ISSN 0915-6364

NATIONAL INSTITUTE FOR FUSION SCIENCE

The Screening Length of Interatomic Potential in Atomic Collisions

Y. Yamamura, W. Takeuchi and T. Kawamura

(Received - Dec. 10, 1997)

NIFS-DATA-45 Mar. 1998

RESEARCH REPORT
NIFS-DATA Series

NAGOYA, JAPAN

The Screening Length of Interatomic Potential in Atomic Collisions

Y. Yamamura[a)], W. Takeuchi[a)] and T. Kawamura

National Institute for Fusion Science, Toki 509-52, Gihu, Japan

Abstract

In computer studies on the interaction of charged particle with solids, many authors treat the nuclear collision by the Thomas-Fermi screened Coulomb potential. For better agreement with experiment, the screening length is modified sometimes.We investigate the theoretical background for the correction factor of the screening length in the interatomic potential which can bededuced from two steps. The first step is to select the correction factor of an isolated atom so as to match the average radius of the Thomas-Fermi electron distribution with that of the Hartree-Fock electron distribution, where we use the Clementi and Roetti's table. The second step is to determine the correction factor of the screening length of the interatomic potential by using a combination rule. The correction factors obtained for the screening length are in good agreement with those determined by the computer analysis of the Impact Collision Ion Scattering Spectroscopy (ICISS) data.

Key words: interatomic potential, screening length, shell correction, Thomas-Fermi electron distribution, Hartree-Fock electron distribution

Permanent address:

[a)] Okayama University of Science, Ridai-cho, Okayama 700, Japan

1. Introduction

The interatomic potential is one of the most important quantities in the theory of interaction of charged particles with solids. There are a large number of works about this problem. In many applications involving the use of interatomic potentials in physics and material science it is not necessary to know the precise form of the force between the interacting particles. Many authors proposed empirical atomic interactions which provide mathematically tractable, analytical expression for the pairwise interaction between two atoms and ions.

In computer simulation of the interaction of charged particle with solids, many authors treat the nuclear collision by the Thomas-Fermi screened Coulomb potential by adjusting the screening length to experiment. It is very surprising that there is no clear theoretical background for the correction of the screening length. Recent development of computer simulation ask a more precise treatment of nuclear collisions, using a well-established analytical interatomic potential, and the light ion scattering is asked to be treated reasonably within the same framework.

There are two approaches for an analytical model of the interatomic potential. The first approach is based on the Thomas-Fermi (TF) statistical model for an isolated atom. The TF screened Coulomb potential of an isolated atom of the atomic number Z is given as

$$V(r) = \frac{Ze}{r}\phi(r/a_{TF}) \quad , \tag{1}$$

where the a_{TF}, the TF screening length, is given by

$$a_{TF} = 0.4685\, Z^{-1/3} \quad (\text{Å}), \tag{2}$$

and the screening function $\phi(x)$ is the solution of the dimensionless TF equation

$$x^{1/2}\frac{d^2\phi(x)}{dx^2} = \phi(x)^{3/2} \quad . \tag{3}$$

The earliest extension to an interatomic potential between two atoms of atomic numbers Z_1 and Z_2 was considered by Firsov [1,2]. Firsov applied the first-order perturbation theory, assuming that the

electron distribution will be distored so that the total energy of two atoms is a minimum for any patricular separetion, and finally suggested that the interatomic potential would be best describe using reduced distance by a screening length of the form [2]

$$a_F = \frac{0.4685}{(Z_1^{1/2} + Z_2^{1/2})^{2/3}} \text{ (Å)} \quad . \tag{4}$$

Lindhard [3] also suggested using the atomic TF screening function for the interatomic screening function with a screening length of the form

$$a_L = \frac{0.4685}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \text{ (Å)} \quad . \tag{5}$$

The screening length presented by eqs. (4) and (5) do not differ significantly from each other.

A large number of approximate analytical solutions of eq. (3) have been proposed. Perhaps the earliest and well-known of these is the Sommerfeld asymptotic form [4]:

$$\phi(x)_{Som} = \{1 + (x/144^{1/3})^{\lambda}\}^{-c} \quad , \tag{6}$$

where $c\lambda = 3$. By fitting this equation for large x, Sommerfeld arrived at the value $\lambda = 0.772$. In later work March normalized the radial momentum function using the Sommerfeld approximation and modified the value of λ to 0.8034 [5]. A number of workers have proposed analytical solutions involving exponentials or combinations of powers and exponentials. Moliére gave an approximation in the form of three exponentials [7]:

$$\phi(x)_{Mol} = 0.35e^{-0.3x} + 0.55e^{-1.2x} + 0.10e^{-6.0x} \quad . \tag{7}$$

The second approach is to find the interatomic potential by calculating numerically the two-center TF problem, where the interatomic potential is defined by the difference between the total energy of the two atom system and the sum of the energies of two isolated atoms. In an attempt to find an analytic

function which accurately predicts the interatomic potential between atoms, Wilson et al. proposed the so-called "Kr-C" or "Kr-Si" potentials, using the Hartree-Fock (HF) atomic state wave functions [7]. The Kr-C potential is often used and it has the form

$$\phi(x)_{KrC} = 0.1909451e^{-0.278544x} + 0.473674e^{-0.63717x} + 0.335381e^{-1.919249x}, \quad (8)$$

where the reduced length is given by $x = r/a_F$.

Extending the work of Wilson et al, Ziegler, Biersack and Littmark (ZBL) performed detailed calculations of solid-state interatomic potential for 261 atom pairs and arrived at the following universal screening function [8]:

$$\phi(x)_{ZBL} = 0.028171e^{-0.20162x} + 0.28022e^{-0.4029x} + 0.50986e^{-0.94229x} + 0.18175e^{-3.1998x}, \quad (9)$$

where the reduced distance is given by $x = r/a_{ZBL}$ with the definition of

$$a_{ZBL} = \frac{0.4685}{(Z_1^{0.23} + Z_2^{0.23})} \text{ (Å)} . \quad (10)$$

Nakagawa and Yamamura [9] used the relativistic electron densities of Carlson et al. [10] in a statistical local-density calculation of the interactions of many pairs of atoms similar to ZBL, where the atoms were confined to Wigner-Seitz cells representing the densities of the approximate solids. They proposed the averaged modified Lenz-Jensen (AMLJ) potential of the form

$$\phi(r)_{AMLJ} = \exp(-\alpha_1 r + \alpha_2 r^{3/2} - \alpha_3 r^2) , \quad (11)$$

where $\alpha_1 = 1.706\,(Z_1^{0.307} + Z_2^{0.307})^{2/3}/a_B$, $\alpha_2 = 0.916\,(Z_1^{0.169} + Z_2^{0.169})/a_B^{3/2}$, $\alpha_3 = 0244$ $(Z_1^{0.0418} + Z_2^{0.0418})^2/a_B^2$ (a_B : Bohr radius). The AMLJ potential is not "universal": the three parameters show different Z-dependencies so that the shape of the function varies with the atoms involved in the encounter.

Even if the Hartree-Fock electron density is employed in place of the TF electron density, the second

approaches such as the ZBL、Kr-C and AMLJ interatomic potentials use the statistical model. For example, the authors must employ the assumption that the kinetic energy of the electrons is proportional to the 5/3 power of the electron density. It means that these interatomic potentials cannot be applied to the two-atom encounter in which a light atom is included. Unfortunately, there is no simple interatomic potential which treats reasonably the light-atom scattering. Therefore, in the computer simulation of the Impact-Collision-Ion-Scattering-Spectroscopy (ICISS) surface scattering [11] and light-ion sputtering [12], the authors used the screening function with the modified screening length, i.e, $a_m = q\times$(screening length). The correction factor, q, ranges from 0.6 to 1.0 which depends on the ion-target combination. O'Conner and MacDonald [13] proposed the empirical formula, $q = 0.69 + 0.0051\ (Z_1 + Z_2)$ for the Firsov screening length in the Moliére potential.

