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A COMPARATIVE TEST OF THE MODELS OF ATOMIC CAPTURE OF NEGATIVE PARTICLES USING 321 EXPERIMENTAL COULOMB-CAPTURE RATIOS

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1. INTRODUCTION

Exotic (muonic and hadronic) atoms can be considered as new nuclear probes used in practically all fields of physical sciences, from particle physics to materials sciences and biophysics. However, the basic problem of exotic atoms, their formation via Coulomb capture of heavy negative particles, has not been solved yet. The experimentalist working in this field needs a simple calculation method for estimating the probability $W_M(Z_k)$ of formation of an exotic atom Z_kM^- when the M^- particle is stopped in a sample consisting of elements Z_1, Z_2, etc. (Z_k denotes both the element and its atomic number). For that, several models have been suggested. A direct test of the models is the comparison of their predictions with the experimental values of the so-called Coulomb capture or atomic capture ratio:

$$A(Z_1,Z_2) = \frac{W_M(Z_1)}{W_M(Z_2)} . \qquad (1)$$

Usually, that comparison is made for a more or less arbitrarily chosen group of binary compounds, in most cases a subset of the data on oxides. The aim of the present work is to compare the predictions of the various models with the 321 available Coulomb capture ratios measured in simple binary gas mixtures, alloys, and compounds of composition $(Z_1)_k(Z_2)_\ell$.[1-38] First, we summarize the theoretical basis of the different models,[39-59] then we make attempts to modify them by introducing adjustable parameters and fitting their predictions to the experimental data. Finally, we compare the predictions of the different models. We do not give an exhaustive bibliography on exotic atoms here, the reader is advised to consult Ref. 60 for that.

2. ATOMIC CAPTURE - GENERAL CONSIDERATIONS

Let us summarize the common basis of the various descriptions of the atomic capture: the theoretical statements which seem to be supported by unambiguous experimental evidence or which most of the recently published theoretical works agree upon.

A) The atomic capture process is similar for all negative particles, muons or hadrons.[39-42,44-58] In the following we shall use the general term "meson".

B) The slowing down and atomic capture of mesons are competing processes in the kinetic energy region $E_M < 10$ keV, where their velocities approach those of the atomic electrons.[40-42,46-47] However, in contradiction to the earlier assumptions,[39,41-42,44-45,49-52,58] the capture rates of mesons in atoms are not proportional to the atomic stopping powers. This has been predicted theoretically[46,56] and observed experimentally.[35]

C) The Auger process (meson capture through electron ejection) is responsible for all the details of the meson capture because for almost every meson transition from the continuum to an atomic bound state the Auger cross sections dominate the radiative ones.[40-44,46-47,49-58]

D) In dense systems the mesons do not slow down to thermal velocities as they are captured at much higher energies, $E_M \gtrsim 10$ eV.[40,43,46-47,53,56,58]

E) In the energy region 10 eV < E_M < 10 keV, where most of the mesons are captured, the meson wave function has many oscillations over the dimensions of the atom. This justifies a quasi-classical treatment of the capture process.[39-42,44-45,47,49,55]

F) In a mixture of elements of $c_1Z_1 + c_2Z_2$ type (where Z_1, Z_2 are the atomic numbers and c_1, c_2 the atomic concentrations) the atomic capture rates are proportional to the concentrations. This virtually evident statement has been thoroughly tested both theoretically[47,52,56] and experimentally.[1,3-4,11,19-20,26-27,29,31,35] A concentration dependence is predicted for the atomic capture in the lighter elements[56] but was not found in the mixtures of ^{3}He with other gases.[35]

G) A chemical compound is usually treated, in first approximation, as a mixture of elements. However, molecular effects have been observed in mesic X-rays and atomic capture rates (see for example reviews[41-42,53]). Therefore, at least for compounds of light elements, the influence of the chemical bond has to be considered.

H) In the case of exotic hydrogen atoms a transfer of the meson from the hydrogen nucleus (proton, deuteron, or triton) to the heavy atom was observed (see reviews[41-42,53]). The transfer is assumed to proceed via collisions of the small, neutral, and fast exotic hydrogen atom with the heavy nucleus.[61] According to the experimental observations[35] and the present theoretical picture of the transfer process, there is no particle transfer from atom ZM^- if $Z > 1$.

3. EXPERIMENTAL INFORMATION

The Coulomb capture ratio seems to be the best observable quantity for testing the models of the atomic capture process. In the present paper we made an attempt to collect all available atomic capture ratios measured in binary mixtures of elements and simple binary compounds.[1-38] We rejected, however:

- the hydrogen-containing compounds and mixtures where the transfer effect obscures the atomic capture information;[19,41-42,53]
- the compounds with complicated chemical bond structure, e.g. $C_6C\ell_6$ or the peroxides;
- the data which are related but not atomic capture ratios in the strict sense, e.g. line intensity ratios.[11,13,16-18,...]

As a result, we have 321 experimental data points taken from Refs. 1-10, 12-18, 20-38. Unfortunately, there are systematic differences among the data measured at different places and times, using different methods, for the same compounds.[48] Due to these and other inherent systematic errors, it is very difficult to perform a proper statistical test of the various theories. Following the generally accepted method, we shall compare the goodness of agreement between theory and experiment using the quantities:

$$\chi_n^2 = \sum_{i=1}^{n} \left(\frac{A_{exp} - A_{theor}}{\sigma_{exp}} \right)^2 \qquad (2a)$$

$$\chi_r^2 = \chi_n^2/(n-p) \qquad (2b)$$

where $A_{exp} \pm \sigma_{exp}$ is the measured value, A_{theor} is a theoretical prediction and p is the number of fitted parameters. Quantities (2a) and (2b) are called - somewhat inaccurately - total chi-square and reduced chi-square.[22,45,48,54]

The "best" parameters of the various models were estimated by minimizing (2). The computations have been performed using the MINUIT program[62] on the VAX-11/780 computer at TRIUMF.

In Table 1 we enlist our efforts to improve the models in order to obtain a better goodness of fit (χ^2). In Tables 2 through 7 the experimental data are presented in comparison with the predictions of five different models for various groups of chemical systems: mixtures, oxides, sulphides, halides, alloys and nitrides (BN). Table 8 summarizes the χ^2-values for the various groups and models.

4. DISCUSSION OF THE ATOMIC CAPTURE MODELS

As mentioned earlier, our aim is to aid the experimentalists in choosing among calculation methods when estimating atomic capture probabilities. To start with, we try to reproduce the gross atomic number dependence (Z-dependence) of the atomic capture probabilities, possibly including the quasi-periodic oscillations first observed by Zinov et al.[8] on oxides (see Fig. 1); the consideration of molecular and solid-state effects[11-13,17-18,28,31,34,40-42,53-54] comes next.

In their classic paper[39] Fermi and Teller estimated the capture probabilities of mesons in atoms to be roughly proportional to their atomic numbers (Z-law):

$$A(Z_1,Z_2) = Z_1/Z_2 \ . \tag{3}$$

Relation (3) has been deduced using the assumption that the capture rates are proportional to the stopping powers of the atoms. This is in contradiction with consideration B) when studied in detail, but has been commonly used for estimating the capture rates.

The Z-law underwent numerous experimental tests[1-38] and modifications. Baijal et al.[6] observed that the experimental capture ratios could be described as follows:

$$A(Z_1,Z_2) = \left(\frac{Z_1}{Z_2}\right)^n \ , \tag{4}$$

and most of the results happened to be in the region $0.5 \leq n \leq 1.5$ ($n = 1$ corresponds to the (3) Z-law).

Zinov et al. proposed a modified, empirical Z-law for metallic halides and alloys[8]:

$$A(Z_1,Z_2) = 0.66\ (Z_1/Z_2) \ . \tag{5}$$

Vogel et al.,[47] using a semi-classical approximation with the Thomas-Fermi model of the atom, deduced a Z-dependence similar to Eqs. (3) and (4):

$$A(Z_1,Z_2) = (Z_1/Z_2)^{7/6} \ . \tag{6}$$

It has been shown in several works[6,8,33,48] that the Z-law cannot give a satisfactory prediction of the atomic capture ratios in any of its forms (3-6). We

