Mean Excitation Energy of the Elements for Proton Penetration in Matter

by
Rong-Fu Hsu
Department of Physics
National Taiwan Normal University

ABSTRACT

In this paper we propose a semiemperical model for the mean excitation energy, I, for all elements. By making use of the Monte Carlo technigue and the lowest (class 1) ionization potentials of the elements, we find that the mean excitation energy, I, can be expressed by $I_{z\pm1,s} = I_{z,s} + i_{z\pm1,s}$ where I is the lowest ionization potential and the subscripts Z and S are respectively refered to the atomic number and the periodic order of the element.

The I-values from our model are compared with those obtained from six other theoretical models as well as the average experimental values. It is found that our I-values are in good agreement with the experimental data for most elements and our model is over all much better than the others.

I. Introduction

The knowledge of the mean excitation energy (I-value) of an element is necessary for computing the stoppong power or the range of a charged particle in the given element. The energy deposited per unit absorber mass, i.e., the absorbed dose from charged particles, is proportional to the stopping power of the absorber. Also, the amount of energy deposited in an ionization chamber or shielding material depends upon stopping power. Data on the variation of stopping power or range with particle energy are often used to determine energies and masses in nuclear cross-section measurements. But to calculate the stopping power we have to know the mean excitation energy and the corresponding shell corrections of the absorber[1, 2, 3, 4].

Dalton and Turner[5] analyzied the nine key experiments before 1966 for the absolute stopping power, relative stopping power, and range of most elements and obtained the I-values with shell corrections. After 1967, many attempts have been made to construct sufficiently accurate theoretical I-value models as well as to obtain more precise experimental measurements. But there are still discrepencies between the theoretical estimates and the experimental measurements. Furthermore, so far there are no systematic I-values for all elements available both theoretically and experimentally. Therefore an analysis of the I-values from the recent experimental measurements and the different theoretical models seems to be useful. It will also be useful to search for a semiempirical model for I-values which might lead to a better understanding of the experimental results.

In section II, we briefly discuss the existing theoretical models for I-values. As a theoretical background we also review the stopping power formula in this section. The average experimental I-values obtained from analyzing the fourteen key experiments are given in section III. Based on the core electron theory for the interaction between the incident charged particles and atoms and by making use of the Monte Carlo technigue one can construct a semiempirical model for the mean excitaiton energy, I, for all elements. The details of this model is given in sectionIV. In section V we discuss in somewhat detail the comparism of our model with others.

II. Analysis of the Theoretical I-values

We start from a brief review of the stopping power formula. Then we summerize the existing theoretical I-value models. The details for obtaining the I-values from each model have been presented in the previous paper by the author[6]. The result is listed in Table 1.

A. Stopping Power Formula

The basic theoretical groundwork of the stopping power formula was laid down by Bohr[7] in 1913. But the first quantum mechanical solution was obtained by Bethe[8, 9, 10] using the Born approzimation. Bethe's theory expresses the energy loss per unit path length for a completely stripped heavy ion of atomic number z and velocity v as

$$-\frac{dE}{dS} = \frac{4\pi z^2 e^4}{mv^2} NZ \left[\ln \frac{2mv^2}{I(1-\beta)} - \beta^2 \right]. \qquad (1)$$

where m and e are the electron mass and charge, N is the number of atoms per unit volume, Z is the atomic number of stopping material and $\beta = v/c$, the velocity of the incident particle relative to the velocity of light.

If the velocity of the incident particles v is not large compared to the Bohr-orbit velocity of the atomic electrons v_e in the stopping material, Equation (1) predicts too high a value for the energy loss. The inner electrons in intermediate and high atomic number elements have velocities such that the condition $v \gg v_e$ cannot always be satisfied. Also, the requirement may not be met when low energy incident particles slow down in low Z materials. For these reasons shell correction terms are included in the stopping power formula.. Walske[11, 12] has suggested a theoretical corrections for electrons in the K- and L- shells, and Bichsel[13, 14] has extended the theory to include the M-shell. Sachs and Richardson[15] have proposed a theoretical correction to include all shells. Dixon[16] also used Bischsel and Walske's derivation to obtain the all shell corrections. By making use of the shell correction, equation (1) is then to be weitten as

$$-\frac{dE}{dS} = \frac{4\pi z^2 e^4}{mv^2} NZ \left[\ln \frac{2mv^2}{I(1-\beta^2)} - \beta^2 - \frac{\sum_i C_i}{Z} \right], \qquad (2)$$

where C_i is the shell correction of the i-th shell.

Due to polorization of the medium, the reduction in the energy loss of charged particles must also be considered. Sternheimer[17] summarized the theory and presented the results as a density effect, δ.

Hence, the total average energy loss by ionization per unit path length per density of the absorber medium is

$$-\frac{dE}{\rho dS} = \frac{4\pi^2 z^2 e^4}{mv^2} NZ \left[\ln \frac{2mv^2}{I(1-\beta^2)} - \beta^2 - \frac{\sum_i C_i}{Z} - \frac{\delta}{2} \right], \quad (3)$$

Below about 200 MeV, δ is negligible in comparison to the experimental errors. I-values may be obtained using equation (3) from experimental values of range or stopping power, provided the shell corections are known.