The motivation of this paper is to show what physical quantity is the measure of determining this q-value. One of the most promising candidates seems to be the average radius of the electron density. For this purpose, first of all, we decide the correction factor of the screening length for an isolated atom so as to match the average radius of the TF electron distribution with that of the Hartree-Fock electron distribution for an isolated atom and then we calculate the correction factor of two-center TF system by using a combination rule for the screening length corresponding to the Firsov, Lindhard and ZBL screening length formula.

2. The Thomas-Fermi electron distribution for an isolated atom

The TF electron distribution, n(r), shows no shell structure, and is given by

$$4\pi r^2 n(r)dr = Zx^{1/2}\phi(x)^{3/2}dx \quad , \tag{12}$$

using the TF differential equation (3).

Rigorously speaking, the empirical screening functions, eqs. (6) and (7), mentioned in the previous section are not exact solutions of eq. (3), and so we cannot use eq. (12) for the TF electron distribution. We must use the Poisson equation for the TF electron distribution. Then, we have

$$4\pi r^2 n(r)dr = Zx\frac{d^2\phi(x)}{dx^2}dx \quad . \tag{13}$$

Here, we will propose a new TF screening function corresponding to the AMLJ potential which for convenience will be called "Yamamura" screening function in this paper:

$$\phi(x)_{Yam} = \exp(-1.35x + 0.586x^{3/2} - 0.093x^2) \quad . \tag{14}$$

Three parameters of the Yamamura potential are determined from the Moliére screening function by the least square method.

The whole profiles of the electron distributions are characterized by the average radius $< r >$ and the radial spread $< r^2 >$. Table 1 shows the average reduced radius $< x >$ and the corresponding radial spread $< x^2 >$ of the TF electron distributions calculated from Moliére, Kr-C, ZBL, Sommerfeld and Yamamura screening functions. Rigorously speaking, the Kr-C and ZBL screening functions should not be used for calculating the electron distribution of an isolated atom, because these two screening functions are determined from the ion pair interaction. Since the screening length of the ZBL potential is small, the $< x >$ and $< x^2 >$ of the ZBL electron distribution are smallest among these five potentials. In Fig. 1 we compare these five screening functions. The ZBL potential shows the lowest values in the whole region, because its screening length is shorter than the TF screening length. The Sommerfeld, Moliére and Yamamura potentials have nearly equal values for $x < 6$, and the Moliére and Yamamura potentials behave similarly until $x = 8$. The Yamamura potential drops rapidly for $x > 10$.

3. The correction factor of the screening length for an isolated atom

It is not established how to determine the correction factor, q-value, for the screening length of an isolated atom. In this paper, we determine the q-value of an isolated atom so as to match the average radius of the TF electron distribution with that of the Hartree-Fock electron distribution for an isolated atom, where we use the double-zeta functions listed in Clementi and Roetti's table [14]. The q-value for an isolated atom is obtained by

$$q = \frac{< r >_{HF}}{a_{TF} < x >_{TF}} \quad , \tag{15}$$

where $< r >_{HF}$ is the average radius of the Hartree-Fock electron distribution, and $< x >_{TF}$ is the

average reduced radius of the TF electron distribution which depends on the empirical screening function listed in Table 1. Table 2 shows the q-values for different screening functions listed in Table 1 and they are plotted in Fig. 2 as a function of the Z number. The shell effect of the electron distribution is clearly observed in the present q-values. Here, it must be noted that the expansion coefficients listed in Clementi and Roetti's table do not satisfy the normalization for lithium atom.

Another important quantity for the profile of the electron distribution is the radial spread $< r^2 >$. In Fig. 3 we plot the relative deviation $(< r^2 >_{HF} - < r^2 >_{TF})/< r^2 >_{HF}$ for present five screening functions, where the correction factor q is taken into account for the calculation of $< r^2 >_{TF}$. Fig. 3 says that Moliére, ZBL, Kr-C and Yamamura TF electron distributions will give reasonable profiles within about 15% accuracy, except for $Z \leq 10$. For light atom ($Z \leq 10$) the ZBL and Yamamura TF electron distributions are better than the Moliére one. From the viewpoint of electron distribution the Yamamura screening function with the modified screening length, $q_{Yam} \times a_{TF}$, gives similar results to the ZBL and Kr-C screening function with the present modified screening length for a wide range of the atomic number, though it has only three parameters.

In Figs. 4 through 17 we plot the Hartree-Fock electron distribution, the TF electron distributions with the modified screening length and those with the original TF screening length, in the broad solid line, broad gray line and thin solid line, respectively, for the present five TF screening functions, where H, He, Li, Be, B, C, Ne, Ar, Ni, Cu, Kr, Xe, Au and U are considered as isolated atoms. For hydrogen, helium and lithium atoms the TF electron distributions are different from the Hartree-Fock electrons distributions even if $< r >_{HF} = < r >_{TF}$. Especially, the Moliére distribution have a sharp peak near $r = 0$ because of the third term $\exp(-6.0 x)$ of the Moliére screening function.

It must be noted that the TF electron distribution n(r) diverge at $r = 0$ as is seen from eq. (13). This is why the TF electron distributions cannot describe the Hartree-Fock electron distributions of light atoms such as H, He and Li. It is interesting that ZBL, Kr-C and Yamamura TF screening functions give reasonably good profiles for Beryllium ($Z = 4$) and Boron ($Z = 5$) even if their atomic numbers are small. As the atomic number increases, the TF electron distributions show good agreement with the Hartree-Fock distributions. The TF electron distributions with the present modified screening lengths are much better than those with the original screening length for all cases. It is very interesting that ZBL and Kr-C screening functions give very good electron densities for an isolated atom if one

uses the present modified screening length though they are not an approximate solutions of the TF equation, (3).

4. The correction factor of the screening length in the interatomic potential

For the encounter of atomic number Z_1 and Z_2, there are three screening formula, Firsov, Lindhard and ZBL, of the screening length in the interatomic potential. Let us consider the Z_1 and Z_2 in these formulas as the screening length of the isolated atom. Then, we have the following combination rules for the screening length of the interatomic potential:

Firsov: $$\left(\frac{1}{a_F}\right)^{\frac{3}{2}} = \left(\frac{1}{a_1}\right)^{\frac{3}{2}} + \left(\frac{1}{a_2}\right)^{\frac{3}{2}}, \tag{16}$$

Lindhard: $$\left(\frac{1}{a_L}\right)^{2} = \left(\frac{1}{a_1}\right)^{2} + \left(\frac{1}{a_2}\right)^{2}, \tag{17}$$

ZBL: $$\left(\frac{1}{a_{ZBL}}\right) = \left(\frac{1}{a_1}\right)^{0.69} + \left(\frac{1}{a_2}\right)^{0.69}, \tag{18}$$

where a_1 and a_2 are the screening lengths of the isolated atoms with atomic number Z_1 and Z_2, respectively, given by eq. (2). In principle, the Kr-C and ZBL potentials are the interatomic potential proposed for the interacting two-atom system. Therefore, the direct application of the present approach to the Kr-C and ZBL potentials is not suitable. The Sommerfeld screening function is not good from the viewpoint of its electron distribution. Then, we will use the Moliére and Yamamura potentials and use the Firsov formula, eq. (16), for the screening length. These two potentials resemble each other, except for light atoms (see Fig. 4 and 5) and at large distance (see Fig. 1). Table 3 shows the q-value for several typical the Z_1 and Z_2 combinations, where H, He, Li, Be, C, O, Ne, Na, Si, Ar, K, Ni, Cu, Kr, Ag, Xe W, and Au are picked as the projectile (Z_1).