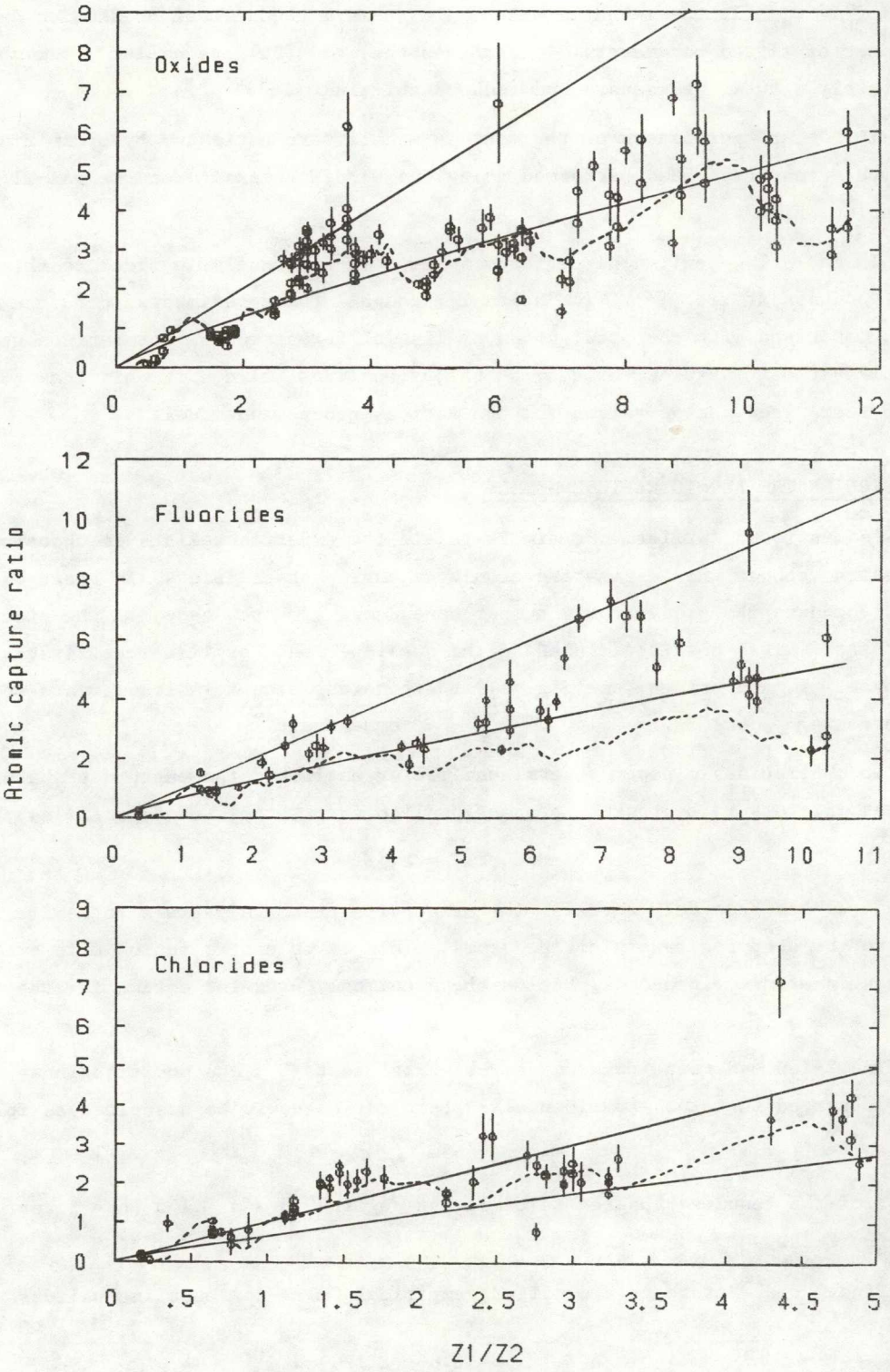

Fig. 1. Atomic capture ratios $A(Z_1,Z_2)$ measured in oxides, fluorides and chlorides[1-38] against the ratio of the corresponding atomic numbers Z_1/Z_2. Note the characteristic oscillations in each case. The upper solid line corresponds to the Fermi-Teller Z-law and the lower one to the (7) modified Z-law. The dashed curve represents the predictions of the SPP model with the (26) parameter values (i.e. model 4 in Tables 2 through 8).

tried to find an "optimal" Z-law by fitting parameters a and b of the general expression

$$A(Z_1,Z_2) = a(Z_1/Z_2)^b \ . \qquad (7)$$

As seen from Table 1, the best fit was obtained at a = 0.69 and b = 0.86 with a much χ_r^2 than for (3). This "empiric" Z-law is close to (5) but with a somewhat weaker Z-dependence.

Having considered the energy loss of the meson in the atom along a trajectory which is close enough to the nucleus for the meson to be subsequently captured in an atomic orbit, H. Daniel[45] deduced a Z-dependence of the following form

$$A(Z_1,Z_2) = \frac{Z_1^{1/3}\ell n(0.57Z_1)}{Z_2^{1/3}\ell n(0.57Z_2)} \ , \qquad (8)$$

which fitted the atomic capture ratios measured in metal halides rather well.[16,45] Later, in order to describe the oscillations observed in oxides,[8] Daniel[55] revised Eq. (8) by including the atomic radii R(Z):

$$A(Z_1,Z_2) = \frac{Z_1^{1/3}\ell n(0.57Z_1)R(Z_2)}{Z_2^{1/3}\ell n(0.57Z_2)R(Z_1)} \ . \qquad (9)$$

This expression predicts the oscillations in the oxides fairly well.[33] However, its use is hindered by the somewhat undefined nature of the R(Z) radius. In his paper[55] Daniel used the metallic radii of the metal atoms and the ionic radius $R(O^{-2})$ of the oxygen. At the same time most of the oxides have a highly covalent chemical bond, and there are considerable differences between the atomic, metallic, covalent and ionic radii. Even the best-defined crystal ionic radii have high systematic uncertainties: "Numerical values of the radii of the ions may vary depending on how they were measured. They may have been calculated from wave functions and determined from the lattice spacings or crystal structure of various salts. Different values are obtained depending on the kind of salt used or the method of calculating." (Quotation from Ref. 63.) Equation (9) is highly instructive for the theory of atomic capture but - in our opinion - cannot be used for predicting atomic capture ratios.

Daniel's formula (8) gives a poor agreement with the experimental data; the surprisingly high χ^2 is mostly due to the systems with light elements such as He, Li, Be, B. We made attempts to improve Eq. (8) by using the form:

$$A(Z_1,Z_2) = \frac{Z_1^{1/3}\ell n(aZ_1+b)}{Z_2^{1/3}\ell n(aZ_2+b)} \ . \qquad (10)$$

As shown in Table 1, the best fit was obtained at a = 0.83 and b = 0.69 but with a reduced χ^2 still considerably higher than that for Z-law (7).

A Z-dependence, somewhat similar to Eq. (8), has been empirically found by Petrukhin and Suvorov[19] in an experimental study of pion capture in mixtures of hydrogen with noble gases. After the removal of the contribution of pion transfer, the

observed atomic capture ratios A(Z,H) could be well approximated by

$$A(Z,H) \propto (Z^{1/3}-1) \ . \tag{11}$$

Vasilyev et al.[48] have generalized expression (11) in the form

$$A(Z_1,Z_2) = \frac{A(Z_1,H)}{A(Z_2,H)} = \frac{Z_1^{1/3}-1}{Z_2^{1/3}-1} \tag{12}$$

and compared its predictions with the Coulomb capture ratios available at that time. Equation (12), as shown in Table 1, approximated the experimental values much better than the Z-law (3) and somewhat better than (8).

Another line of the descriptions of the atomic capture data has been initiated by Schneuwly, Pokrovsky and Ponomarev (SPP).[53,54] They formulated a model where the $\rho(E)$ efficiency of an electron in atomic capture depends on the electron binding energy E:

$$\rho(E) = \begin{cases} 1 \text{ for } E \leq E_o \\ 0 \text{ for } E > E_o \end{cases} \tag{13}$$

(rigid boundary[53]), or

$$\rho(E) = \begin{cases} 1 & \text{for } E \leq E_o \\ \exp\left[-\left(\frac{E-E_o}{E_c}\right)^2\right] & \text{for } E > E_o \end{cases} \tag{14}$$

(smooth boundary[54]), where E_o and E_c are parameters. Following the idea of Gerstein et al.,[41] after the meson has knocked off an electron, it is presumably trapped in an atomic or a molecular orbit. Thus the capture ratio is defined as

$$A(Z_1,Z_2) = \frac{n_1+2\nu_1\omega}{n_2+2\nu_2(1-\omega)} \tag{15}$$

where n_1 and n_2 are the effective electron numbers of atoms Z_1 and Z_2:

$$n_i = \sum_j \rho(E_j^i) n_j^i \ . \tag{16}$$

Here E_j^i is the energy and n_j^i is the population of level j in atom Z_i; ν_1 and ν_2 are the corresponding valencies. ω is the transition probability of the meson from the molecular orbit to the atomic orbit of atom Z_1, and is assumed to have one of the following forms:

$$\omega_1 = \left(1 + \frac{p_2 q_2}{p_1 q_1}\right)^{-1} \tag{17}$$

for a long-lived mesic molecular state, or

$$\omega_2 = p_1\beta_1 + (1-p_1\beta_1-p_2\beta_2)q_1 \tag{18}$$

for a short-lived mesic molecular state.[54] The p_i's are the valence electron densities expressed in terms of σ, the ionicity of the Z_1-Z_2 bond:

$$p_1 = \frac{1}{2}(1-\sigma); \quad p_2 = \frac{1}{2}(1+\sigma) \ . \tag{19}$$

The transition from molecular state to atomic states is described by the quantities q and β:

$$q_1 = \left[1 + \left(\frac{Z_2}{Z_1}\right)^2\right]^{-1} \quad ; \quad q_2 = 1 - q_1 \tag{20}$$

$$\beta_1 = \frac{n_1}{n_1+2\nu_1} \quad ; \quad \beta_2 = \frac{n_2}{n_2+2\nu_2} \, . \tag{21}$$

It is shown in Ref. 54 that Eqs. (14-16) and (18-21), i.e. the smooth boundary approximations with ω_2 and parameters

$$E_o = 15 \text{ eV} \; ; \quad E_c = \begin{cases} E_1 = 70 \text{ eV if } Z \leq Z_o = 18 \\ E_2 = 100 \text{ eV if } Z > Z_o = 18 \end{cases} , \tag{22}$$

can describe the atomic capture ratios measured in oxides better than any of the simple relations (3-6), (8), (12). However, it is mentioned in Ref. 54 that the (22) parameter values are not optimized in the least-squares sense. Our attempts to optimize the SPP model are summarised in Table 1. We have tried to find an improvement for both the rigid- and smooth-boundary approximations, using both forms, (17) and (18), of the ω transition probability. The rigid-boundary model has only one parameter, the E_o cut-off energy. The smooth-boundary model has been fitted with two different $\rho(E)$ efficiency functions: the original Gaussian (14) and a Fermi function

$$\rho(E) = \frac{1}{1+\exp\{(E-E_o)/E_c\}} \, . \tag{23}$$

In Table 1, if Z_o is not presented among the parameters, then we have used $E_c = E_1$ with no change in the width. We also tried to find improvement in the q_1 probability by fitting the exponent x in:

$$q_1 = \left[1 + \left(\frac{Z_2}{Z_1}\right)^x\right]^{-1} \, . \tag{24}$$

It is quite clear from Table 1 that the best agreement is given by the SPP model in any form. Furthermore, the agreement between predictions and experimental values is much better for the smooth-boundary approximation. The best fits are obtained when using the original SPP model with modified parameters. The cut-off energy E_o tends to be zero in every case. The increase in the E_c width at $Z > 18$ suggested in Ref. 54 seems to be well established; its removal increases the χ_r^2 value, and the fitting changes the Z_o value only slightly (from $Z_o = 18$ to 15-17). The fitted values of exponent x in (24), x = 1.7-1.8, are not far from the original 2, and these changes do not affect the obtained χ_r^2 value very much. The goodness of fit is not sensitive to the actual form of the $\rho(E)$ distribution, whether it is Gaussian or Fermian. It is, however, sensitive to the actual form of the transition probability of the meson from the molecular to atomic orbit, preferring the short-lived molecular state described by Eq. (18).

In Tables 2 through 7 the experimental data are presented together with the theoretical predictions of five models from Table 1: the generalised Z-law (7) with a = 0.69 and b = 0.86; the modified model of Daniel (10) with a = 0.83 and b = 0.69; the model (12) of Vasilyev et al. and two versions of the SPP model with Gaussian efficiency function (14) and ω_2 probability. We did not feel any justification for the removal of experimental data from the comparison as removing a dozen of those with the biggest deviations does not affect the final picture.