B. Theoretical I-value Models

The mean excitation potential, I, is defined in the stopping power equation to be the mean value of the energy transfer in a charged particle – atomic electron collision which produces and excitation event. All of the atomic electrons are considered to participate in the collision process. Fano[18] defined the mean excitation potential as

$$\mathrm{In}\ I = \Sigma_n f_n \ln E_n , \qquad (4)$$

where f_n and E_n are the dipole oscillator strength and the excitation energy of the transition from its ground state to the excited state n respectively. The summation is extended to the various virtual oscillators of strength f_n and excitation frequency $E_n/\hbar$. In principle I could be obtained from equation (4). However, the determination of I from this definition presents serious difficulties since the oscillator strengths are not generally well known in the desired energy range. Most elements have excitation energies (E_n) in the range 10 eV to 1000 eV, and in this range the oscillator strengths (f_n) are poorly known.

Bloch[19] made a generalization on the basis of the Thomas-Fermi statistical approach and showed that the mean excitation potential I of an atom should be proportional to the atomic number Z,

$$I = KZ.$$

Since the value of K was not specified, attempts have been made to evaluate K from the experimentally derived values of I for some known media. It is known that the values of K thus obtained differ for different media and that for media of low atomic numbers, these values are unexpectedly high. Further, in the absence of any definite trend in the variation of K with Z, it is difficult to make interpolations or extrapolations on the basis of the avaiable data to obtain the value of I for an unknown medium with any degee of certainty. Five different semiempirical equations models have been proposed before 1967:

1. Bloch[19] (1933)

$$I = KZ, \text{ where } K \text{ is about } 15 \text{ eV for low } Z \text{ absorbers,}$$

$$K \text{ is about } 10 \text{ eV for high } Z \text{ absorbers.}$$

2. Barkas and Berger[20] (1964), based on H, Be, Al.

$$\frac{I_{adj}}{Z} = 12 + \frac{7}{Z} \quad , \quad I_{adj} \leqslant 163 \text{ eV}$$

3. Sternheimer[17] (private communication to Barkas and Berger), based on Al, Cu, Pb.

$$\frac{I_{adj}}{Z} = 9.76 + 58.8/Z^{1.19} \quad , \quad I_{adj} > 163 \text{ eV}$$

4. Dixon[16] (1967), based on Al, Si, Fe, Pb.

$$\frac{I}{Z} = 9.81 + 35.5/Z$$

5. Dalton and Turner[5] (1967)

$$I = (10.2 \pm 2.07) + (11.8 \pm 0.55)\, Z, \text{ for } Z \leqslant 13$$

$$I = (56.1 \pm 8.76) + (8.61 \pm 0.37)\, Z, \text{ for } Z > 13$$

In 1968, Kamikawai, Watanabe, and Amemiya[21] used the variational method without integration over a frequency parameter to calculate the mean excitation energy I in two ways. The first one is the procedure involving a matrix diagonalization. In the case of small number of variational parameters, this method can easily be applied. The second one is the procedure by expressing I in terms of matrix power series. The matrices, which are independent of frequency parameter, can easily be calculated using a vector function. These methods, as well as the direct calculation, involving integration over ω, are applied to the hydrogen molecular. They obtain 18.2 eV for the I-values of the hydrogen molecular.

In 1969, Futrelle and McQuarrie[22] used linear programming method to calculate rigorous upper and lower bounds to quantum-mechanical properties and have illustrated it by calculating the upper and the lower bound to the mean excitation energy of hydrogen, helium, neon, argon and krypton. In this method the knowledge of certain oscillator strength sum rules were used. The sum rules themselves have been calculated in most cases in an approximate way so that inaccuracies in the sum rules will be reflected in their otherwise rigorous bounds. The bounds they obtained for I are:

H, $14.0 \leqslant I\,(\mathrm{eV}) \leqslant 15.2$ He, $14.1 \leqslant I\,(\mathrm{eV}) \leqslant 43.5$;
Ne, $90 \leqslant I\,(\mathrm{eV}) \leqslant 181$; Ar, $64 \leqslant I\,(\mathrm{eV}) \leqslant 295$;
Kr, $88 \leqslant I\,(\mathrm{eV}) \leqslant 476$.

In 1972, Bell, Bish, and Gill[23] used both the Hartree-Fock wavefunctions to evaluate atomic expection values and the reliability of the interpolation with separate atomic subshell contribution scheme to obtain the I value of He, Ne, Ar, Kr, Xe, and Rn. The calculated results are: Helium, 2.92 Rydberg; Neon, 8.97 Rydberg; Argon, 12.8 Rydberg; Krypton, 24.3 Rydberg; and Xeron, 33.1 Rydberg, where 1 Rydberg is equivalent to 13.59994 eV.

In 1972 Chu and Powers[24] used Lindhard and Scharff's[25] theory with a Hartree-Fock-Slater[26] charge distribution to calculate the I-value in the stopping power. The calculation were based on:

(1) it is at the high-velocity limit and therefore the I value is independent of velocity.

(2) the Hartree-Fock-Slater wave functions for an isolated atom, instead of the wave functions for the valence electrons in metals are used, and the effect of

chemical binding on valence electrons in diatomic molecules is neglected. The calculated I values for all elements are listed on Table 1.