In the past, many authors have determined the correction factors of the screening length by adjusting a computer simulation to experimental data in the field for the ICISS [11, 15-38] analysis and light-ion sputtering [12]. In the computer simulation of the sputtering yield, the correction factor also reflects ambiguities in the collision events of ion-target and target-target combinations and those in the electronic energy loss. On the other hand, the ICISS analysis is simple and usually the effect of

the electronic energy loss is small. Therefore, in Table 4, we compared the q-values determined by the ICISS computer analysis with present theoretical q-values for various ion-target combinations. In the ICISS experiments not all experimental data are obtained at 180° backscattering angle, but the scattering angles range from 140° to 180°. In the ICISS computer analysis, all authors in Table 4 used the Moliére potential with the modified Firsov screening length, $a_m = q \times a_F$.

As is seen from Table 4, the present q-values are in reasonably good agreement with those of the ICISS computer analysis for almost all cases (about 80%) . Chang et al. [37] used q = 0.65 for both 2 keV Na $\rightarrow$ Cu and Na $\rightarrow$ Pt and these values are much less than the present values. They determined their correction factors by fitting their calculations to the experimental shadow cones measured by Niehus and Comsa [39] who used the 144° ICISS technique. The 144° ICISS technique is sometimes dangerous for determining the shadow cone experimentally. It appears that the agreement between the present q-values and the ICISS-q values is not good for the covalent crystals such as TiC, Si, NbC, and HfC. It seems that we should use the solid state electron density in place of the atomic electron density for determining the correction factor of the screening length for covalent crystal.

5. Conclusion

In order to investigate the interaction of a charged particle with solids as in the ICISS analysis and sputtering yield calculations by computer simulation, many authors treat the nuclear collision by the Thomas-Fermi screened Coulomb potential by adjusting the screening length to experiment. In this paper, we propose a new way to determine the correction to the screening length of the interatomic potential. First of all we decide the correction factor of the screening length for an isolated atom so as to match the average radius of the TF electron distribution with that of the Hartree-Fock electron distribution. After that, we calculate the correction for the screening length of two-center TF system by using the screening-length combination rule. The correction for the screening length in the Moliére interatomic potential are in good agreement with those determined by the ICISS computer analysis.

From the viewpoint of electron distribution in an isolated atom, the ZBL and Yamamura screening functions give good profiles of electron distributions for $Z \geq 4$ if the present modified screening lengths is used. The Kr-C potential is good enough for light elements.

References

[1] O.B. Firsov, Dokl. Akad. Nauk USSR 91 (1953) 515.

[2] O.B. Firsov, Sov. Phys. JETP 6 (1958) 534.

[3] J.Lindhard, V.Nielson and M.Scharff, Mat. Fys. Medd. Dan. Vid. Selsk. 36 (1968) no.10.

[4] A. Sommerfeld, Z. Phys. 78 (1932) 283.

[5] N.H. March, Proc. Cambridge Phil. Soc. 46 (1950) 356.

[6] G.Moliere, Z. Naturforsch. 2A (1947) 133.

[7] W.D. Wilson, L.G. Haggmark and J. Biersack, Phys. Rev. B15 (1977) 2458.

[8] J.F. Ziegler, J.P. Biersack and U. Littmark, "The stopping and range of ions in solids" (Pergamon press, New York, 1985).

[9] S.T. Nakagawa and Y. Yamamura, Radia. Eff. 105 (1988) 239.

[10] T.A. Carlson, C.C. Lu, T.C. Tucker, C.W. Nestor, Jr., and F.B. Malik, ORNL-4614 UC-34-Physics (1970).

[11] W. Takeuchi and Y. Yamamura, Nucl. Instr. Meth. B84 (1994) 443.

[12] Y. Yamamura and H. Tawara, At. Data and Nucl. Data Table, 62 (1996) 149.

[13] D.J. O'Connor and R.J. MacDonald, Radiat. Eff. 34 (1977) 247.

[14] E. Clementi and C. Roetti, At. Data and Nucl. Data Table, 14 (1974) 177.

[15] Th. Fauster and M.H. Metzner, Surf. Sci. 166 (1986) 29.

[16] M. Voetz, H. Niehus, J. O'Connor and G. Comsa, Surf. Sci. 292 (1993) 211.

[17] W. Takeuchi, private communication (1997).

[18] R. Spitzl, H. Niehus and G. Comsa, Surf. Sci. 250 (1991) L355.

[19] H. Durr, Th. Fauster and R. Schneider, Surf. Sci. 244 (1991) 237

[20] R.S. Daley, J.H Huang and R.S. Williams, Surf. Sci. 202 (1988) L577.

[21] R.-P. Blum, D. Ahlbehrendt and H. Niehus, Surf. Sci. 366 (1996) 107.

[22] M. Aono, Y. Hou, R. Souda, C. Oshima, S. Otani, Y. Ishizawa, K. Matsuda and R. Shimizu, Jpn. J. Appl. Phys. 21 (1982) L670.

[23] J.H Huang and R.S. Williams, Phys. Rev. B38 (1988) 4022.

[24] M. Aono, R. Souda, C. Oshima and Y. Ishizawa, Surf. Sci. 168 (1986) 713.

[25] J.A. Yarmoff, D.M. Cyr, J.H. Huang, S. Kim and R.S. Williams, Phys. Rev. B33 (1986) 3856.

[26] W. Hayami, R. Souda, T. Aizawa and Y. Ishizawa, Surf. Sci. 303 (1994) 247.

[27] Y. Li and B.E. Koel, Surf. Sci. 330 (1995) 193.

[28] J.H. Huang, R.S. Daley, D.K. Shuh and R.S. Williams, Surf. Sci. 186 (1987) 115.

[29] W. Hayami, R Souda, T.Aizawa, S. Otani and Y. Ishizawa, Surf. Sci. 276 (1992) 299.

[30] W. Soszka, Surf. Sci. 249 (1991) 289.

[31] K. Umezawa, A. Takahashi, T. Yumura, S. Nakanishi and W.M. Gibson, Surf.Sci. 365 (1996) 118.

[32] Th. Fauster, H. Durr and D. Hartwig, Surf. Sci. 178 (1986) 657.

[33] R.M. Charatan and R.S. Williams, Surf. Sci. 289 (1993) 163.

[34] T.C.Q. Noakes, D.A. Hutt, C.F. McConville and D.P. Woodruff, Surf. Sci. 372 (1997) 117.

[35] W. Takeuchi and Y. Yamamura, Nucl. Instr. and Meth. B72 (1992) 363.

[36] J. Moller, H. Niehus and W. Heiland, Surf. Sci. 166 (1986) L111.

[37] C.S. Chang, U. Knipping and I.S.T. Tsong, Nucl. Instr. and Meth. B18 (1986) 11.

[38] W.D. Roos, J. du Plessis, G.N. van Wyk, E. Taglauer and S. Wolf, J. Vac Sci. Technol. A14 (1996) 1648.

[39] H. Niehus and G. Comsa, Surf. Sci. 140 (1984) 18.