In Table 8 the total χ^2-values are presented for the six groups of binary systems and the five chosen models. For the mixtures where no chemical effects are involved, formula (12) gives the best predictions; for the compounds the SPP model is the best. Therefore, we made an attempt to improve on formula (12) by including the terms of the molecular orbits from Eq. (15). With adjustable parameters a and b, it assumed the following form:

$$A(Z_1,Z_2) = \frac{Z_1^{1/3} - a + b(2\nu_1\omega)}{Z_2^{1/3} - a + b(2\nu_2(1-\omega))} \cdot \qquad (25)$$

For the probability ω of the transition from the molecular to an atomic orbit on Z_1 we used Eq. (18), the fast transition approximation. From the results presented in Table 1 it is clear that we got back the initial (12) form for the atomic capture in the mixtures, and including molecular effects does not improve the χ_r^2 considerably.

5. CONCLUSION

We tested the various descriptions of the atomic capture of mesons against 321 experimental atomic capture ratios. The comparison shows that there is no adequate model for the atomic capture yet. The model proposed by Schneuwly, Pokrovsky and Ponomarev gives the best agreement with the measured data, with zero boundary and slightly modified parameters:

$$E_o = 0 \; ; \quad E_c = \begin{cases} E_1 = 86 \text{ eV for } Z \leq 15 \\ E_2 = 119 \text{ eV for } Z > 15 \end{cases} \cdot \qquad (26)$$

For mixtures of elements (gases) the use of the (12) empirical formula is recommended. To facilitate the application of the SPP model for the estimation of atomic capture probabilities, we enclose a list of the effective electron numbers Z_{eff}, calculated by using models 4 and 5 of Tables 2 through 7 for the elements of the periodic system (see Table 9). The Z_{eff} value listed in Table 9 corresponds to the effective number of all electrons in the atom. The effective number of the core electrons, n, used in Eq. (15), can be obtained from Z_{eff} by subtracting ν, the actual number of valence electrons:

$$n = Z_{eff} - \nu \; . \qquad (27)$$

This is a good approximation as the binding energies of the valence electrons are much smaller than those of the core electrons (i.e. $\nu \approx \nu_{eff}$).

Finally, we emphasize the need for an adequate method of estimating the probability of Coulomb capture of mesons in atoms. As shown by the reduced χ_r^2-value obtained in the best case ($\chi_r^2 = 14 \gg 1$), at present the agreement between theory and experiment is far from being satisfactory.

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Table 1. Comparison of atomic capture models

Function	Degrees of freedom	Parameters	Total CHI square	Reduced CHI square
Model : Original Z-law	321	-	42152.6	131.32
Model : Z-law A(Z1,Z2)=A*(Z1/Z2)**B	320	A= 1.00 B= 0.73 +/- 0.002	21837.5	68.24
Model : Z-law A(Z1,Z2)=A*(Z1/Z2)**B	320	A= 0.61 +/- 0.001 B= 1.00	14418.4	45.06
Model : Z-law A(Z1,Z2)=A*(Z1/Z2)**B	319	A= 0.69 +/- 0.0004 B= 0.86 +/- 0.0008	12877.8	40.37
Model : Vasilyev et al W(Z)= Z**(1/3) - 1	321	-	21905.3	68.24
Model : Vasilyev et al Modified version (eq.25)	319	A= 1.00 +/- 0.000 B= 0.28 +/- 0.004	18145.8	56.88
Model : Daniel W(Z)=Z**(1/3)*log(A*Z+B)	321	A= 0.57 Original B= 0.00 values	192280.7	599.01
Model : Daniel W(Z)=Z**(1/3)*log(A*Z+B)	320	A= 1.28 +/- 0.0015 B= 0.00	20332.9	63.54
Model : Daniel W(Z)=Z**(1/3)*log(A*Z+B)	321	A= 1 B= 0	21166.4	65.94
Model : Daniel W(Z)=Z**(1/3)*log(A*Z+B)	321	A= 1 B= 1	20621.6	64.24
Model : Daniel W(Z)=Z**(1/3)*log(A*Z+B)	319	A= 0.83 +/- 0.009 B= 0.69 +/- 0.002	20202.1	63.33
Model : SPP Rigid boundary Omega-1	320	E0= 92.13 +/- 0.27 X = 2	8342.8	26.07
Model : SPP Rigid boundary Omega-2	320	E0= 92.60 +/- 0.44 X = 2	8773.1	27.42
Model : SPP Smooth boundary Gaussian distribution Omega-1	319	E0= 13.11 +/- 0.02 E1= 75.68 +/- 0.44 X = 2	6267.8	19.65
Model : SPP Smooth boundary Gaussian distribution Omega-1	318	E0= 10.59 +/- 0.44 E1= 79.98 +/- 0.51 E2= 73.00 +/- 0.74 Z0= 18 X = 2	6201.4	19.50
Model : SPP Smooth boundary Gaussian distribution Omega-2	319	E0= 00.00 +/- 0.01 E1= 88.76 +/- 0.15 X = 2	5386.3	16.88
Model : SPP Smooth boundary Gaussian distribution Omega-2	318	E0= 15 Original E1= 70 parameters E2= 100 Z0= 18 X = 2	4972.5	15.64
Model : SPP Smooth boundary Gaussian distribution Omega-2	318	E0= 00.00 +/- 0.12 E1= 85.24 +/- 0.76 E2= 111.86+/- 0.94 Z0= 18 X = 2	4738.8	14.90
Model : SPP Smooth boundary Gaussian distribution Omega-2	317	E0= 00.00 +/- 0.19 E1= 86.12 +/- 0.31 E2= 119.06+/- 0.60 Z0= 15 (fitted) X = 2	4578.6	14.44

Table 1. Comparison of atomic capture models (cont'd)

Function	Degrees of freedom	Parameters	Total CHI square	Reduced CHI square
Model : SPP Smooth boundary Gaussian distribution Omega-2	317	E0= 00.00 +/- 0.07 E1= 84.74 +/- 0.33 E2= 113.65+/- 1.53 Z0= 18 X = 1.71 +/- 0.03	4704.9	14.84
Model : SPP Smooth boundary Gaussian distribution Omega-2	316	E0= 00.00 +/- 0.02 E1= 85.74 +/- 0.25 E2= 121.09+/- 0.56 Z0= 15 (fitted) X = 1.69 +/- 0.01	4540.3 ------	14.37 -----
Model : SPP Smooth boundary Fermi distribution Omega-1	319	E0= 77.37 +/- 0.23 E1= 18.72 +/- 0.13 X = 2	6238.1	19.56
Model : SPP Smooth boundary Fermi distribution Omega-1	318	E0= 75.64 +/- 0.57 E1= 20.60 +/- 0.33 E2= 27.18 +/- 0.49 Z0= 18 X = 2	6185.8	19.45
Model : SPP Smooth boundary Fermi distribution Omega-2	319	E0= 48.21 +/- 0.04 E1= 38.79 +/- 0.02 X = 2	5262.2	16.50
Model : SPP Smooth boundary Fermi distribution Omega-2	318	E0= 63.90 +/- 0.22 E1= 33.18 +/- 0.19 E2= 20.53 +/- 0.27 Z0= 18 X = 2	5024.7	15.80
Model : SPP Smooth boundary Fermi distribution Omega-2	317	E0= 63.65 +/- 0.29 E1= 33.98 +/- 0.16 E2= 19.15 +/- 0.22 Z0= 17 (fitted) X = 2	4738.0	14.95
Model : SPP Smooth boundary Fermi distribution Omega-2	317	E0= 63.81 +/- 0.41 E1= 33.38 +/- 0.25 E2= 20.40 +/- 0.33 Z0= 18 X = 1.89 +/- 0.04	5017.8	15.83
Model : SPP Smooth boundary Fermi distribution Omega-2	316	E0= 64.61 +/- 0.39 E1= 33.29 +/- 0.12 E2= 18.58 +/- 0.42 Z0= 17 (fitted) X = 1.84 +/- 0.04	4728.0	14.96

Table 2. Test of atomic capture models for simple binary mixtures

T A R G E T			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
He+He-3	2	2	0.750 +- 0.130	35	0.69	0.2	1.00	3.7	1.00	3.7	1.00	3.7	1.00	3.7
N2+He-3	7	2	3.520 +- 0.230	10	2.03	42.2	3.51	0.0	3.33	0.7	2.58	16.7	2.58	16.7
N2+He-3	7	2	3.740 +- 0.160	35	2.03	114.7	3.51	2.0	3.33	6.7	2.58	52.7	2.58	52.7
O2+He-3	8	2	4.680 +- 0.180	35	2.27	178.8	3.85	21.4	3.70	29.6	3.04	83.5	3.04	83.5
Ne+He-3	10	2	4.130 +- 0.150	35	2.75	84.2	4.44	4.3	4.40	3.1	3.85	3.6	3.85	3.6
Ar+He-3	18	2	4.540 +- 0.160	35	4.57	0.0	6.24	112.3	6.69	181.1	4.22	4.0	4.23	3.7
Kr+He-3	36	2	8.000 +- 0.230	35	8.29	1.6	8.86	13.9	10.49	117.2	7.25	10.6	7.33	8.6
Xe+He-3	54	2	8.660 +- 0.310	35	11.74	99.0	10.69	43.1	13.41	234.3	8.70	0.0	8.78	0.1
N2+O2	7	8	0.834 +- 0.031	28	0.62	49.8	0.91	6.5	0.90	4.4	0.85	0.3	0.85	0.3
He+Ar	2	18	0.150 +- 0.010	9	0.10	20.9	0.16	1.1	0.15	0.0	0.24	75.7	0.24	74.6
He+Ar	2	18	0.210 +- 0.040	27	0.10	7.0	0.16	1.5	0.15	2.3	0.24	0.5	0.24	0.4
N2+Ar	7	18	0.510 +- 0.020	9	0.31	103.8	0.56	7.1	0.50	0.4	0.61	25.6	0.61	24.8
Ne+Ar	10	18	0.610 +- 0.020	9	0.42	93.9	0.71	26.2	0.66	5.4	0.91	227.1	0.91	223.7
Ne+Ar	10	18	0.900 +- 0.120	15	0.42	16.3	0.71	2.4	0.66	4.1	0.91	0.0	0.91	0.0
Ne+Ar	10	18	0.710 +- 0.030	27	0.42	95.9	0.71	0.0	0.66	3.2	0.91	45.1	0.91	44.1
Kr+Ar	36	18	1.340 +- 0.060	27	1.25	2.1	1.42	1.8	1.57	14.4	1.72	39.8	1.73	42.7
Total chi-square for 16 points						910.3		247.3		610.6		588.8		583.3