In 1974 Mukherji[27] calculated the I value of an element of atomic number Z on the basis that the velocity distribution among the orbital electrons of an atom is given by $n(u_s) = f(Z)\, u_s/v_o$, where $n(u_s)$ is the number of obital electrons with velocity less than u_s, v_o is given by $e^2\hbar^{-1}$, and f((Z) assumes the values $0.28Z^{2/3}$ for $Z \leqslant 45.5$ and $Z^{1/3}$ for $Z \geqslant 45.5$. The calculated values for the case of elements with $Z<13$ are in fair agreement with the corresponding experimental values of the mean excitation energies, but for the heavier elements these are appreciably lower than the experimental values. The model may be described by

$$\ln I = \frac{Z-2}{Z} \ln \left[\left(\frac{Z-2}{2.717\, f(Z)} \right)^2 \text{x}\ 13.6 \right] + \frac{2}{Z} \ln (13.6 Z^2),$$

Where $f(Z) = Z^{1/3}$ for $Z \geqslant 45.5$

$f(Z) = 0.28\, Z^{2/3}$ for $Z \leqslant 45.5$

In 1975 Dehmer, Inokuti, and Saxon[28] used the stopping power depending on the moment, of the dipole oscillator-strength distribution to calculate a comprehensive set of partial dipole oscillator strengths and the related moments for the atoms of the first two rows of the periodic table. They derived the moments $S(\mu)$ and $L(\mu) = d\, S(\mu)/\,\mu$ for $-6 \leqslant \mu \leqslant 1$ from the comprehensive Hartree-Slater oscillator distributions for He through Ar. The stopping power depends on L (0) for fast charged particles and therefore the mean excitation energy I can be defined by

$$\ln \left(\frac{I}{R} \right) = \frac{L(0)}{S(0)} = \frac{L(0)}{Z}$$

The I-values for Z=2 through Z=18 obtained by these authors are listed in Table 1.

Crawford[29] used the latest form of the "straight-ahead" stopping power equation as part of a Monte Carlo Nucleon transport program without shell corrections to evaluate the I-value. The "straight-ahead" model assumption that the path of the particle is the shortest distance from entrance to exit in a medium can be corrected in a number of ways. By making use of the Monte Carlo technique Crawford included the multiple scattering correction in his calculations. The result are also listed in Table 1.

The theoretical I-value models discussed above are based on different physical assumptions. These include theoretical oscillator strength distribution (OSD)[22], semiempirical OSD[23], moment theory[28], variation-perturbation theory[21], and local plasma model of Lindhard and Scharff[24]. None of the models considered here represents a comprehensive model for determining the I-value for all elements. A further development in theoretical study is required. Before a better theoretical model is available, it seems to be useful to search for a semiempirical model for I-values which might lead to a better understanting of the experimental results.

III. Analysis of the Experimental I-values

The experiments which yield the information about the mean excitation energy can be classified according to the parameter measured: stopping power relative to a reference absorber, absolute stoppimg power. or range. Thus, what we need to do before analyzing the experimental I-valuesis is to normalize the initial data of different experiments to the same scale or to the same stopping materials. We first introduce the formula relating the relative stopping power, absolute stopping power and range. Then the fourteen key experiments can be analyzied to obtain the I-values based on the same scale. The details of the alanyzing procedure has been presented in the previous paper by the author[6]. The results of the analyzied experimental I-values are listed in Table 2.

A. Description of the Original Experimental Data

1. Measurements of Relative Stopping Power

Equation (2) for the stopping power formular can be rewritten

$$S_D = -\left[\frac{dE}{dS} \right]_D$$

$$= \left(\frac{0.30708}{\beta^2} \right) Z^2 \left(\frac{Z}{A} \right)_D$$

$$\left[f(\beta) - \ln I_D - \left(\sum_i \frac{C_i}{Z} \right)_D \right]. \qquad (5)$$

The subscripts "D" is referred to the standard absorber, and β^2 and $f(\beta)$ can be find in Table 8d-1 of the American Institute of Physics Handbook^{30} (The Third Edition) 1972. The ratio of the thickness of a test absorber to that of the reference absorber for the same incident particle at a given energy with the same energy loss is defined as the relative stopping power. The stopping power of the test absorber is given by equation (5) with the subscript "D" replaced by "R", and the relative stopping power, S, is therefore given by

$$S = \frac{S_R}{S_D} = \frac{(-dE/dS)_R}{(-dE/dS)_D}$$

$$= \frac{Z_R A_D}{Z_D A_R} \left[\frac{f(\beta^2) - \ln I_R - (\sum_i C_i / Z)_R}{f(\beta^2) - \ln I_D - (\sum_i C_i / Z)_D} \right], \qquad (6)$$

where s is measured quantity.

The mean excitation potential, I_R, can be calculated from equation (6) if the shell corrections, $\sum_i C_i/Z$, are known for both the reference (standard) and the test elements. Also I_D must be known for the standard absorber.

2. Measurements of Absolute Stopping Power

The absolute stopping power of an absorber is obtained by a direct determination of the energy lost by charged particles in the absorber. The mean excitation potential, I, of the absorbing material can be calculated from the absolute stopping power directly by using equation (5).

3. Measurements of Range

The range of monoenergetic heavy particles with kinetic energy E is well defined only when the particle losses energy without scattering. The quantity related to range R(E) which can be calculated from stopping power theory is the theoretical mean range R_t (E) in the continuous slowing-down approximation CSDA:

$$R_t (E) = \int_0^E \frac{1}{(-dE/dS)} dE \qquad (7)$$

A small difference between R(E) and R_t(E) is caused by the use of CSDA approximation. Because the stopping power formula does not hold at very low particle velocities, equation (5) cannot be used directly to calculate the mean excitation potential values. This CSDA range equation must be rewritten as

$$R = R_0 (E_0) + \int_{E_0}^{E} \frac{1}{(-dE/dS)} dE, \qquad (8)$$

Where R_o (E_o) is the measured range of particles with some low energy E_o.

The straight ahead model or linear method of determining I from a range measurement is to estimate the probable I-value of the absorber and then to numerically intergrates the reciprocal of the stopping power formula over the energy interval E_o to E. A measured value of R_o (E_o) is added to the result of the numerical integration to obtain the total tange R. The value of I is adjusted until it matches the experimentally measured range.