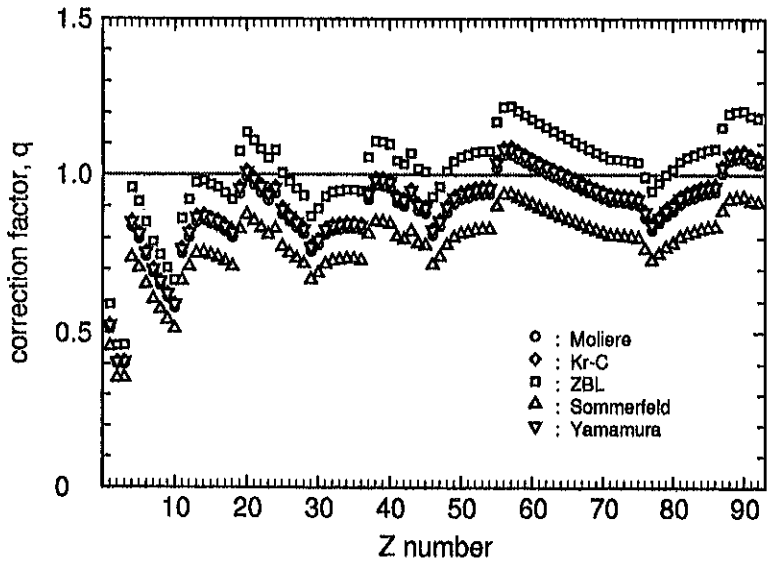

Fig. 2 Plots of q-values as a function of the Z number for various screening functions

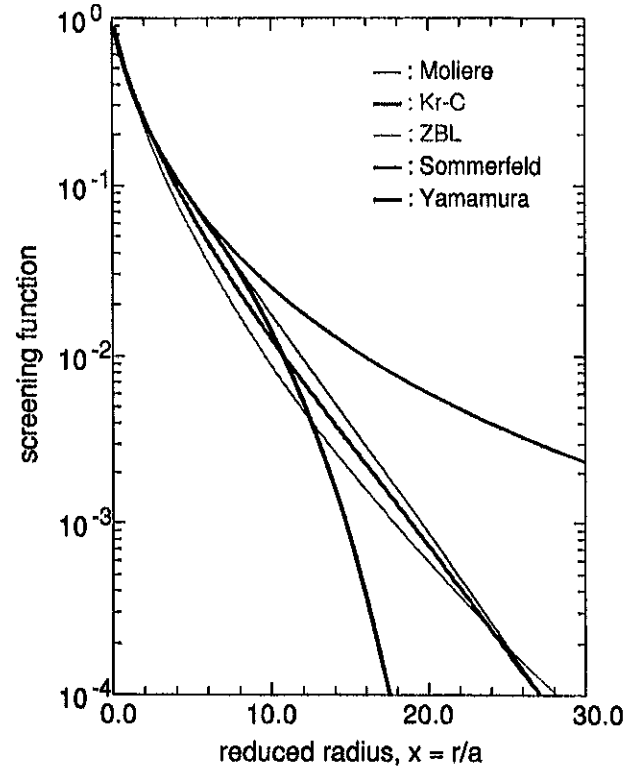

Fig. 1 The screening functions of five models as a function of reduced radius x = r/a

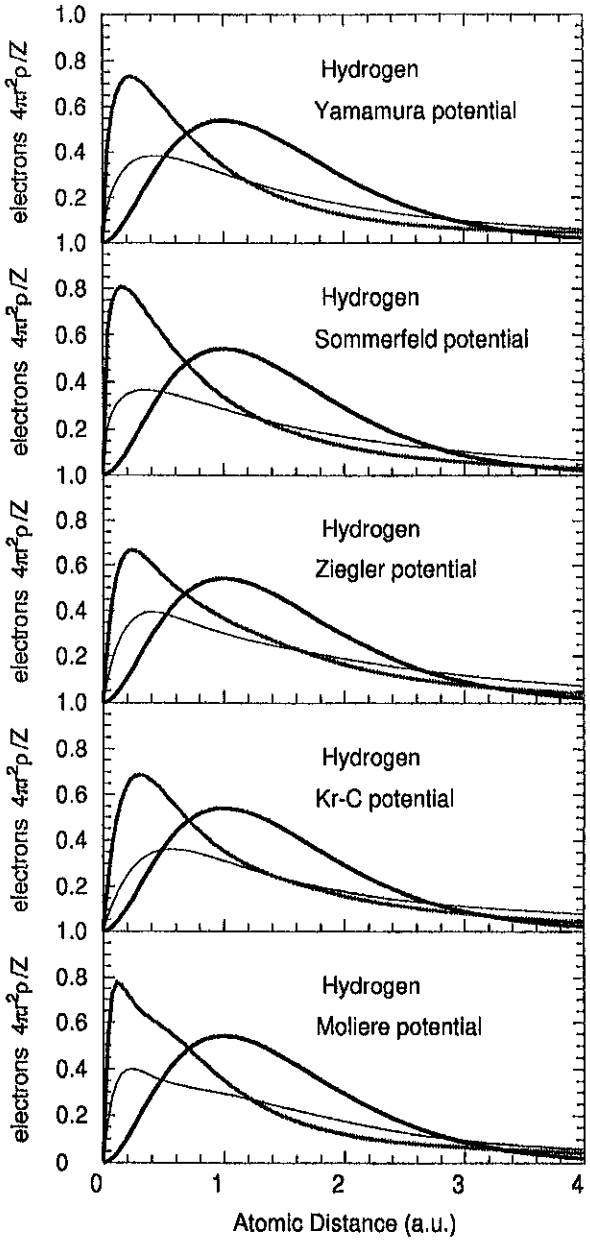

Fig. 4 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Hydrogen

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

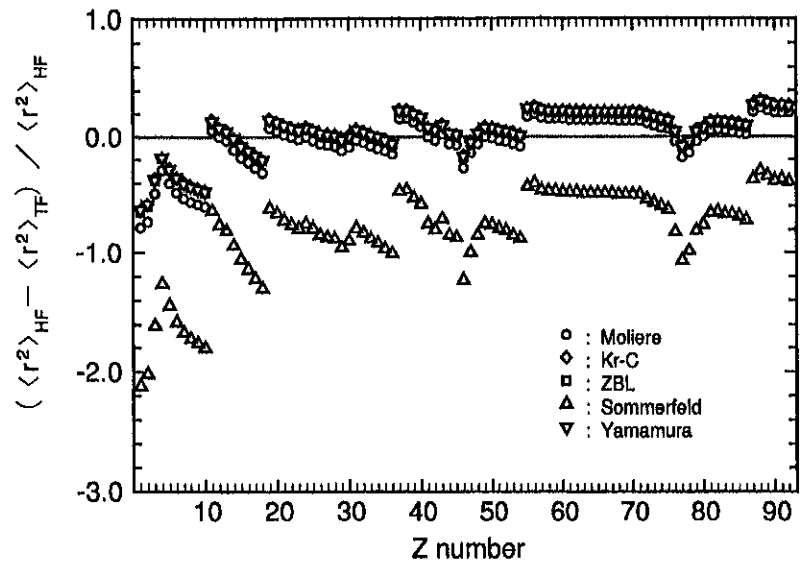

Fig. 3 Plots of $(\langle r^2 \rangle_{HF} - \langle r^2 \rangle_{TF}) / \langle r^2 \rangle_{HF}$ as a function of the Z number for various screening functions