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Guassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 3. Test of atomic capture models for simple binary oxides

TARGET			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Be O	4	8	0.120 +- 0.040	8	0.38	42.3	0.59	136.5	0.55	117.4	0.11	0.1	0.12	0.0
B2 O3	5	8	0.220 +- 0.050	8	0.46	23.2	0.71	96.0	0.68	83.5	0.16	1.5	0.18	0.7
C O	6	8	0.766 +- 0.030	28	0.54	57.4	0.82	2.9	0.79	0.7	0.51	70.2	0.53	64.0
C O2	6	8	0.430 +- 0.020	30	0.54	29.6	0.82	374.7	0.79	326.6	0.30	43.4	0.32	31.3
N O	7	8	0.959 +- 0.030	28	0.62	131.4	0.91	2.4	0.90	4.0	0.77	40.7	0.77	38.0
Mg O	12	8	0.830 +- 0.070	8	0.98	4.5	1.29	43.1	1.36	57.2	1.03	8.5	1.02	7.1
Mg O	12	8	0.830 +- 0.040	24	0.98	13.7	1.29	131.9	1.36	175.2	1.03	26.2	1.02	21.6
Mg O	12	8	0.800 +- 0.020	30	0.98	79.1	1.29	598.9	1.36	782.3	1.03	137.6	1.02	116.7
Mg O	12	8	0.890 +- 0.050	33	0.98	3.1	1.29	63.8	1.36	88.1	1.03	8.4	1.02	6.4
Al2 O3	13	8	0.650 +- 0.060	1	1.05	43.9	1.35	136.6	1.44	173.6	0.93	21.6	0.90	17.6
Al2 O3	13	8	0.850 +- 0.060	8	1.05	10.8	1.35	69.8	1.44	96.8	0.93	1.7	0.90	0.7
Al2 O3	13	8	0.840 +- 0.030	30	1.05	47.9	1.35	290.5	1.44	400.6	0.93	8.8	0.90	4.2
Al2 O3	13	8	0.740 +- 0.040	33	1.05	59.1	1.35	233.6	1.44	306.6	0.93	22.3	0.90	16.3
Si O	14	8	0.960 +- 0.050	33	1.12	9.8	1.41	81.1	1.52	124.9	0.93	0.3	0.91	1.0
Si O2	14	8	0.570 +- 0.050	1	1.12	119.5	1.41	282.3	1.52	360.0	0.90	42.9	0.86	33.2
Si O2	14	8	0.790 +- 0.070	8	1.12	21.8	1.41	78.5	1.52	108.4	0.90	2.4	0.86	0.9
Si O2	14	8	0.860 +- 0.070	22	1.12	13.4	1.41	61.8	1.52	88.5	0.90	0.3	0.86	0.0
Si O2	14	8	0.960 +- 0.040	30	1.12	15.3	1.41	126.6	1.52	195.1	0.90	2.4	0.86	6.5
Si O2	14	8	0.840 +- 0.040	33	1.12	47.8	1.41	203.2	1.52	287.9	0.90	2.1	0.86	0.2
P2 O5	15	8	0.930 +- 0.100	1	1.18	6.5	1.47	28.8	1.59	44.1	0.99	0.4	0.94	0.0
P2 O5	15	8	0.870 +- 0.030	30	1.18	110.1	1.47	395.0	1.59	583.1	0.99	16.8	0.94	5.1
P2 O5	15	8	1.000 +- 0.050	33	1.18	13.7	1.47	86.9	1.59	141.3	0.99	0.0	0.94	1.6
Ca O	20	8	1.360 +- 0.100	8	1.52	2.5	1.71	12.6	1.94	33.9	1.61	6.1	1.58	4.8
Ca O	20	8	1.450 +- 0.090	18	1.52	0.6	1.71	8.6	1.94	29.9	1.61	3.0	1.58	2.0
Ca O	20	8	1.710 +- 0.090	37	1.52	4.6	1.71	0.0	1.94	6.6	1.61	1.3	1.58	2.1
Sc2 O3	21	8	2.780 +- 0.200	8	1.58	35.9	1.76	26.1	2.01	15.0	1.79	24.3	1.76	26.1
Ti O	22	8	2.640 +- 0.190	33	1.65	27.3	1.80	19.5	2.07	9.0	1.97	12.6	1.94	13.7
Ti O2	22	8	2.700 +- 0.200	8	1.65	27.7	1.80	20.2	2.07	10.0	1.99	12.7	1.94	14.4
Ti O2	22	8	1.900 +- 0.100	18	1.65	6.4	1.80	1.0	2.07	2.9	1.99	0.8	1.94	0.2
Ti O2	22	8	1.870 +- 0.190	21	1.65	1.4	1.80	0.1	2.07	1.1	1.99	0.4	1.94	0.1
Ti O2	22	8	2.170 +- 0.110	30	1.65	22.6	1.80	11.2	2.07	0.8	1.99	2.8	1.94	4.3
Ti O2	22	8	2.700 +- 0.130	33	1.65	65.6	1.80	47.7	2.07	23.6	1.99	30.1	1.94	34.1
V2 O3	23	8	2.190 +- 0.180	18	1.71	7.1	1.84	3.7	2.13	0.1	2.14	0.1	2.10	0.2
V2 O4	23	8	2.280 +- 0.230	18	1.71	6.1	1.84	3.6	2.13	0.4	2.15	0.3	2.11	0.6
V2 O4	23	8	2.700 +- 0.190	33	1.71	27.1	1.84	20.3	2.13	9.0	2.15	8.3	2.11	9.8
V2 O5	23	8	3.100 +- 0.200	8	1.71	48.2	1.84	39.4	2.13	23.5	2.17	21.8	2.11	24.4
V2 O5	23	8	2.680 +- 0.140	18	1.71	47.9	1.84	35.7	2.13	15.4	2.17	13.5	2.11	16.5
V2 O5	23	8	2.860 +- 0.200	33	1.71	33.0	1.84	25.8	2.13	13.3	2.17	12.0	2.11	14.0
Cr2 O3	24	8	3.000 +- 0.170	8	1.77	51.9	1.88	43.1	2.19	22.7	2.32	15.8	2.29	17.6
Cr2 O3	24	8	2.040 +- 0.110	18	1.77	5.8	1.88	2.0	2.19	1.9	2.32	6.7	2.29	5.0
Cr2 O3	24	8	2.630 +- 0.130	30	1.77	43.3	1.88	32.9	2.19	11.4	2.32	5.5	2.29	7.0
Cr2 O3	24	8	3.450 +- 0.250	33	1.77	44.9	1.88	39.2	2.19	25.4	2.32	20.3	2.29	21.6
Cr2 O3	24	8	2.650 +- 0.200	36	1.77	19.1	1.88	14.6	2.19	5.3	2.32	2.6	2.29	3.3
Cr O3	24	8	2.960 +- 0.200	30	1.77	35.1	1.88	28.9	2.19	14.8	2.37	8.6	2.31	10.6
Cr O3	24	8	3.520 +- 0.180	33	1.77	94.0	1.88	82.6	2.19	54.5	2.37	40.6	2.31	45.2
Cr O3	24	8	3.230 +- 0.220	36	1.77	43.7	1.88	37.4	2.19	22.3	2.37	15.1	2.31	17.5
Mn O2	25	8	3.000 +- 0.170	30	1.84	46.7	1.92	40.1	2.25	19.5	2.38	13.2	2.34	15.1
Mn O2	25	8	2.600 +- 0.190	33	1.84	16.1	1.92	12.7	2.25	3.4	2.38	1.3	2.34	1.9
Fe2 O3	26	8	2.430 +- 0.240	21	1.90	4.9	1.96	3.8	2.31	0.3	2.57	0.4	2.54	0.2
Fe2 O3	26	8	3.210 +- 0.200	33	1.90	42.8	1.96	38.9	2.31	20.4	2.57	10.1	2.54	11.3
Co2 O3	27	8	3.040 +- 0.290	21	1.96	13.8	2.00	12.9	2.36	5.4	2.69	1.4	2.66	1.7

Table 3. Test of atomic capture models for simple binary oxides (cont'd)