The determination of the relative stopping power involves the measurements of the energy losses in terms of the path lengths of an ionizing particle in a test absorber and a reference absorber. The reference absorber used in measuring relative stopping powers is made of either aluminum or copper. Thus it is necessary to know the I-value and the correct shell corrections for aluminum or copper. In some cases, improved shell correction values permit the reanalysis of an experiment. Thus the recalculated I-values reported in Table 2 takes into account both a normalization of the relative stopping power measurements to I = 163 eV for aluminum or I = 314 eV for copper and the effect of the new shell corrections. The average experimental I-values based on the work of many investigators can then be analyzied.

B. Analysis of Experiments

Before 1967, nine selected key experiments had been analyzied for calculating I-value by Dalton and Turner[5]. Since 1968, fourteen key experiments are essential in deciding the experimental I-value, which are: Crawford[29,31]; Burkig and Mackenzie[32]; Ishiwari, Shiomi, Shirai, and Vemura[33,34]; Andersen, Simonsen, Sorensen, and Vajda[35,36,37]; Swint Prior, and Ramirez[38]; Derrick, Fields, Hyman, Keyes, Fetkovich, Mckenzie, and Wang[39]. The analysis of these key experimental I-values based on the Range and Stopping-Power Table by Barkas & Berger[40] was carried out by the before[6]. The result of the average experimental I-values and the experimental errors for all elements are given in Table 2.

IV. Evaluation of the Mean Excitation Energy for all Elements

A. Semiempirical Model

The ionization potential is defined as the work (expressed in electron volts) required to remove a given electron from its atomic orbit and place it at rest at an infinite distance. The mean excitation parameter, I, is defined to be the mean value of the minimum energy transfer in a proton-atomic electron collision which porduces an ionization event. All of the atomic electrons are considered to participate in the collision process. According to Mukherji's theory[27], if one neglects the minor coupling effect between the electronic bindings, one may attribute the oscillators to the transition probabilities of the individual atomic electrons. Further, since the total oscillator strength for each electron is close to unity for the most significant transitions of the closed shell electrons, one may identify the mean excitation energy I with the mean ionization potential in the first approximation. Keeping this idea in mind, one may consider that, as far as the I-value is concerned, for two adjacent elements in the same period only the lowest ionization potentials are different. This is due to the fact that they have the same core electrons.

Based on this core electron theory, one can find a semiempirical model to evaluate the I-values for all elements rather than merely find a mathematical equation which fits the analyzied experimental I-values obtained in section III. Assume that the lowest ionization potential is of the magnituide of the difference of the mean excitation energy between two adjacent elements. Then the proposed semiempirical formula can be used to determine the correct I-value by making use of both tht Monte Carlo calculation technique for calculating the I-value for one of the elements in each period and the lowest (Class 1) ionization potential reported in the Handbook of Chemistry and Physics[41]. The expression for the semiempirical model is then

$$I_{z\pm1,s} = I_{z,s} \pm i_{z\pm1,s}, \qquad (9)$$

where I is the mean excitation energy and i is the lowest ionization potential, and the subscripts Z and S refers to the atomic number, the order of the period of the element respectively. For example, for the first period elements, $S = 1$, $1 \leqslant Z \leqslant 2$; for the second period elements, $S = 2$, $3 \leqslant Z \leqslant 8$, etc. For the maximum period $S = 8$, and $99 \leqslant Z \leqslant 104$ (the maximum Z is 104, so far).

For the hydrogen atom, only one electron can be involved in a collision. The lowest ionization potential value of 13.60 eV and the x-ray K edge ionization potential of 14 eV are in close agreement. Thus the mean ionization potential is really one electron and should be the same with I = 13.6 eV.

Helium with two electrons has a lowest ionization potential of 24.48 eV and an x-ray K edge ionization potential of 25 eV. Using the semiempirical model, (9), we obtain I = 38.08 eV for helium. Both electrons would be involved in the nucleon - electron collision process. The Class 2 ionization potential of helium is

54.40 eV. The sum of the two ionization potential is 78.88 eV. If the mean value, I, involves both with equal weight then I would be equal to ½ (24.48 + 54.40) = 39.44 eV. The experimental values of 15.7 ± 0.6 for H and 43.0 ± 0.6 eV for He are listed on Table 2, as compared to those of 13.60 and 38.08 for our model.

The problem becomes more complicated in stepping form the first period to the second period. To compute the I-values for the second period, we first choose carbon as the key element. From eq. (2) with the value for the stopping power obtained by Crawford etal[42], we obtain I = 72.34 eV for carbon. The I-values for the rest of the elements in the second period are obtained by adding in turn the lowest ioniztion potential of each element.

As explained before, in our model we assume that within a given period the Class 1 ionization potential represents the difference in the mean excitation potential, I, between any two adjacent elements and that the correct value for I is known for at least one element in the period. Thus we choose aluminum as the key element for the third period. Its I-value can also be obtained from eq. (2) and we have $I_{Al} = 163.0$ eV With the I-value for Al we can then compute the I-values for the rest of the elements in this period according to the semimpirical formula (9). Similarily, the I-values for the fouth period are obtained by choosing Cu as the key element with $I_{Cu} = 313.97$ eV. The results are listed in Table 3. Note that in our computation we neglect the density correction, since the proton energy is lower than 200 MeV. Therefore we use eq. (2) instead of eq. (3).