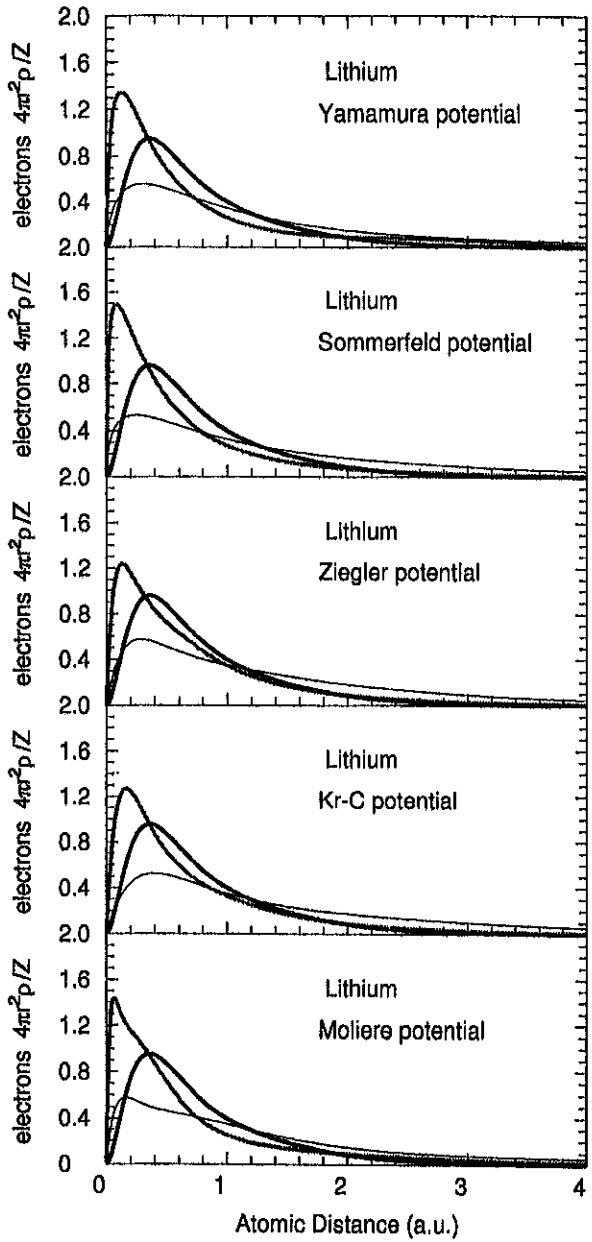

Fig. 6 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Lithium

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

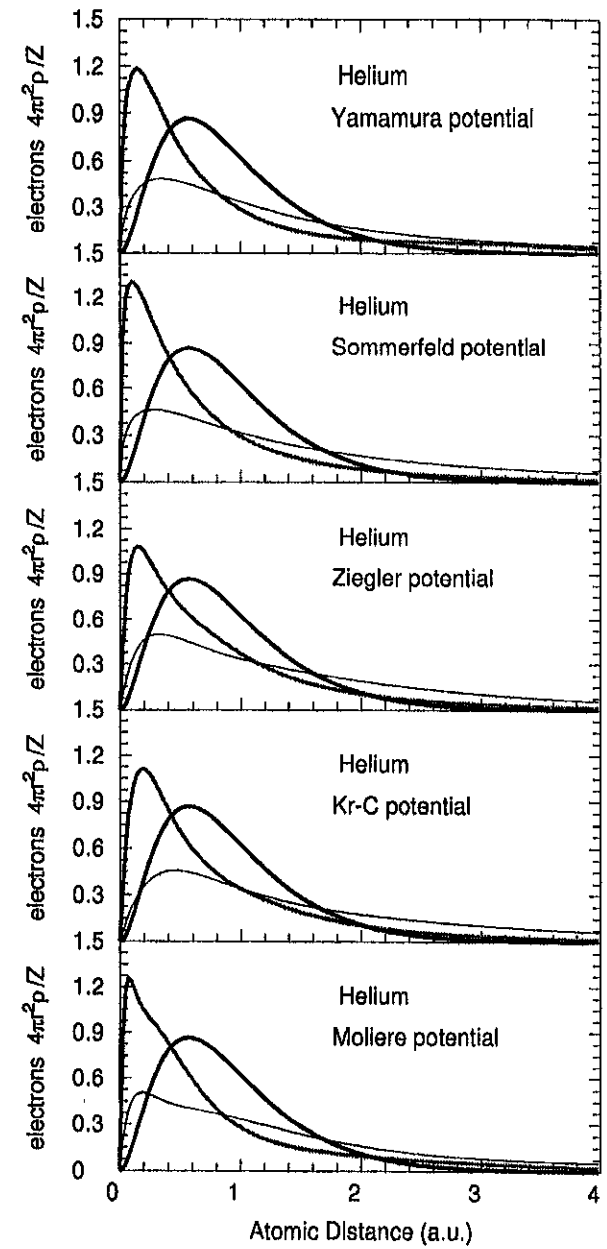

Fig. 5 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Helium

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

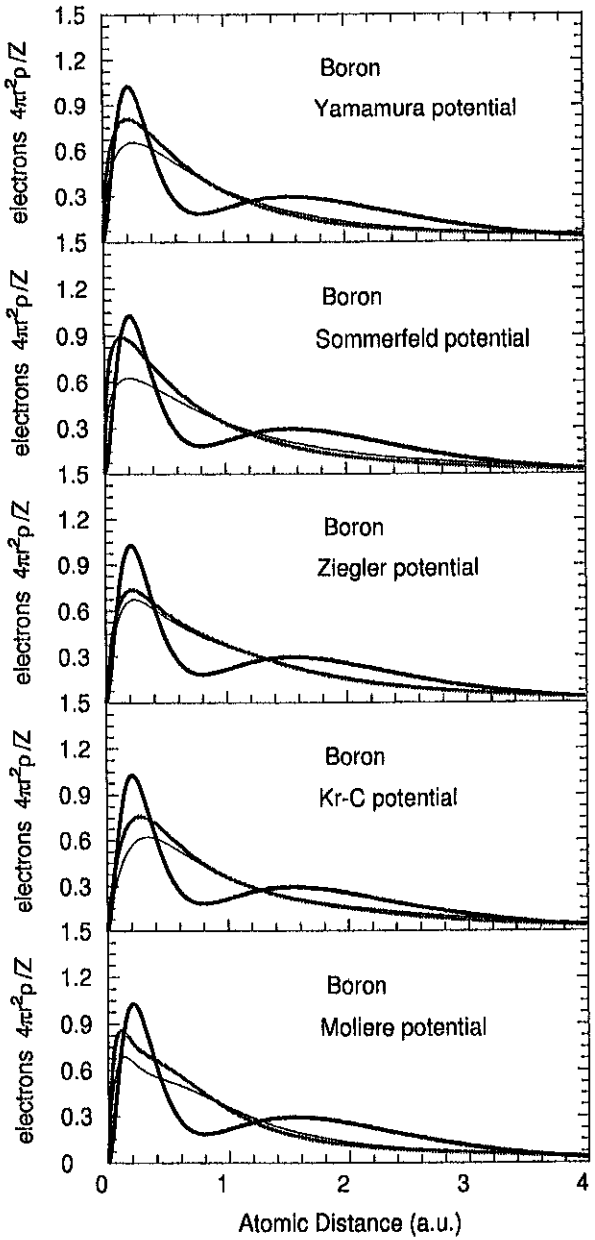

Fig. 8 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Boron

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

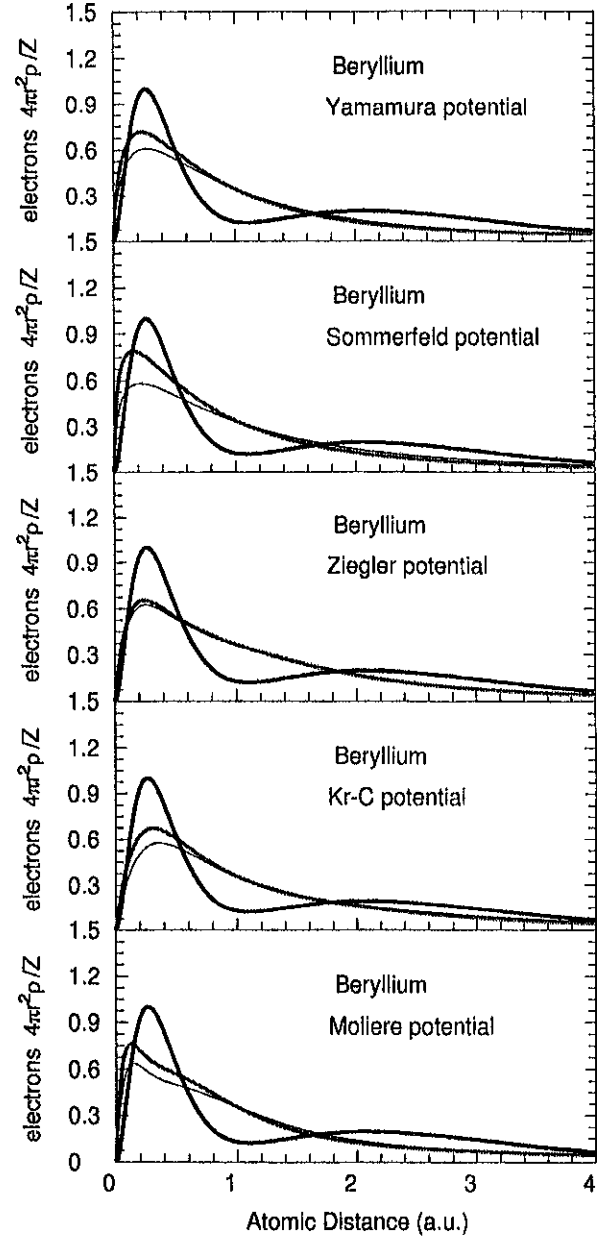

Fig. 7 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Beryllium

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