TARGET			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Co2 O3	27	8	3.700 +- 0.380	33	1.96	20.9	2.00	20.0	2.36	12.4	2.69	7.0	2.66	7.5
Co3 O4	27	8	3.350 +- 0.250	33	1.96	30.7	2.00	29.2	2.36	15.5	2.69	6.9	2.66	7.6
Cu2 O	29	8	3.800 +- 0.900	8	2.09	3.6	2.07	3.7	2.47	2.2	2.97	0.8	2.96	0.9
Cu O	29	8	6.140 +- 0.850	6	2.09	22.7	2.07	22.9	2.47	18.6	3.01	13.6	2.99	13.8
Cu O	29	8	3.600 +- 0.400	8	2.09	14.3	2.07	14.6	2.47	7.9	3.01	2.2	2.99	2.4
Cu O	29	8	4.060 +- 0.230	30	2.09	73.5	2.07	74.7	2.47	47.5	3.01	20.8	2.99	21.8
Cu O	29	8	3.260 +- 0.230	33	2.09	25.9	2.07	26.7	2.47	11.7	3.01	1.2	2.99	1.4
Zn O	30	8	2.220 +- 0.060	7	2.15	1.3	2.11	3.5	2.53	26.5	2.94	144.9	2.92	136.2
Zn O	30	8	2.660 +- 0.320	8	2.15	2.5	2.11	3.0	2.53	0.2	2.94	0.8	2.92	0.7
Zn O	30	8	2.390 +- 0.100	30	2.15	5.7	2.11	8.0	2.53	1.9	2.94	30.5	2.92	28.1
Zn O	30	8	3.060 +- 0.240	33	2.15	14.4	2.11	15.8	2.53	4.9	2.94	0.2	2.92	0.3
Ga2 O3	31	8	2.770 +- 0.200	33	2.21	7.8	2.14	9.9	2.58	0.9	2.95	0.8	2.92	0.6
Ge O2	32	8	2.900 +- 0.210	33	2.27	8.9	2.17	11.9	2.63	1.6	3.01	0.3	2.98	0.1
As2 O3	33	8	3.390 +- 0.250	33	2.33	17.8	2.21	22.4	2.69	8.0	2.99	2.6	2.97	2.9
Se O2	34	8	2.720 +- 0.200	33	2.39	2.6	2.24	5.8	2.74	0.0	3.13	4.2	3.10	3.6
Sr O	38	8	2.120 +- 0.110	37	2.64	21.9	2.36	4.8	2.93	54.3	2.19	0.4	2.18	0.3
Y2 O3	39	8	1.830 +- 0.120	8	2.69	51.9	2.39	21.9	2.98	91.5	2.23	11.0	2.22	10.5
Y2 O3	39	8	2.070 +- 0.130	18	2.69	23.1	2.39	6.1	2.98	48.8	2.23	1.5	2.22	1.3
Y2 O3	39	8	2.190 +- 0.160	33	2.69	9.9	2.39	1.6	2.98	24.2	2.23	0.1	2.22	0.0
Zr O2	40	8	2.380 +- 0.160	8	2.75	5.5	2.42	0.1	3.02	16.2	2.30	0.3	2.28	0.4
Zr O2	40	8	2.620 +- 0.190	33	2.75	0.5	2.42	1.1	3.02	4.5	2.30	2.9	2.28	3.2
Nb2 O5	41	8	2.950 +- 0.230	33	2.81	0.4	2.45	4.8	3.07	0.3	2.49	3.9	2.47	4.4
Mo O3	42	8	3.480 +- 0.230	8	2.87	7.0	2.48	19.1	3.12	2.5	2.71	11.3	2.67	12.4
Mo O3	42	8	3.600 +- 0.290	33	2.87	6.3	2.48	15.0	3.12	2.8	2.71	9.5	2.67	10.3
Tc O2	43	8	3.260 +- 0.310	33	2.93	1.1	2.50	6.0	3.16	0.1	2.78	2.3	2.76	2.6
Pd O	46	8	3.570 +- 0.440	33	3.11	1.1	2.58	5.0	3.29	0.4	3.24	0.6	3.23	0.6
Ag2 O	47	8	3.830 +- 0.320	33	3.16	4.3	2.61	14.6	3.33	2.4	3.17	4.2	3.16	4.3
Cd O	48	8	6.700 +- 1.500	8	3.22	5.4	2.63	7.3	3.38	4.9	3.21	5.4	3.20	5.4
Cd O	48	8	2.470 +- 0.220	18	3.22	11.7	2.63	0.6	3.38	17.0	3.21	11.5	3.20	11.2
Cd O	48	8	2.500 +- 0.280	21	3.22	6.6	2.63	0.2	3.38	9.8	3.21	6.5	3.20	6.3
Cd O	48	8	3.140 +- 0.250	33	3.22	0.1	2.63	4.1	3.38	0.9	3.21	0.1	3.20	0.1
In2 O3	49	8	2.940 +- 0.280	8	3.28	1.5	2.66	1.0	3.42	2.9	3.28	1.5	3.27	1.4
In2 O3	49	8	2.920 +- 0.310	33	3.28	1.3	2.66	0.7	3.42	2.6	3.28	1.3	3.27	1.3
Sn O2	50	8	3.170 +- 0.240	8	3.34	0.5	2.68	4.1	3.46	1.5	3.36	0.6	3.35	0.6
Sn O2	50	8	3.020 +- 0.230	33	3.34	1.9	2.68	2.1	3.46	3.7	3.36	2.2	3.35	2.0
Sb2 O3	51	8	2.790 +- 0.140	6	3.39	18.6	2.71	0.3	3.50	25.8	3.35	16.2	3.35	15.9
Sb2 O3	51	8	3.480 +- 0.350	8	3.39	0.1	2.71	4.9	3.50	0.0	3.35	0.1	3.35	0.1
Sb2 O3	51	8	3.520 +- 0.280	33	3.39	0.2	2.71	8.4	3.50	0.0	3.35	0.4	3.35	0.4
Sb2 O5	51	8	1.730 +- 0.090	8	3.39	341.8	2.71	118.2	3.50	387.4	3.45	365.1	3.43	358.4
Te O2	52	8	3.220 +- 0.250	33	3.45	0.9	2.73	3.8	3.54	1.7	3.48	1.0	3.47	1.0
Ba O	56	8	2.270 +- 0.220	8	3.68	41.0	2.83	6.4	3.70	42.3	2.77	5.2	2.78	5.4
Ba O	56	8	1.450 +- 0.180	21	3.68	153.2	2.83	58.4	3.70	156.4	2.77	53.8	2.78	54.5
La2 O3	57	8	2.210 +- 0.250	21	3.73	37.2	2.85	6.5	3.74	37.4	2.78	5.2	2.79	5.4
La2 O3	57	8	2.730 +- 0.330	33	3.73	9.3	2.85	0.1	3.74	9.4	2.78	0.0	2.79	0.0
Ce O2	58	8	3.700 +- 0.400	21	3.79	0.1	2.87	4.3	3.78	0.0	3.01	3.0	3.01	2.9
Ce O2	58	8	4.500 +- 0.550	33	3.79	1.7	2.87	8.8	3.78	1.7	3.01	7.3	3.01	7.3
Nd2 O3	60	8	5.130 +- 0.350	33	3.90	12.3	2.91	40.1	3.85	13.3	3.21	30.1	3.21	29.9
Sm2 O3	62	8	3.090 +- 0.340	8	4.01	7.4	2.96	0.2	3.93	6.1	3.44	1.0	3.44	1.1
Sm2 O3	62	8	4.400 +- 0.740	33	4.01	0.3	2.96	3.8	3.93	0.4	3.44	1.7	3.44	1.7
Eu2 O3	63	8	3.600 +- 0.400	21	4.07	1.4	2.98	2.4	3.97	0.8	3.55	0.0	3.55	0.0
Eu2 O3	63	8	4.340 +- 0.460	33	4.07	0.3	2.98	8.8	3.97	0.7	3.55	2.9	3.55	2.9

Table 3. Test of atomic capture models for simple binary oxides (cont'd)

TARGET			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Gd2 O3	64	8	5.520 +- 0.330	33	4.13	17.8	3.00	58.3	4.00	21.2	3.55	35.6	3.55	35.5
Dy2 O3	66	8	4.700 +- 0.500	21	4.24	0.9	3.04	11.0	4.07	1.6	3.94	2.3	3.94	2.3
Dy2 O3	66	8	5.790 +- 0.610	33	4.24	6.5	3.04	20.3	4.07	7.9	3.94	9.2	3.94	9.2
Yb2 O3	70	8	3.180 +- 0.340	8	4.46	14.1	3.12	0.0	4.21	9.3	4.49	15.0	4.49	14.8
Yb2 O3	70	8	6.850 +- 0.420	33	4.46	32.5	3.12	78.8	4.21	39.4	4.49	31.4	4.49	31.7
Lu2 O3	71	8	4.400 +- 0.500	21	4.51	0.0	3.14	6.3	4.25	0.1	4.60	0.2	4.59	0.1
Lu2 O3	71	8	5.310 +- 0.580	33	4.51	1.9	3.14	14.0	4.25	3.3	4.60	1.5	4.59	1.5
Ta2 O5	73	8	6.000 +- 0.600	21	4.62	5.3	3.18	22.1	4.32	7.9	4.89	3.4	4.88	3.5
Ta2 O5	73	8	7.200 +- 0.730	33	4.62	12.5	3.18	30.3	4.32	15.6	4.89	10.0	4.88	10.1
W O3	74	8	4.700 +- 0.500	21	4.67	0.0	3.20	9.0	4.35	0.5	5.06	0.5	5.05	0.5
W O3	74	8	5.750 +- 0.670	33	4.67	2.6	3.20	14.5	4.35	4.4	5.06	1.1	5.05	1.1
Tl2 O3	81	8	4.000 +- 0.500	21	5.05	4.4	3.33	1.8	4.58	1.4	4.28	0.3	4.31	0.4
Tl2 O3	81	8	4.810 +- 0.570	33	5.05	0.2	3.33	6.8	4.58	0.2	4.28	0.9	4.31	0.8
Pb O	82	8	4.560 +- 0.530	6	5.11	1.1	3.34	5.3	4.61	0.0	4.00	1.1	4.03	1.0
Pb O	82	8	5.800 +- 0.700	8	5.11	1.0	3.34	12.3	4.61	2.9	4.00	6.6	4.03	6.4
Pb O	82	8	4.100 +- 0.400	21	5.11	6.3	3.34	3.6	4.61	1.6	4.00	0.1	4.03	0.0
Pb O	82	8	4.880 +- 0.550	33	5.11	0.2	3.34	7.8	4.61	0.2	4.00	2.6	4.03	2.4
Bi2 O3	83	8	4.300 +- 0.500	8	5.16	3.0	3.36	3.5	4.65	0.5	3.90	0.6	3.93	0.6
Bi2 O3	83	8	3.100 +- 0.400	21	5.16	26.5	3.36	0.4	4.65	14.9	3.90	4.0	3.93	4.3
Bi2 O3	83	8	3.770 +- 0.430	33	5.16	10.4	3.36	0.9	4.65	4.1	3.90	0.1	3.93	0.1
Th O2	90	8	2.900 +- 0.400	21	5.53	43.3	3.48	2.1	4.86	24.1	3.25	0.8	3.27	0.8
Th O2	90	8	3.570 +- 0.500	33	5.53	15.4	3.48	0.0	4.86	6.7	3.25	0.4	3.27	0.4
U O2	92	8	3.600 +- 0.400	21	5.64	25.9	3.51	0.0	4.92	10.9	3.65	0.0	3.66	0.0
U O2	92	8	4.650 +- 0.550	33	5.64	3.2	3.51	4.3	4.92	0.2	3.65	3.3	3.66	3.2
U O3	92	8	6.000 +- 0.500	8	5.64	0.5	3.51	24.7	4.92	4.6	3.74	20.5	3.75	20.3
Total chi-square for 127 points						3005.6		5194.8		6265.4		1708.5		1642.8

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Guassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 4. Test of atomic capture models for simple binary halides