B. Calculation Procedure

The stopping power for incident protons in the energy range from 8 to 186 MeV of seven elements had been remeasured by Crawford's group 1977. The I-values of these seven elements are then computed by using the new Monte Carlo Approach PROTOS III computer program with shell corrections. The details of the computer program was given in "Joint Meeting, Texas Section of The American Association of Physics Teachers" by Crawford and the author[43]. The calculated I-values of these seven elements are: Be-53.34 eV, C-72.34 eV, Al-163.0 eV, Si-172.3 eV, Fe-300.9 eV, Cu-313.97 eV, and Pb-743.95 eV.

With the aid of CDC computer in Chung-San Technology in Science, the I-values for all elements can be obtained from eq. (9). The results of this calculation are listed in Table 3.

C. Results

1. Individual Corrected I-values:

Figure 1 shows that the mean excitation energy, I, plotted against the atomic number, Z. The noted "*" mark represents the I–value obtained from the model proposed in this paper. The average experimental I values and the I-values from different theoretical models are also shown in Fiqure 1 for comparison. The I-values obtained from our model are also listed in Table 3.

From Figure 1 we see that the I-values obtained from our semiempirical model fit the experimental average I-values very well except $19 \leqslant Z \leqslant 27$.

2. Suggested I/Z Average Value:

Figure 2 shows I/Z plotted against Z, and we see that I/Z values fit the experimental data very well except $19 \leqslant Z \leqslant 27$. The discrepancy may be caused by such as Fano[18] stated that the interpolation should be dependable to a few per cent of the value of I in this region or by the well known fact of specially strong magnetic dipole moment in 3d-shell effect. It may also be improved in the 4-th period simply by changing the key element.

V. Conclusions

An examination of Figure 1 shows that the new calculated values of I are generally in better agreement with experimental averaged I-values than the other theoretical I-value models, except in the case of $19 \leqslant Z \leqslant 27$. In the case of the lighter elements, the calculated I-values are also in fair agreement with the corresponding values by Mukherji[27]. For the heavier elements, the calculated I-values appear to be rather in excellent agreement with the experimental I-values.

In view of the fact that our I-values are rather in good agreement with the so far available experimental data, the predicted I-values for those elements without experimental data seems to be reliable. Therefore our model might be useful in constructing a better theoretical description for the proton penetration phenomienon.

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TABLE 1

Values of I (in eV) Calculated from Theoretical Model

First Period

Element	Chu &[23] Powers	Kamikawai,[26] Watmanabe & Amemiya	Dehmer,[27] Inokuti & Saxon	Futrelle &[21] Mcquarrie	Bell,[22] Besh & Gill	Crawford[28] Model	Average Experimental Value
1 H atomic				14.0⩽I⩽15.2		13.6	15.6±0.6
1 H molecular		18.2					18.5±0.3
2 He	49.08±0.5		38.82±2.0	41.1⩽I⩽43.5	39.7±0.8	38.1	43.0±0.6

TABLE 1 – Continued

Second Period

Element	Chu &[23] Powers	Mukherji[26]	Dehmer,[27] Inokuti & Saxon	Bell,[22] Bish & Gill	Crawford[28] Model	Average Experimental Value
3 Li	38.85±0.4	43.32	34.02±1.7		45.7	37.4±0.7
4 Be	45.72±0.5	56.75	38.62±1.9		55.0	61.1±0.9
5 B	56.85±0.6		49.00±2.5		63.2	
6 C	72.24±0.7	83.49	62.01±3.1		74.8	79.1±1.0
7 N	90.65±0.9	95.45	76.91±3.8		89.3	89.3±2.0
8 O	111.60±1.1	106.5	93.50±4.7		102.9	101.5±2.3
9 F	135.09±1.4		111.8± 5.6		120.3	
10 Ne	160.09±1.6	126.5	131.3± 6.6	122.0±2.4	141.9	126.8±2.1

TABLE 1 – Continued

Third Period

Element	Chu &[23] powers	mukherji[26]	Dehmer[27] Inokuti & sacon	Bell,[22] Bish & Gill	Crawford[28] Model	Average Experimental Value
11 Na	148.61±1.5		123.6±6.2		149.4	
12 Mg	149.40±1.5				157.0	
13 Al	150.93±1.5	152.4	124.3±6.2		163.0	163.4±1.7
14 Si	158.34±1.6	160.3	131.5±6.6		171.2	172.3±2.7
15 P	168.45±1.7				181.6	
16 S	180.16±1.8				192.0	
17 Cl	193.46±1.9		164.0±8.2		205.0	176±3.5
18 Ar	207.90±2.1	189.0	177.4±8.9	174.1±3.5	220.8	198±3.3

TABLE 1 – Continued

Fourth Period

Element	Chu &[23] Powers	Mukherji[26]	Bell,[22] Bish & Gill	Crawford[28] Model	Average Experimental Value
19 K	197.22±2.0			242.5	
20 Ca	196.00±2.0			248.6	188.3±2.6
21 Sc	207.48±2.1			255.2	205.2±0.6
22 Ti	221.10±2.2			262.0	225.5±2.6
23 V	235.52±2.4			268.7	240.5±3.5
24 Cr	260.64±2.6			275.5	244.2±0.7
25 Mn	266.75±2.7			282.9	258.5±0.8
26 Fe	283.04±2.8	238.3		290.8	282.9±2.9
27 Co	301.32±3.0			298.6	285.7±3.3
28 Ni	319.48±3.2			306.3	302.6±3.1
29 Cu	350.61±3.5	255.0		314.0	317.2±3.3
30 Zn	358.20±3.6			323.4	316.5±4.5
31 Ga	359.29±3.6			329.4	
32 Ge	365.44±3.7			337.2	
33 As	373.56±3.7			347.1	
34 Se	382.84±3.8			356.8	
35 Br	393.40±3.9			368.6	
36 Kr	404.28±4.0		330.5±66	382.6	362.6±3.3