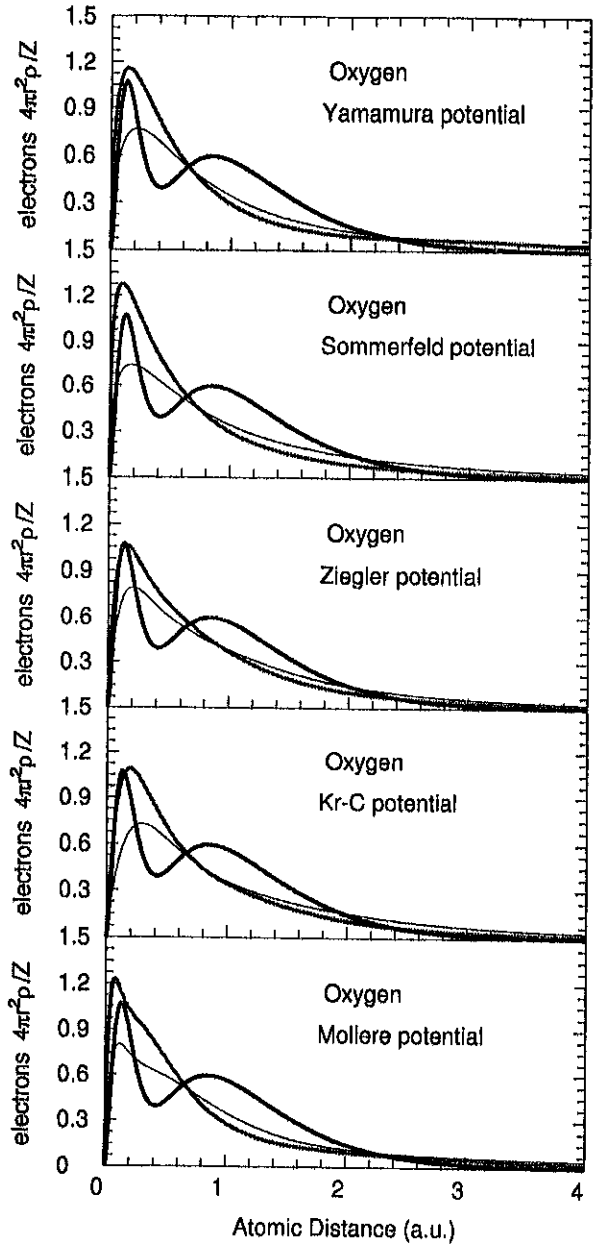

Fig.10 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Oxygen

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

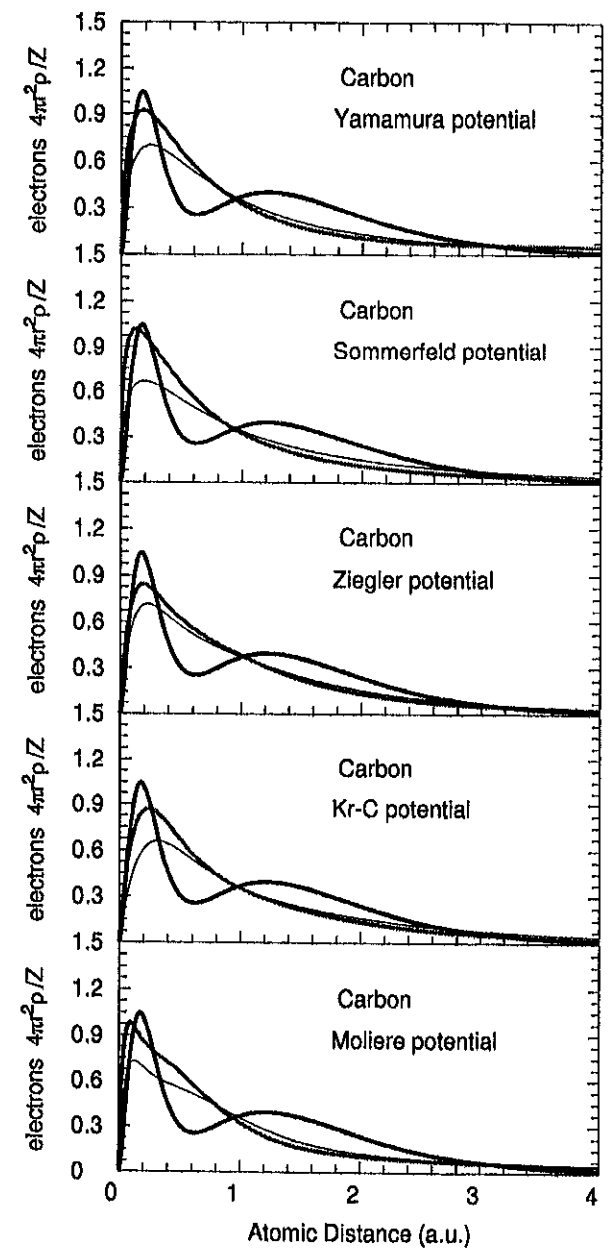

Fig. 9 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Carbon

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

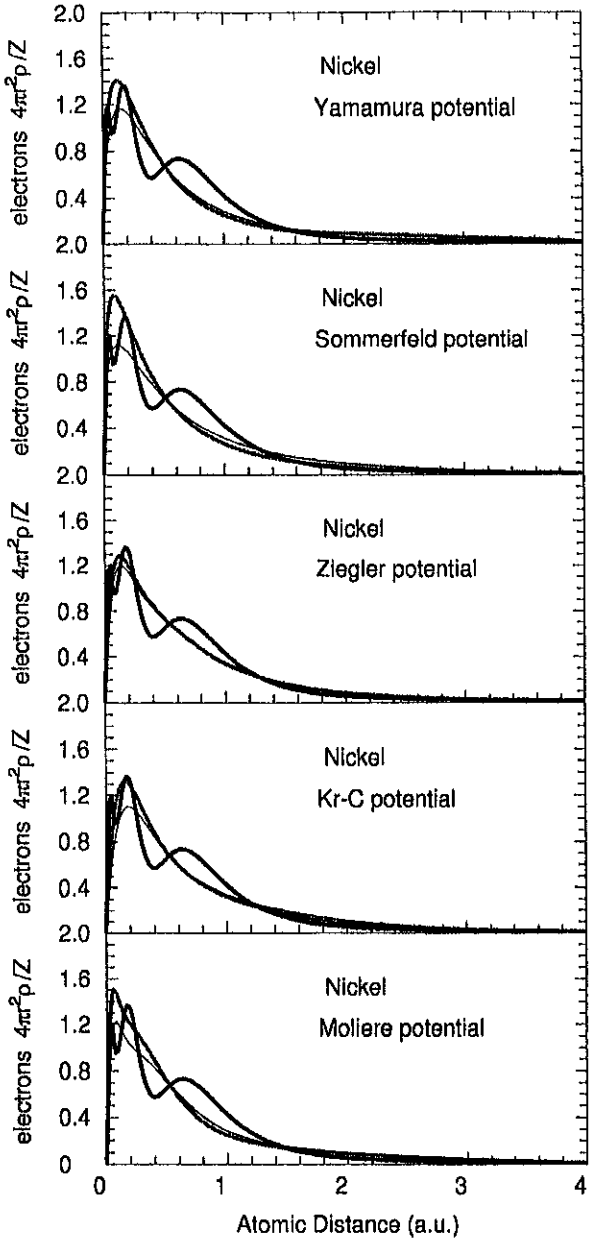

Fig.12 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Nickel

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

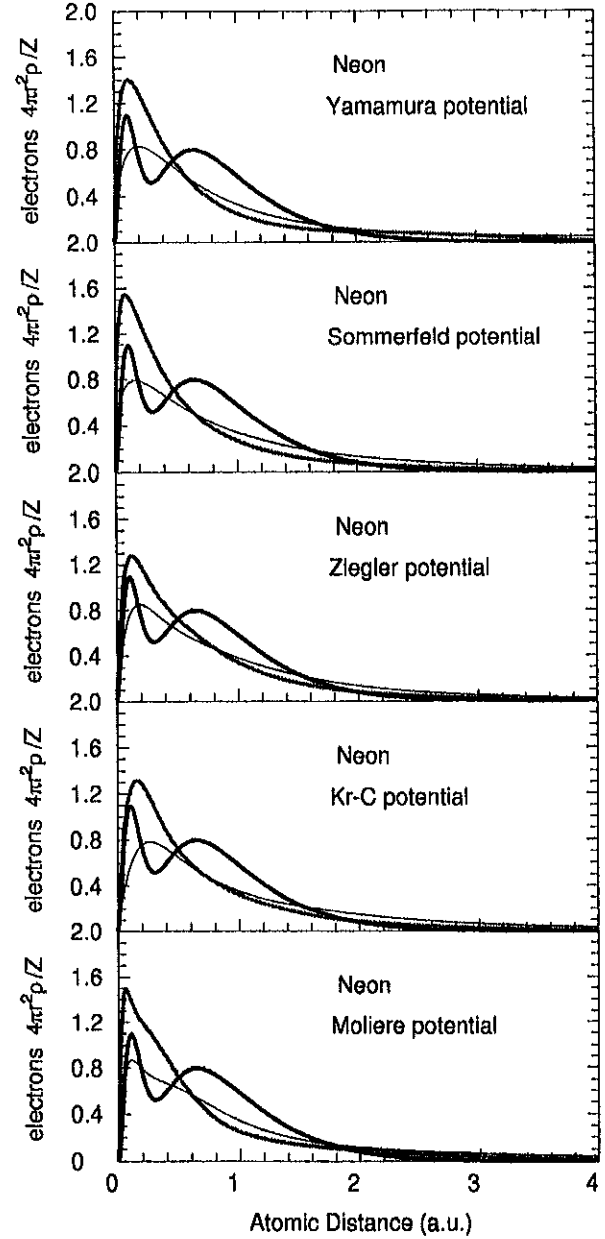

Fig.11 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Neon

