22.90
2	2	3	9.59	9.45
4	2	3	15.01	15.17
1	3	3	23.80	23.05
3	3	3	12.69	12.65
0	4	3	5.01	4.99
2	4	3	3.70	3.99
4	4	3	8.77	8.90
1	5	3	12.95	12.94
3	5	3	10.56	10.69
0	6	3	7.30	7.24
2	6	3	10.85	10.69
1	7	3	5.20	5.11
0	0	4	25.13	23.68
2	0	4	34.00	33.83
4	0	4	10.98	11.44
1	1	4	13.58	13.45
3	1	4	8.41	8.53
0	2	4	5.51	5.20
2	2	4	16.67	16.50
1	3	4	16.68	16.79
3	3	4	10.79	11.04
0	4	4	10.62	10.78
2	4	4	4.60	4.32
1	5	4	1.16	1.31
0	6	4	2.54	2.40
1	1	5	2.83	2.57
0	2	5	20.06	20.16
2	2	5	5.48	5.60
1	3	5	9.04	9.37
0	4	5	11.85	11.81
0	0	6	5.32	5.57
1	1	6	4.55	4.64
0	2	6	1.84	1.73
0	4	6	6.71	6.82
-5	-5	1	11.37	11.13

REFERENCES

1. G. H. Stout and L. H. Jensen. X-ray Structure Determination: A Practical Guide. The Macmillan Company, London. 1968.

2. H. Lipson and W. Cochran. The Crystalline State, vol. III: The Determination of Crystal Structures, 3rd. edn. G. Bell and Sons, Ltd., London. 1966.

3. M. J. Buerger. Crystal Structure Analysis. J. Wiley and Sons, Inc., New York. 1960.

4. M. J. Buerger. Vector Space. J. Wiley and Sons, Inc., New York. 1959.

5. M. M. Woolfson. X-ray Crystallography. Cambridge University Press. 1970.

6. International Tables for X-ray Crystallography, vols. I-III. Kynoch Press, Birmingham. Vol. I, 1952; vol. II, 1959; and vol. III, 1962.

7. N. L. Paddock. Quart. Rev. (London) 18, 168 (1964).

8. D. P. Craig and N. L. Paddock. In 'Nonbenzenoid Aromatics,' vol. 2. Academic Press, New York. 1971.

9. D. P. Craig and N. L. Paddock. J. Chem. Soc., 4118 (1962).

10. J. Trotter and S. H. Whitlow. J. Chem. Soc. A, 460 (1970).

11. N. V. Mani and A. J. Wagner. Acta Cryst. B27, 51 (1971).

12. A. L. Macdonald and J. Trotter. Canad. J. Chem. 52, 734 (1974).

13. J. Trotter and S. H. Whitlow. J. Chem. Soc. A, 455 (1970).

14. W. C. Marsh and J. Trotter. J. Chem. Soc. A, 1482 (1971).

15. W. Harrison and J. Trotter. J. Chem. Soc. Dalton Trans., 61 (1973).

16. A. J. C. Wilson. Nature. 150, 151 (1942).

17. I. L. Karle, K. S. Dragonette and S. A. Brenner. Acta Cryst. 19, 713 (1965).

18. Ref. 6, vol. III.

19. M. W. Dougill. J. Chem. Soc., 3211 (1963).

20. S. Rettig and J. Trotter. Canad. J. Chem. 51, 1295 (1973).

21. A. Wilson and D. F. Carroll. J. Chem. Soc., 2548 (1960).

22. E. Giglio. Ric. Sci. Suppl. 30, 721 (1960).

23. M. I. Davis and I. C. Paul. Acta Cryst. A25, Part S3, S116 (1969).

24. E. Giglio and R. Puliti. Acta Cryst. 22, 304 (1967).

25. F. R. Ahmed, P. Singh and W. H. Barnes. Acta Cryst. B25, 316 (1969).

26. M. W. Dougill. J. Chem. Soc., 5471 (1961).

27. R. S. Mulliken. J. Amer. Chem. Soc. 74, 811 (1952).

28. L. Pauling. The Nature of the Chemical Bond, 3rd edn. Cornell University Press, New York. 1960.

29. O. Hassel and C. Rømming. Acta Chem. Scand. 10, 696 (1956).

30. O. Hassel, C. Rømming and T. Tufte. Acta Chem. Scand. 15, 967 (1961).

31. O. Hassel and H. Hope. Acta Chem. Scand. 14, 391 (1960).

32. K. O. Strømme. Acta Chem. Scand. 13, 268 (1959).

33. W. H. Zachariasen. J. Amer. Chem. Soc. 62, 1011 (1940).

34. J. Park. Private Communication.

35. J. Karle and I. L. Karle. Acta Cryst. 21, 849 (1966).

36. J. Karle and H. Hauptman. Acta Cryst. 14, 217 (1961).

37. J. Karle and H. Hauptman. Acta Cryst. 9, 635 (1956).

38. M. G. B. Drew. Private communication (1969). see eg. M. G. B. Drew, D. H. Templeton, and A. Zalkin. Acta Cryst. B25, 261 (1969).

39. O. Kennard, W. D. S. Motherwell, D. G. Watson, J. C. Coppola and A. C. Larson. Acta Cryst. B25 (1969). Suppl. Abstracts Internat. Union Crystallography, 8th General Assembly and Congress. Abstract IX 44, 588.

40. P. W. R. Corfield and S. G. Shore. J. Amer. Chem. Soc. 95, 1480 (1973).

41. R. F. Stewart. J. Chem. Phys. 53, 205 (1970).

42. I. Nitta and K. Osaki. X-Rays. 5, 37 (1948).

43. J. L. Galigne. Acta Cryst. B27, 2429 (1971).

44. T. Sugawara, M. Kakudo, Y. Saito and I. Nitta. X-Rays.6, 85 (1951).

45. A. Pabst. J. Chem. Phys. 11, 145 (1943).

46. I. Nahringbauer. Acta Cryst. B24, 565 (1968).

47. S. C. Jain, S. S. Tavale and A. B. Biswas. Acta Cryst. B25, 584 (1969).

48. S. S. Tavale, L. M. Pant and A. B. Biswas. Acta Cryst. 16, 566 (1963).

49. S. S. Tavale, L. M. Pant and A. B. Biswas. Acta Cryst. 14, 1281 (1961).

50. G. A. Jeffrey and G. S. Parry. J. Amer. Chem. Soc. 76, 5283 (1954).

51. D. W. J. Cruickshank. Acta Cryst. 2, 65 (1949).