TABLE 1 – Continued

Fifth Period

Element	Chu &[23] Powers	Mukherji[26]	Bell,[22] Bish & Gill	Crawford[28] Model	Average Experimental Value
37 Rb	391.83±3.9			392.0	
38 Sr	388.36±3.9			396.2	
39 Y	395.07±4.0			401.0	
40 Zr	404.00±4.0			408.3	373.4±1.1
41 Nb	421.89±4.2			415.2	406.2±7.9
42 Mo	433.02±4.3			422.0	420.4±6.0
43 Tc	436.45±4.4			429.3	
44 Ru	458.04±4.6			436.6	
45 Rh	471.60±4.7			444.1	436.1±8.5
46 Pd	497.72±5.0			452.4	454.4±8.9
47 Ag	500.08±5.0	349.3		460.0	475.3±3.9
48 Cd	503.52±12.6			469.0	460.5±9.0
49 In	502.25±12.6			474.8	478.4±9.3
50 Sn	505.50±12.6	377.2		482.1	496.7±5.9
51 Sb	510.00±12.8			490.8	
52 Te	519.48±13.0			499.8	
53 I	523.11±13.1			510.2	
54 Xe	530.28±13.3		450.1±9.0	522.4	517.5±6.2

TABLE 1 – Continued

Sixth Period

Element	Chu &[23] Powers	Mukherji[26]	Crawford[28] Model	Average Experimental Value
72 Hf	743.04±18.6		707	
73 Ta	752.63±18.8		715	686.4±7.8
74 W	762.20±19.1	618.9	726	706.3±8.9
75 Re	773.25±19.3		734	
76 Os	784.32±19.6		742	
77 Ir	796.18±19.9		751	706.2±13.8
78 Pt	317.44±20.4		760	736.1±8.6
79 Au	830.29±20.8	673.0	769	769.4±7.8
80 Hg	832.00±27.5		779	
81 Ti	829.44±27.4		786	
82 Pb	838.86±27.7	705.7	793	798.2±9.7
83 Bi	834.15±27.5		800	
84 Po	838.32±27.7		808	
85 At	844.05±27.9		818	
86 Rn	849.68±28.0		829	

TABLE 2

Average value of I (in eV) Obtained from Experimental Data

First Period

Element	Barkas[18] & Berger	Bakker & Segre	Brolley & Robe	Thompson	Zrelov & Stoletov	Derrick[39]	Average	Average Error in Average Value
1 H_2 moluclar	18.7±0.1		20.0	21.9	13.6		18.8	±0.1
1 H-saturated		17.5		18.6			18.1	±0.5
1 H-unsaturated				15.7			15.7	±0.6
2 He	42.0±0.2		44.3±0.9			42.7±0.6 *	43.0	±0.6

TABLE 2 – Continued

Second Period

Element	Barkas[18] & Berger	Dalton[19] & Turner	Crawford[28]	Barkig &[31] Mackenzie	Swint[38]	Average	Average Error in Average Value
3 Li		37.4±0.7				37.4	±0.7
4 Be	60.0±0.3	61.7±1.2	53.34	66.8±1.3		61.1	±0.9
6 C	78.0±0.4	81.2±1.6	72.14		88.5	79.1	±1.0
7 N	131±0.7	89.6±1.8			88.5±2.2	89.3	±2.0
8 O		101±2.0			103.4±2.6	101.5	±2.3
10 Ne		132±2.6			117.3±2.9	126.8	±2.1

Table 2 – Continued

Third Period

Element	Barkas[18] & Berger	Dalton &[19] Turner	Crawford[28]	Burkin &[31] Mackenzie	Ishiwari[33]	Andersen[35]	Swint[38]	Average	Average Error in Average Value
13 Al	163.0±0.8	163±3.3	163.0	163±3.1	166±0.6	162.4±0.6		163.4	±1.7
14 Si			172.3					172.3	±2.7
17 Cl		176±3.5						176	±3.5
18 Ar	210.0±1.1	189±3.8					195.1±4.9	198.0	±3.3

TABLE 2 – Continued

Fourth Period

Element	Barkas & Berger[18]	Dalton & Turner[19]	Crawford[28]	Burkig & Mackenzie[31]	Ishiwari[33]	Andersen[35]	Swint[38]	Average	Average Error in Average Value
20 Ca		187±3.7		192.1±3.6		185.8±0.6		188.3	±2.6
21 Sc						205.2±0.6		205.2	±0.6
22 Ti		224±4.5		227.8±4.3	233±0.9	217.0±o.7		225.5	±2.6
23 V		250±5.0		244.9±4.7		226.5±0.7		240.5	±3.5
24 Cr						244.2±0.7		244.2	±0.7
25 Mn						258.5±0.8		258.5	±0.8
26 Fe	273.0±1.4	277±5.5	300.9	291 ±5.5	280±1.1	275.4±0.8		279	±2.9
27 Co		290±5.8				281.4±0.8		286	±3.3
28 Ni	304.0±1.5	312±6.2		310 ±5.9	299±1.2	288.0±0.9		306	±3.1
29 Cu	314.0±1.5	316±6.3	313.8	319 ±6.1	323±1.3	317.1±0.9		316	±3.3
30 Zn		319±6.4		323 ±6.1		307.1±0.9		321	±4.5
36 Kr	381.0±1.9	350±7.0					356.7±0.9	362.6	±3.3