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

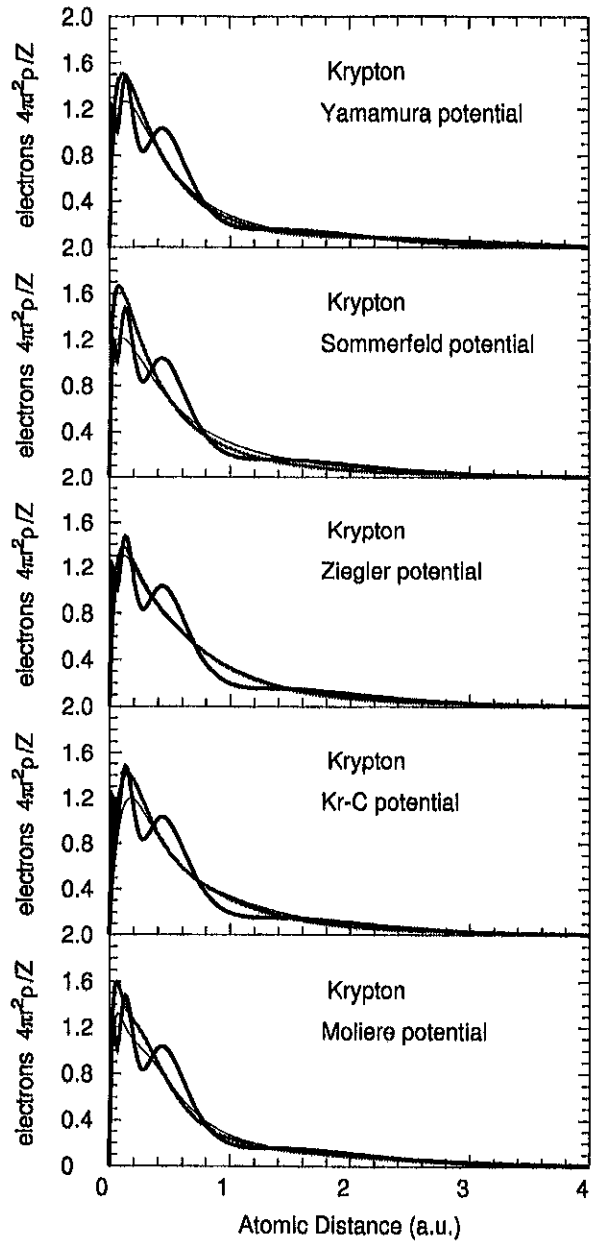

Fig.14 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Krypton

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

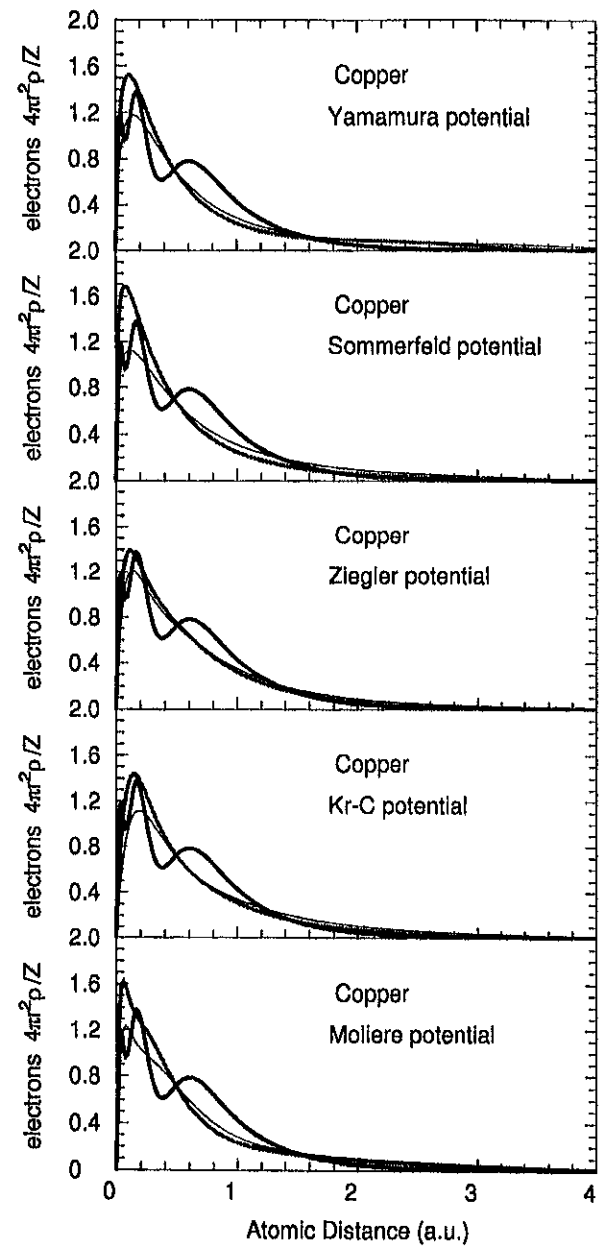

Fig.13 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Copper

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

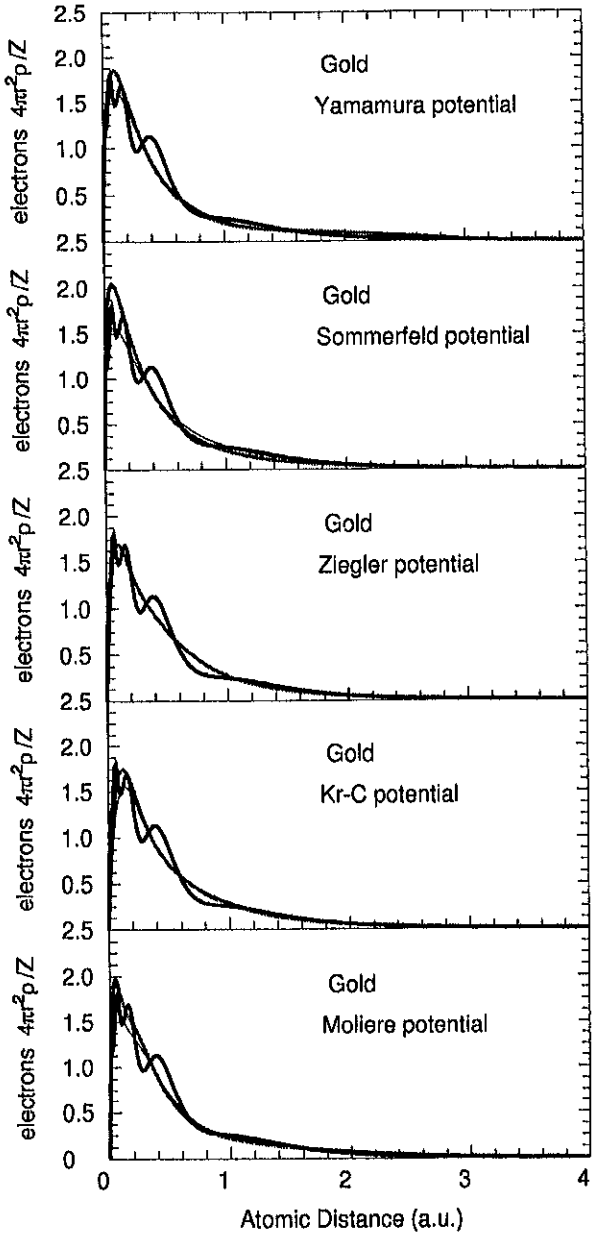

Fig.16 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Gold

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

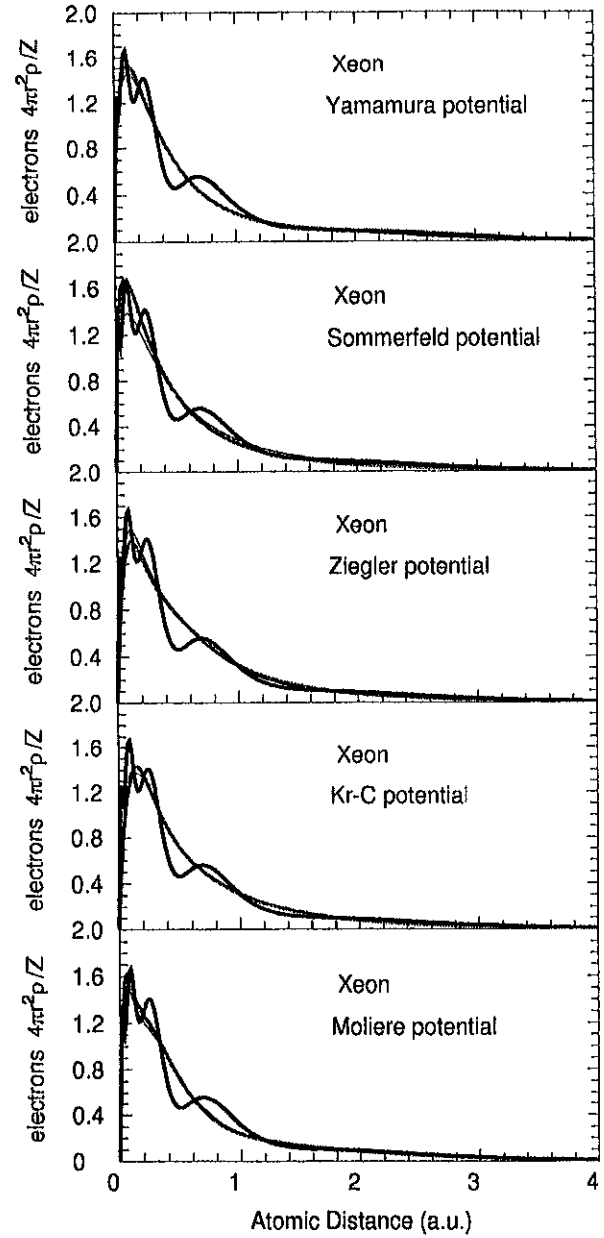

Fig.15 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Xeon