TARGET			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Li F	3	9	0.280 +- 0.030	8	0.27	0.2	0.41	18.6	0.38	11.6	0.17	13.3	0.17	12.6
Li F	3	9	0.100 +- 0.080	25	0.27	4.4	0.41	15.0	0.38	12.4	0.17	0.8	0.17	0.8
Na F	11	9	1.560 +- 0.120	8	0.82	38.0	1.13	12.6	1.16	10.9	0.91	29.4	0.91	29.6
Na F	11	9	0.960 +- 0.050	25	0.82	7.8	1.13	12.0	1.16	16.6	0.91	1.0	0.91	1.1
Mg F2	12	9	0.920 +- 0.030	25	0.88	1.5	1.19	83.3	1.24	114.0	0.76	27.9	0.76	29.4
Al F3	13	9	0.900 +- 0.300	16	0.95	0.0	1.25	1.4	1.31	1.9	0.60	1.0	0.59	1.1
Al F3	13	9	0.950 +- 0.170	38	0.95	0.0	1.25	3.1	1.31	4.6	0.60	4.3	0.59	4.5
S F6	16	9	1.040 +- 0.100	14	1.13	0.8	1.41	13.5	1.52	23.2	0.75	8.2	0.73	9.4
K F	19	9	1.890 +- 0.180	23	1.31	10.3	1.54	3.7	1.71	1.0	1.15	16.8	1.15	16.9
Ca F2	20	9	1.470 +- 0.260	25	1.37	0.1	1.59	0.2	1.77	1.3	1.18	1.3	1.17	1.3
Ti F4	22	9	2.440 +- 0.310	38	1.49	9.4	1.67	6.2	1.89	3.2	1.31	13.4	1.30	13.6
V F4	23	9	3.200 +- 0.290	38	1.55	32.5	1.71	26.5	1.94	18.8	1.43	37.4	1.42	37.8
Mn F2	25	9	2.160 +- 0.210	38	1.66	5.6	1.78	3.3	2.05	0.3	1.72	4.4	1.72	4.4
Fe F3	26	9	2.440 +- 0.390	25	1.72	3.4	1.82	2.6	2.11	0.7	1.80	2.7	1.80	2.7
Co F2	27	9	2.380 +- 0.320	25	1.77	3.6	1.85	2.7	2.16	0.5	1.94	1.9	1.94	1.9
Ni F2	28	9	3.090 +- 0.230	38	1.83	30.0	1.89	27.4	2.21	14.7	2.02	21.6	2.02	21.5
Zn F2	30	9	3.280 +- 0.200	38	1.94	44.7	1.95	44.2	2.31	23.7	2.16	31.1	2.17	30.9
Rb F	37	9	2.410 +- 0.180	38	2.33	0.2	2.16	1.9	2.63	1.5	1.76	13.1	1.77	12.5
Sr F2	38	9	1.830 +- 0.280	25	2.38	3.9	2.19	1.6	2.67	9.1	1.60	0.7	1.61	0.6
Y F3	39	9	2.540 +- 0.190	38	2.44	0.3	2.21	2.9	2.72	0.9	1.53	28.0	1.54	27.6
Zr F4	40	9	2.330 +- 0.490	25	2.49	0.1	2.24	0.0	2.76	0.8	1.51	2.8	1.51	2.8
Ag F2	47	9	3.200 +- 0.230	38	2.86	2.2	2.42	11.6	3.04	0.5	2.32	14.5	2.33	14.3
Cd F2	48	9	3.980 +- 0.540	16	2.91	3.9	2.44	8.1	3.08	2.8	2.34	9.2	2.35	9.2
Cd F2	48	9	3.250 +- 0.370	38	2.91	0.8	2.44	4.8	3.08	0.2	2.34	6.0	2.35	6.0
Sn F2	50	9	2.300 +- 0.150	38	3.02	22.7	2.49	1.5	3.16	32.7	2.37	0.2	2.39	0.3
Sb F3	51	9	3.690 +- 0.420	16	3.07	2.2	2.51	7.9	3.19	1.4	2.35	10.2	2.36	10.0
Sb F3	51	9	2.980 +- 0.300	38	3.07	0.1	2.51	2.5	3.19	0.5	2.35	4.4	2.36	4.3
Sb F5	51	9	4.600 +- 0.710	25	3.07	4.7	2.51	8.7	3.19	3.9	2.28	10.7	2.28	10.7
Cs F	55	9	3.650 +- 0.350	25	3.27	1.2	2.60	9.1	3.34	0.8	2.20	17.3	2.21	16.8
Ba F2	56	9	3.320 +- 0.400	25	3.32	0.0	2.62	3.1	3.38	0.0	2.05	10.0	2.07	9.7
La F3	57	9	3.930 +- 0.280	38	3.37	3.9	2.64	21.3	3.41	3.4	1.97	48.8	1.99	48.0
Ce F3	58	9	5.400 +- 0.340	38	3.43	33.7	2.66	65.0	3.45	33.0	2.14	92.1	2.15	91.2
Nd F3	60	9	6.720 +- 0.440	38	3.53	52.7	2.70	83.5	3.52	53.0	2.30	100.8	2.32	100.1
Gd F3	64	9	7.300 +- 0.700	38	3.73	26.0	2.78	41.7	3.65	27.2	2.58	45.5	2.59	45.2
Dy F3	66	9	6.800 +- 0.500	38	3.83	35.3	2.82	63.5	3.72	38.0	2.87	61.7	2.89	61.3
Er F3	68	9	6.800 +- 0.500	38	3.93	33.0	2.85	62.3	3.78	36.4	3.10	54.9	3.10	54.6
Yb F3	70	9	5.100 +- 0.600	38	4.03	3.2	2.89	13.6	3.85	4.4	3.32	8.8	3.33	8.7
Ta F5	73	9	5.920 +- 0.410	38	4.18	18.1	2.94	52.7	3.94	23.3	3.42	37.2	3.43	37.0
Hg F2	80	9	4.640 +- 0.330	38	4.52	0.1	3.06	22.8	4.15	2.2	3.32	16.0	3.35	15.2
Tl F	81	9	5.200 +- 0.600	38	4.57	1.1	3.08	12.5	4.18	2.9	3.14	11.8	3.17	11.4
Pb F2	82	9	9.600 +- 1.400	3	4.61	12.7	3.10	21.6	4.21	14.8	2.92	22.8	2.96	22.5
Pb F2	82	9	4.700 +- 0.400	8	4.61	0.0	3.10	16.1	4.21	1.5	2.92	19.8	2.96	19.0
Pb F2	82	9	4.170 +- 0.470	25	4.61	0.9	3.10	5.2	4.21	0.0	2.92	7.1	2.96	6.7
Bi F3	83	9	4.740 +- 0.450	5	4.66	0.0	3.11	13.1	4.24	1.2	2.76	19.4	2.79	18.8
Bi F3	83	9	3.940 +- 0.360	38	4.66	4.0	3.11	5.3	4.24	0.7	2.76	10.8	2.79	10.2
Th F4	90	9	2.320 +- 0.520	25	5.00	26.5	3.22	3.0	4.44	16.6	2.24	0.0	2.26	0.0
U F4	92	9	2.800 +- 1.200	2	5.09	3.7	3.25	0.1	4.49	2.0	2.51	0.1	2.52	0.1
U F4	92	9	6.080 +- 0.600	5	5.09	2.7	3.25	22.2	4.49	7.0	2.51	35.5	2.52	35.1
Li Cl	3	17	0.140 +- 0.020	7	0.16	0.6	0.28	50.0	0.24	25.4	0.16	1.4	0.16	1.6
Li Cl	3	17	0.190 +- 0.080	32	0.16	0.2	0.28	1.3	0.24	0.4	0.16	0.1	0.16	0.1
Be Cl2	4	17	0.056 +- 0.005	32	0.20	815.8	0.37	4040.8	0.32	2749.6	0.05	0.4	0.06	0.3

Table 4. Test of atomic capture models for simple binary halides (cont'd)