TABLE 2 –Continued

Fifth Period

Element	Barkas[18] & Berger	Dalton &[19] Turner	Burkig &[31] Mackenzie	Ishiwari[33]	Andersen[35]	Average	Average Error in Average Value
40 Zr					373.4±1.1	373.4	±1.1
41 Nb		407±8.1	405±7.7			406.2	±7.9
42 Mo		422±8.4	414±7.9	425±1.7		420.4	±6.0
45 Rh		440±8.8	432±8.2			436.1	±8.5
46 Pd		456±9.1	453±8.6			454.4	±8.9
47 Ag	487.0±2.4	466±9.3		462±1.8	496.4±2.0	475.3	±3.9
48 Cd		462±9.2	459±8.7			460.5	±9.0
49 In		481±9.6	476±9.0			478.4	±9.3
50 Sn	516.0±2.6	486±9.7	477±9.1	507±2.0		496.7	±5.9
54 Xe	555.0±2.8	480±9.6				517.5	±6.2

TABLE 2 – Cotinued

Sixth Period

Element	Barkas[18] & Berger	Dalton[19] & Turner	Crawford[28]	Burkig[31] & Muckenzie	Ishiwari[33]	Andersen[35]	Average	Average Error in Average Value
64 Gd						577.6±3.5	577.6	±3.5
73 Ta		692±13.8		645±12.3	713±2.9	695.4±2.1	686.4	± 7.8
74 W	748.0±3.7	704±14.1		667±12.7			706.3	±10.1
77 Ir		730±14.6		682±13.0			706.2	±13.8
78 Pt	787.0±3.9	711±14.2		699±13.3	748±3.0		736.1	± 8.6
79 Au	797.0±4.0	760±15.2		721±13.7	739±3.2	775.9±3.1	769.4	± 7.8
82 Pb	826.0±4.1	767±15.3	840	771±14.7		787 ±4.7	798.2	± 9.7
90 Th		698±14.0		704±13.4			701	±13.7
92 U	923.0±4.6	856±17.2				846 ±6.8	875	± 9.5

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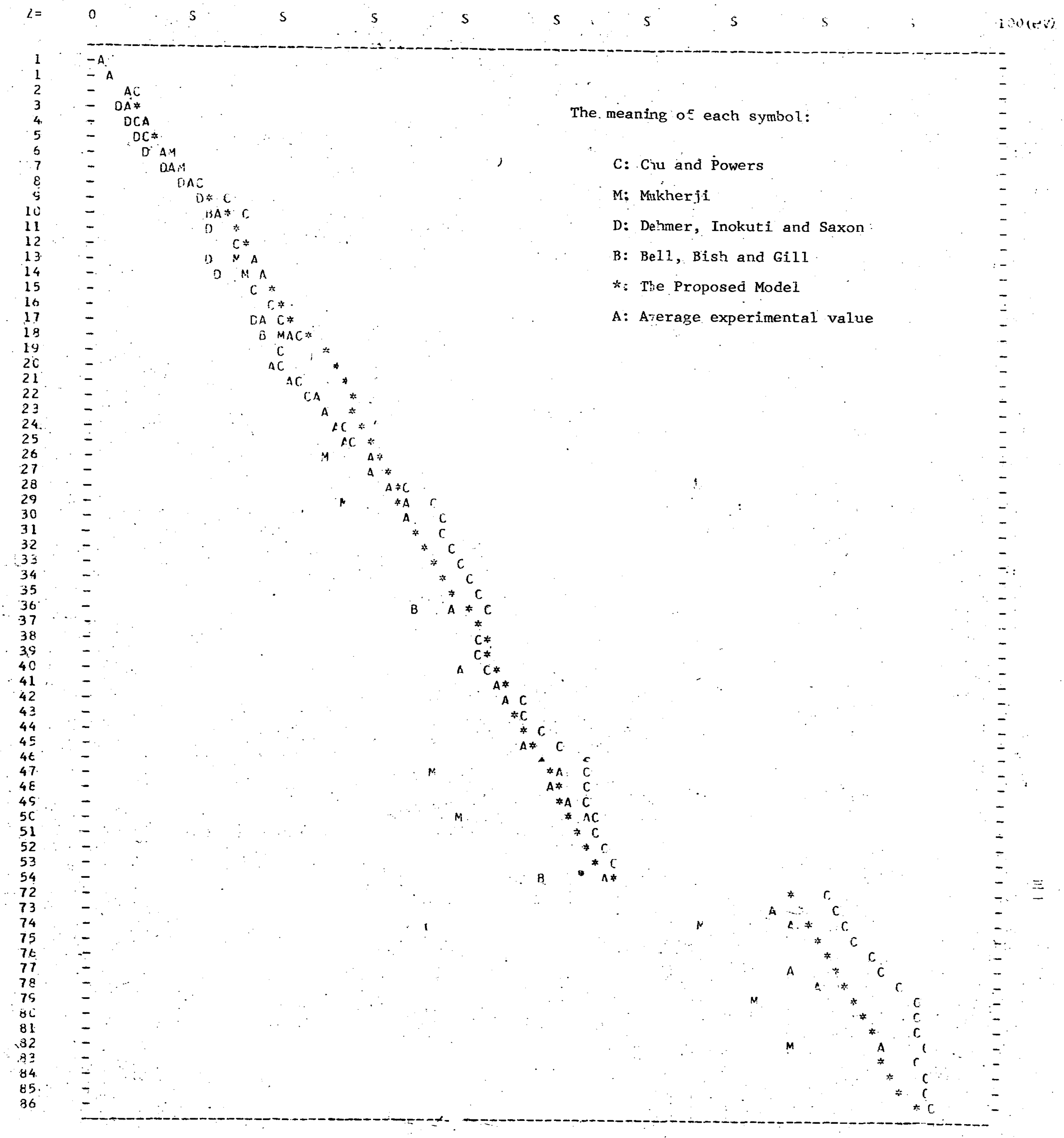
由質子撞擊物質之資料，評估各原素之平均激發能

Fig. 1 FIGURE OF I BY Z.