TARGET			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
C Cl4	6	17	0.980 +- 0.190	1	0.28	13.5	0.52	5.9	0.46	7.6	0.06	23.2	0.09	22.2
Na Cl	11	17	1.050 +- 0.080	8	0.47	51.7	0.78	11.5	0.73	15.7	0.83	7.6	0.83	7.7
Na Cl	11	17	0.680 +- 0.040	13	0.47	26.4	0.78	6.1	0.73	1.8	0.83	13.9	0.83	13.8
Na Cl	11	17	0.790 +- 0.030	18	0.47	110.6	0.78	0.1	0.73	3.6	0.83	1.7	0.83	1.6
Na Cl	11	17	0.680 +- 0.060	22	0.47	11.7	0.78	2.7	0.73	0.8	0.83	6.2	0.83	6.1
Na Cl	11	17	0.710 +- 0.070	23	0.47	11.3	0.78	1.0	0.73	0.1	0.83	2.9	0.83	2.9
Na Cl	11	17	0.692 +- 0.019	29	0.47	131.0	0.78	21.0	0.73	4.7	0.83	52.0	0.83	51.5
Na Cl	11	17	0.770 +- 0.130	32	0.47	5.2	0.78	0.0	0.73	0.1	0.83	0.2	0.83	0.2
Na Cl	11	17	0.790 +- 0.030	32	0.47	110.6	0.78	0.1	0.73	3.6	0.83	1.7	0.83	1.6
Mg Cl2	12	17	0.760 +- 0.040	32	0.51	38.6	0.82	2.3	0.78	0.3	0.69	2.8	0.69	2.7
Al Cl3	13	17	0.630 +- 0.210	16	0.55	0.2	0.86	1.2	0.83	0.9	0.53	0.2	0.53	0.2
Al Cl3	13	17	0.662 +- 0.016	22	0.55	50.9	0.86	153.2	0.83	108.0	0.53	68.8	0.53	64.9
Al Cl3	13	17	0.470 +- 0.250	32	0.55	0.1	0.86	2.4	0.83	2.1	0.53	0.1	0.53	0.1
P Cl5	15	17	0.830 +- 0.410	32	0.62	0.3	0.93	0.1	0.92	0.0	0.38	1.2	0.39	1.2
P Cl5	15	17	0.820 +- 0.040	32	0.62	25.1	0.93	8.0	0.92	5.9	0.38	118.9	0.39	116.3
K Cl	19	17	1.160 +- 0.030	13	0.76	178.4	1.06	10.7	1.08	7.3	1.05	13.2	1.05	14.1
K Cl	19	17	1.160 +- 0.110	16	0.76	13.3	1.06	0.8	1.08	0.5	1.05	1.0	1.05	1.1
K Cl	19	17	1.150 +- 0.050	18	0.76	61.1	1.06	3.1	1.08	2.0	1.05	3.9	1.05	4.2
K Cl	19	17	1.190 +- 0.120	23	0.76	12.9	1.06	1.1	1.08	0.9	1.05	1.3	1.05	1.4
K Cl	19	17	1.140 +- 0.020	29	0.76	362.4	1.06	15.3	1.08	9.4	1.05	19.7	1.05	21.5
K Cl	19	17	1.140 +- 0.150	32	0.76	6.4	1.06	0.3	1.08	0.2	1.05	0.4	1.05	0.4
K Cl	19	17	1.140 +- 0.060	32	0.76	40.3	1.06	1.7	1.08	1.0	1.05	2.2	1.05	2.4
Ca Cl2	20	17	1.560 +- 0.170	8	0.79	20.3	1.09	7.6	1.12	6.8	1.08	7.9	1.08	8.1
Ca Cl2	20	17	1.270 +- 0.030	22	0.79	252.3	1.09	35.6	1.12	26.2	1.08	39.4	1.08	41.3
Ca Cl2	20	17	1.370 +- 0.240	32	0.79	5.8	1.09	1.4	1.12	1.1	1.08	1.4	1.08	1.5
Ca Cl2	20	17	1.410 +- 0.070	32	0.79	77.6	1.09	20.8	1.12	17.6	1.08	22.0	1.08	22.6
V Cl3	23	17	1.960 +- 0.360	32	0.89	8.8	1.17	4.8	1.23	4.2	1.41	2.3	1.41	2.4
V Cl3	23	17	2.030 +- 0.110	32	0.89	106.5	1.17	60.6	1.23	53.5	1.41	31.3	1.41	32.2
Cr Cl3	24	17	1.910 +- 0.350	32	0.93	7.9	1.20	4.1	1.26	3.5	1.55	1.0	1.54	1.1
Cr Cl3	24	17	2.150 +- 0.100	32	0.93	149.3	1.20	90.4	1.26	79.3	1.55	35.7	1.54	36.9
Mn Cl2	25	17	2.290 +- 0.320	32	0.96	17.2	1.22	11.1	1.29	9.7	1.63	4.3	1.62	4.3
Mn Cl2	25	17	2.480 +- 0.140	32	0.96	117.7	1.22	80.4	1.29	71.8	1.63	36.9	1.62	37.4
Fe Cl3	26	17	2.010 +- 0.350	32	0.99	8.4	1.25	4.7	1.33	3.8	1.73	0.6	1.72	0.7
Co Cl2	27	17	2.090 +- 0.290	32	1.03	13.4	1.27	7.9	1.36	6.3	1.85	0.7	1.84	0.7
Ni Cl2	28	17	2.340 +- 0.310	32	1.06	17.1	1.30	11.3	1.39	9.4	1.93	1.7	1.92	1.8
Zn Cl2	30	17	2.170 +- 0.300	32	1.12	12.1	1.34	7.6	1.45	5.7	2.06	0.1	2.05	0.2
Rb Cl	37	17	1.780 +- 0.110	18	1.35	15.5	1.48	7.2	1.66	1.2	1.62	2.0	1.63	1.9
Rb Cl	37	17	1.750 +- 0.180	23	1.35	5.0	1.48	2.2	1.66	0.3	1.62	0.5	1.63	0.5
Rb Cl	37	17	1.530 +- 0.190	32	1.35	0.9	1.48	0.1	1.66	0.5	1.62	0.2	1.63	0.3
Zr Cl4	40	17	2.060 +- 0.430	32	1.44	2.1	1.54	1.5	1.74	0.6	1.48	1.8	1.47	1.9
Nb Cl5	41	17	3.250 +- 0.580	32	1.47	9.4	1.56	8.5	1.77	6.6	1.58	8.3	1.56	8.5
Mo Cl5	42	17	3.220 +- 0.580	32	1.50	8.8	1.58	8.0	1.79	6.1	1.71	6.8	1.68	7.0
Pd Cl2	46	17	2.750 +- 0.360	32	1.62	9.8	1.64	9.4	1.89	5.7	2.24	2.0	2.22	2.1
Ag Cl	47	17	0.800 +- 0.200	2	1.65	18.3	1.66	18.5	1.92	31.2	2.25	52.5	2.24	51.9
Ag Cl	47	17	2.500 +- 0.250	32	1.65	11.4	1.66	11.3	1.92	5.4	2.25	1.0	2.24	1.1
Cd Cl2	48	17	2.260 +- 0.260	16	1.68	4.9	1.68	5.0	1.94	1.5	2.25	0.0	2.24	0.0
Cd Cl2	48	17	2.220 +- 0.300	32	1.68	3.2	1.68	3.3	1.94	0.9	2.25	0.0	2.24	0.0
Sn Cl4	50	17	2.360 +- 0.400	16	1.74	2.4	1.71	2.7	1.99	0.9	2.27	0.1	2.25	0.1
Sn Cl2	50	17	1.980 +- 0.220	16	1.74	1.1	1.71	1.5	1.99	0.0	2.29	2.0	2.28	1.9
Sn Cl2	50	17	2.040 +- 0.310	32	1.74	0.9	1.71	1.1	1.99	0.0	2.29	0.6	2.28	0.6
Sb Cl3	51	17	2.550 +- 0.390	16	1.77	3.9	1.72	4.5	2.01	1.9	2.30	0.4	2.29	0.4

Table 4. Test of atomic capture models for simple binary halides (cont'd)

T A R G E T			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Sb Cl5	51	17	2.300 +- 0.450	16	1.77	1.4	1.72	1.6	2.01	0.4	2.29	0.0	2.27	0.0
Te Cl4	52	17	2.070 +- 0.500	32	1.80	0.3	1.74	0.4	2.04	0.0	2.34	0.3	2.32	0.3
Cs Cl	55	17	1.750 +- 0.090	7	1.89	2.6	1.78	0.1	2.11	15.6	2.03	9.6	2.03	9.9
Cs Cl	55	17	2.070 +- 0.210	23	1.89	0.7	1.78	1.9	2.11	0.0	2.03	0.0	2.03	0.0
Cs Cl	55	17	2.210 +- 0.230	32	1.89	1.9	1.78	3.4	2.11	0.2	2.03	0.6	2.03	0.6
Ba Cl2	56	17	2.670 +- 0.330	32	1.92	5.1	1.80	7.0	2.13	2.7	1.93	5.1	1.93	5.0
Ta Cl5	73	17	3.680 +- 0.620	32	2.42	4.2	2.02	7.1	2.48	3.7	3.35	0.3	3.32	0.3
W Cl6	74	17	7.200 +- 0.930	32	2.44	26.1	2.04	30.8	2.50	25.5	3.43	16.4	3.41	16.7
Hg Cl2	80	17	3.910 +- 0.440	32	2.61	8.7	2.11	16.8	2.62	8.7	3.19	2.7	3.20	2.6
Tl Cl	81	17	3.690 +- 0.370	32	2.64	8.0	2.12	18.1	2.63	8.1	2.98	3.7	3.00	3.5
Pb Cl2	82	17	3.160 +- 0.240	8	2.67	4.2	2.13	18.5	2.65	4.5	2.81	2.1	2.83	1.9
Pb Cl2	82	17	4.230 +- 0.450	32	2.67	12.0	2.13	21.8	2.65	12.3	2.81	9.9	2.83	9.7
Bi Cl3	83	17	2.550 +- 0.410	32	2.70	0.1	2.14	1.0	2.67	0.1	2.70	0.1	2.71	0.2
Na Br	11	35	0.372 +- 0.013	29	0.26	81.0	0.54	164.9	0.46	43.6	0.44	24.9	0.43	22.6
K Br	19	35	0.420 +- 0.070	16	0.41	0.0	0.73	20.2	0.67	13.1	0.54	3.1	0.54	2.9
K Br	19	35	0.590 +- 0.060	23	0.41	9.2	0.73	5.8	0.67	1.9	0.54	0.6	0.54	0.7
K Br	19	35	0.583 +- 0.014	29	0.41	156.2	0.73	117.3	0.67	41.8	0.54	8.3	0.54	9.5
Cd Br2	48	35	0.950 +- 0.120	16	0.91	0.1	1.16	3.1	1.21	4.8	1.13	2.3	1.12	2.1
Li I	3	53	0.770 +- 0.300	2	0.06	5.6	0.16	4.1	0.12	4.7	0.08	5.3	0.08	5.3
Li I	3	53	0.060 +- 0.010	4	0.06	0.0	0.16	100.9	0.12	32.4	0.08	3.9	0.08	3.7
Na I	11	53	0.290 +- 0.030	8	0.18	13.8	0.44	26.4	0.36	4.8	0.38	9.2	0.38	8.7
Al I3	13	53	0.480 +- 0.180	16	0.21	2.3	0.49	0.0	0.40	0.2	0.21	2.3	0.21	2.2
K I	19	53	0.500 +- 0.050	8	0.29	18.4	0.61	4.4	0.52	0.2	0.47	0.3	0.47	0.4
K I	19	53	0.500 +- 0.080	16	0.29	7.2	0.61	1.7	0.52	0.1	0.47	0.1	0.47	0.2
K I	19	53	0.540 +- 0.060	23	0.29	18.0	0.61	1.2	0.52	0.1	0.47	1.3	0.47	1.4
Ag I	47	53	1.450 +- 0.250	8	0.62	11.0	0.95	4.1	0.93	4.3	0.97	3.6	0.97	3.7
Cd I2	48	53	1.000 +- 0.200	8	0.63	3.4	0.96	0.0	0.94	0.1	0.97	0.0	0.97	0.0
Cd I2	48	53	1.000 +- 0.120	16	0.63	9.3	0.96	0.1	0.94	0.2	0.97	0.1	0.97	0.1
Pb I2	82	53	1.220 +- 0.110	8	1.00	3.8	1.21	0.0	1.29	0.4	1.22	0.0	1.22	0.0
Total chi-square for 131 points						3897.6		6222.5		4129.7		1661.6		1653.0

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Quassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 5. Test of atomic capture models for simple binary sulphides

T A R G E T			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Ca S	20	16	1.570 +- 0.040	13	0.84	336.7	1.13	122.1	1.16	102.9	1.29	49.6	1.27	56.2
Fe S	26	16	3.030 +- 0.170	38	1.05	136.0	1.29	104.6	1.38	93.8	2.14	27.7	2.10	29.8
Cu S	29	16	1.890 +- 0.180	6	1.15	16.9	1.36	8.6	1.48	5.1	2.54	13.1	2.50	11.5
Zn S	30	16	1.820 +- 0.360	7	1.18	3.1	1.39	1.5	1.52	0.7	2.50	3.6	2.46	3.2
Zn S	30	16	2.690 +- 0.170	38	1.18	78.4	1.39	58.8	1.52	47.7	2.50	1.2	2.46	1.8
As2 S3	33	16	2.010 +- 0.180	38	1.29	16.2	1.45	9.6	1.61	4.9	2.51	7.9	2.47	6.5
Sr S	38	16	1.900 +- 0.170	38	1.45	6.9	1.55	4.1	1.76	0.7	1.85	0.1	1.83	0.2
Mo S2	42	16	2.700 +- 0.200	38	1.58	31.2	1.63	28.7	1.87	17.3	2.26	4.8	2.20	6.3
Ag2 S	47	16	2.280 +- 0.140	38	1.74	14.7	1.72	16.2	2.00	4.0	2.73	10.5	2.69	8.7
Cd S	48	16	2.500 +- 0.160	38	1.77	20.5	1.73	23.0	2.02	8.8	2.79	3.3	2.74	2.3
Sb2 S3	51	16	2.460 +- 0.150	6	1.87	15.5	1.78	20.4	2.10	5.8	2.91	8.9	2.86	7.1
Sb2 S3	51	16	2.430 +- 0.180	38	1.87	9.7	1.78	13.0	2.10	3.4	2.91	7.1	2.86	5.7
Ba S	56	16	3.590 +- 0.200	38	2.03	61.1	1.86	74.9	2.22	47.0	2.37	36.9	2.35	38.6
Pb S	82	16	2.870 +- 0.350	6	2.81	0.0	2.20	3.7	2.77	0.1	3.50	3.3	3.48	3.1
Pb S	82	16	2.670 +- 0.160	38	2.81	0.8	2.20	8.6	2.77	0.4	3.50	27.0	3.48	25.8
Total chi-square for 15 points						747.8		497.6		342.5		205.0		206.7

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Guassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 6. Test of atomic capture models for simple binary alloys

TARGET			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
Ag Li 1.72	47	3	20.100 +- 5.840	6	7.35	4.8	5.90	5.9	7.96	4.3	11.51	2.2	11.54	2.2
Cd Mg 0.18	48	12	3.140 +- 0.250	20	2.27	12.0	2.04	19.3	2.48	6.9	3.11	0.0	3.10	0.0
Sn Mg 1.79	50	12	2.730 +- 0.300	31	2.35	1.6	2.08	4.7	2.55	0.4	3.32	3.8	3.29	3.5
Cu Al2	29	13	3.500 +- 0.360	5	1.38	34.8	1.53	29.8	1.72	24.5	4.02	2.1	3.93	1.4
Cu Al2	29	13	4.160 +- 0.500	5	1.38	31.0	1.53	27.6	1.72	23.9	4.02	0.1	3.93	0.2
Cu Al 8.6	29	13	10.300 +- 0.430	7	1.38	430.7	1.53	415.6	1.72	398.3	4.02	213.1	3.93	219.4
Cu Al 2.03	29	13	3.560 +- 0.060	29	1.38	1325.3	1.53	1140.7	1.72	942.4	4.02	59.6	3.93	38.3
Cu Al 0.17	29	13	3.490 +- 0.110	29	1.38	369.4	1.53	316.3	1.72	259.5	4.02	23.5	3.93	16.1
Cu Al 0.05	29	13	2.520 +- 0.310	29	1.38	13.6	1.53	10.1	1.72	6.7	4.02	23.5	3.93	20.7
Ni Ca 0.13	28	20	1.640 +- 0.160	31	0.92	20.2	1.19	8.0	1.25	6.1	1.71	0.2	1.71	0.2
Nb V 29.3	41	23	1.670 +- 0.240	20	1.13	5.0	1.33	2.0	1.44	0.9	1.23	3.4	1.21	3.7
Nb V	41	23	1.070 +- 0.050	20	1.13	1.7	1.33	26.6	1.44	55.1	1.23	9.7	1.21	7.9
Nb V 0.05	41	23	0.980 +- 0.170	20	1.13	0.8	1.33	4.2	1.44	7.4	1.23	2.1	1.21	1.8
Nb V 21.74	41	23	1.160 +- 0.090	26	1.13	0.1	1.33	3.5	1.44	9.8	1.23	0.5	1.21	0.3
Nb V 5.49	41	23	1.260 +- 0.060	26	1.13	4.4	1.33	1.3	1.44	9.1	1.23	0.3	1.21	0.7
Nb V 1.03	41	23	1.170 +- 0.050	26	1.13	0.5	1.33	10.0	1.44	29.4	1.23	1.3	1.21	0.7
Nb V 0.25	41	23	1.230 +- 0.060	26	1.13	2.5	1.33	2.7	1.44	12.4	1.23	0.0	1.21	0.1
Nb V 0.05	41	23	1.110 +- 0.100	26	1.13	0.1	1.33	4.7	1.44	11.0	1.23	1.3	1.21	1.0
Cu Ni 0.92	29	28	1.080 +- 0.050	20	0.71	54.4	1.02	1.6	1.02	1.3	1.08	0.0	1.08	0.0
Au Cu 5.56	79	29	1.890 +- 0.180	6	1.63	2.0	1.59	2.8	1.82	0.1	1.65	1.8	1.65	1.8
Ag Zn	47	30	2.200 +- 0.700	4	1.02	2.9	1.24	1.9	1.32	1.6	1.08	2.6	1.07	2.6
Ag Zn 3.06	47	30	0.970 +- 0.050	29	1.02	0.8	1.24	28.7	1.32	48.6	1.08	4.4	1.07	4.1
Ag Zn 0.17	47	30	1.080 +- 0.170	29	1.02	0.1	1.24	0.9	1.32	2.0	1.08	0.0	1.07	0.0
Ag Zn 0.05	47	30	0.970 +- 0.110	29	1.02	0.2	1.24	5.9	1.32	10.1	1.08	0.9	1.07	0.8
Te Se 1.63	52	34	1.020 +- 0.080	20	0.99	0.1	1.22	6.3	1.29	11.8	1.26	8.7	1.24	7.4
Ni Y 0.19	28	39	1.300 +- 0.180	31	0.52	18.8	0.85	6.2	0.81	7.3	1.23	0.1	1.24	0.1
Au Ag 0.67	79	47	1.270 +- 0.120	20	1.08	2.5	1.26	0.0	1.35	0.5	1.50	3.7	1.51	3.9
Total chi-square for 27 points						2340.5		2087.2		1891.1		369.0		338.9

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Guassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 7. Test of atomic capture models for simple binary nitrides

T A R G E T			EXPERIMENT		CALCULATED ATOMIC CAPTURE RATIOS AND CHI-SQUARES									
Name	Z1	Z2	A(Z1/Z2)	Ref.	Model 1		Model 2		Model 3		Model 4		Model 5	
B N	5	7	0.236 +- 0.012	17	0.52	546.9	0.78	2037.7	0.75	1856.7	0.28	16.0	0.31	37.9
B N diam	5	7	0.235 +- 0.020	18	0.52	198.3	0.78	736.3	0.75	671.0	0.28	6.0	0.31	14.0
B N graph	5	7	0.258 +- 0.020	18	0.52	167.2	0.78	675.2	0.75	612.8	0.28	1.7	0.31	6.7
B N cubic	5	7	0.233 +- 0.011	34	0.52	664.8	0.78	2451.9	0.75	2235.4	0.28	21.5	0.31	48.9
B N hexag	5	7	0.275 +- 0.012	34	0.52	405.4	0.78	1754.8	0.75	1587.2	0.28	0.6	0.31	8.5
Total chi-square for 5 points						1982.7		7655.9		6963.0		45.7		116.0

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Quassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 8. Total chi-squares for the groups

Group	Data #	Model 1	Model 2	Model 3	Model 4	Model 5
mixtures	16	910.3	247.3	610.6	588.8	583.3
oxides	127	3005.6	5194.8	6265.4	1708.5	1642.8
halides	131	3897.6	6222.5	4129.7	1661.6	1653.0
sulphides	15	747.8	497.6	342.5	205.0	206.7
alloys	27	2340.5	2087.2	1891.1	369.0	338.9
nitrides	5	1982.7	7655.9	6963.0	45.7	116.0
All	321	12884.4	21905.3	20202.4	4578.6	4540.7

Models:

1.) Modified Z-law: 0.69*(Z1/Z2)**0.86
2.) Z**(1/3)-1 by Vasilyev et al.
3.) Daniel's model modified: Z**(1/3)*log(0.83*Z+0.69)
4.) SPP model: Omega-2 with Guassian cutoff (E0=0, E1=86 eV, E2=119 eV, Z0=15, q(Z)=Z**2)
5.) SPP model: Omega-2 with Gaussian cutoff (E0=0, E1=86 eV, E2=121 eV, Z0=15, q(Z)=Z**1.69)

Table 9. Effective Z-values calculated for SPP model with omega-2 and Gaussian cutoff

Z	Z1-eff	Z2-eff	Z	Z1-eff	Z2-eff	Z	Z1-eff	Z2-eff
1	0.98	0.98	32	14.93	15.04	63	18.63	18.77
2	1.86	1.86	33	14.61	14.74	64	18.76	18.90
3	2.15	2.15	34	14.26	14.39	65	19.98	20.11
4	2.25	2.25	35	13.85	13.99	66	20.69	20.81
5	2.96	2.96	36	13.47	13.61	67	21.43	21.55
6	3.89	3.89	37	12.52	12.66	68	22.20	22.30
7	4.79	4.79	38	11.78	11.92	69	22.99	23.09
8	5.64	5.64	39	11.59	11.71	70	23.81	23.91
9	6.43	6.43	40	11.70	11.80	71	24.19	24.28
10	7.14	7.14	41	12.24	12.32	72	24.53	24.61
11	7.00	7.00	42	12.73	12.80	73	24.74	24.83
12	6.46	6.46	43	13.35	13.41	74	24.85	24.96
13	5.68	5.68	44	14.00	14.06	75	24.75	24.89
14	5.24	5.24	45	14.68	14.75	76	24.52	24.68
15	5.34	5.34	46	15.61	15.68	77	25.10	25.26
16	6.68	6.74	47	16.01	16.09	78	24.23	24.43
17	7.12	7.16	48	16.32	16.40	79	23.73	23.96
18	7.84	7.86	49	16.43	16.53	80	22.58	22.83
19	8.50	8.52	50	16.44	16.56	81	21.24	21.50
20	9.10	9.13	51	16.42	16.55	82	20.05	20.32
21	9.83	9.87	52	16.34	16.47	83	19.07	19.31
22	10.54	10.58	53	16.25	16.39	84	18.40	18.62
23	11.21	11.26	54	16.15	16.30	85	17.98	18.17
24	12.16	12.21	55	15.50	15.66	86	17.80	17.97
25	12.47	12.54	56	14.90	15.06	87	17.28	17.44
26	13.06	13.14	57	14.65	14.81	88	16.86	17.02
27	13.65	13.73	58	15.77	15.93	89	16.70	16.86
28	14.20	14.29	59	16.27	16.42	90	16.64	16.81
29	15.23	15.31	60	16.81	16.96	91	17.49	17.65
30	15.32	15.42	61	17.40	17.55	92	17.95	18.11
31	15.19	15.29	62	18.01	18.16			

Parameters :

Z1-eff : E0=0, E1=86, E2=119, Z0=15, X=2
Z2-eff : E0=0, E1=86, E2=121, Z0=15, X=1.69