NINE OF VALUE (I) REPRESENTED BY ONE SCALE



The meaning of each symbol:

C: Chu and Powers

M: Mukherji

D: Dehmer, Inokuti and Saxon

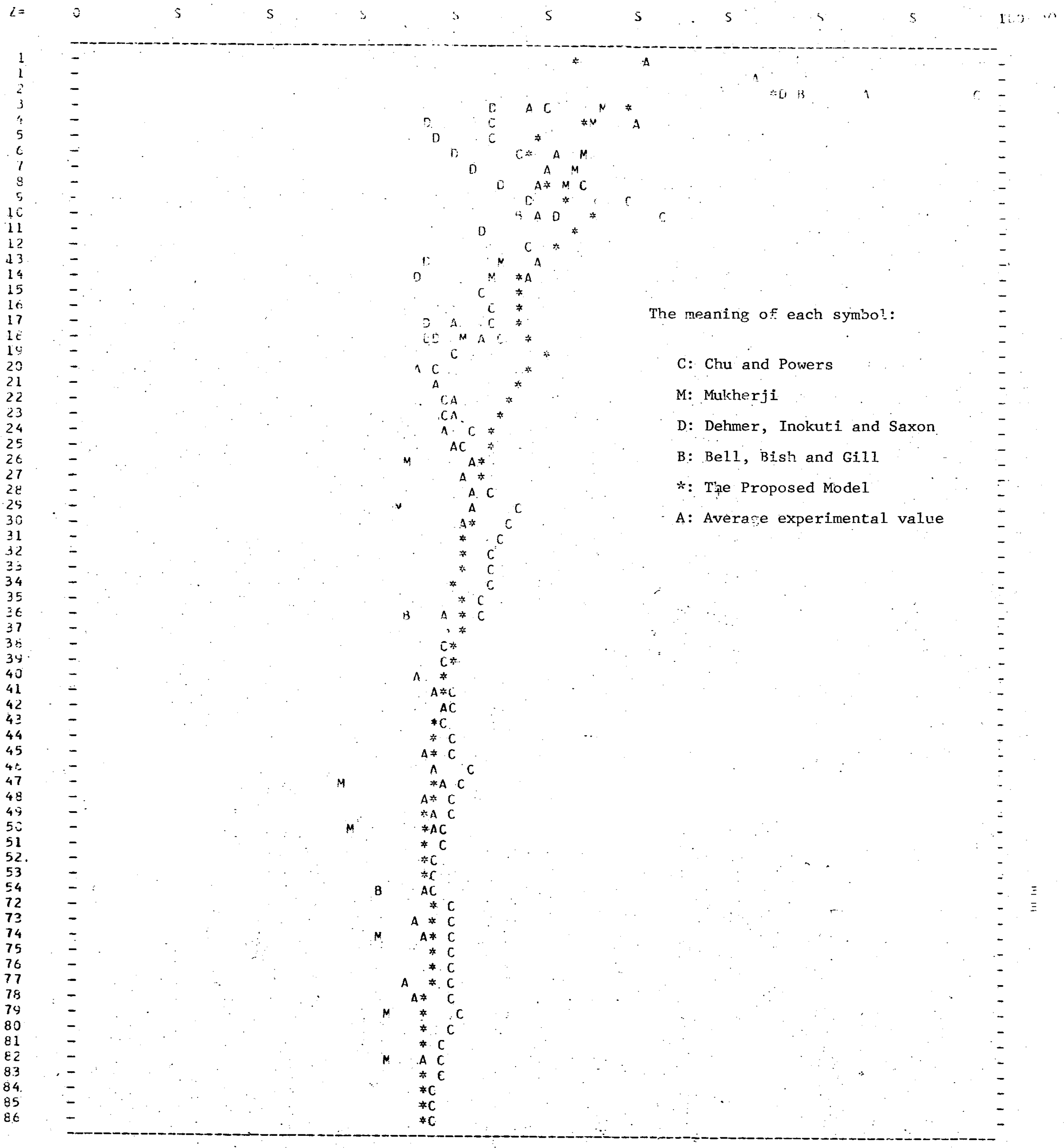
B: Bell, Bish and Gill

*: The Proposed Model

A: Average experimental value

Fig.2 FIGURE OF I/Z BY Z

ONE OF VALUE (I/Z) REPRESENTED BY FOUR SCALES



中文摘要

由質子撞擊物質之資料評估各元素之平均激發能

（物理系　許榮富）

本論文旨在提供一半經驗理論模式以評估各元素之平均激發能數值，此模式之計算式是得自運用蒙特卡羅近似值計算技巧及各元素之最低游離能，可以簡化成右式表示之：$I_{Z\pm1,S}=I_{Z,S}\pm i_{Z\pm1,S}$，此處 I 係指元素之平均激發能，i 係指該元素之最低游離能，Z 及 S 分別表示該元素於週期表上之原子序及週期位序。

本文所評估之元素平均激發能數值亦分別與得自分析其他六大派理論家所提理論值及另十四實驗家所得之實驗平均值作一比較，結果發現：本文所評估之數值，於極大多數之元素中，均較其他理論值更能與實驗平均值吻合。另一方面，本文亦同時對一些其他理論模式及實驗均未曾作過之元素的平均激發能作一預估。