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

Table 1 The average reduced radius $< x >$ and the spread $< x^2 >$ of various Thomas-Fermi electron distributions

TF screening function	$< x >$	$< x^2 >$
Moliére	3.283	25.64
Kr-C	3.207	22.31
ZBL	2.866	18.07
Sommerfeld	3.724	57.70
Yamamura	3.224	22.65

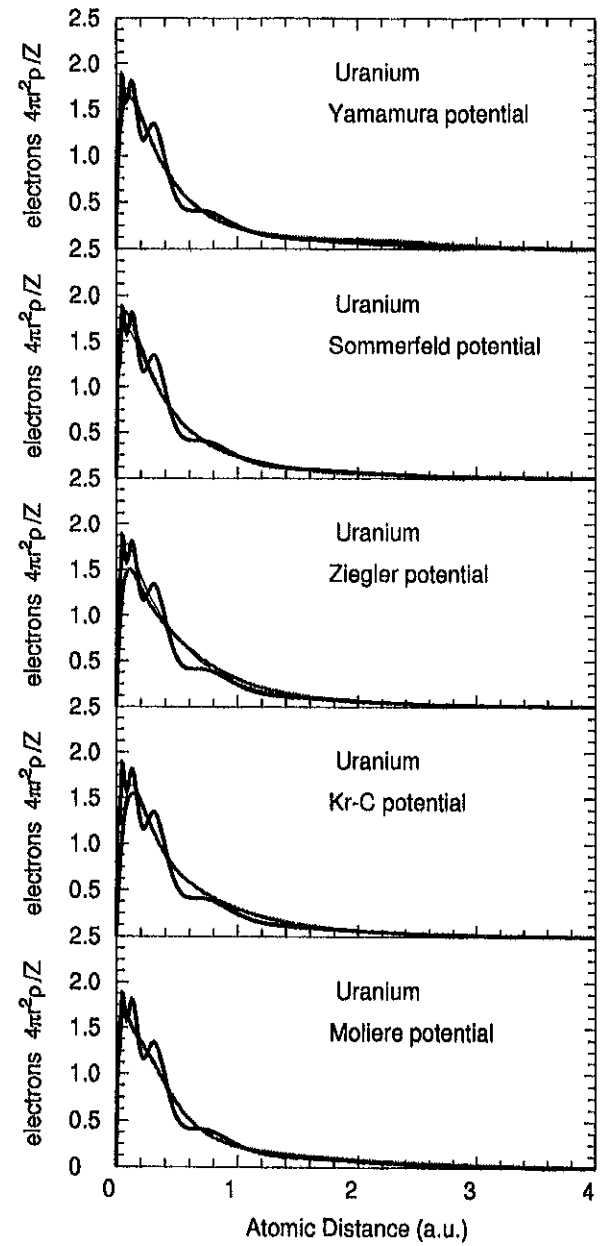

Fig.17 Comparison of various Thomas-Fermi electron distributions with Hartree-Fock electron ditribution for Uranium

——— : Hartree-Fock electron distribution
——— : Thomas-Fermi with the present modified screening length
——— : Thomas-Fermi with the original screening length

Table 2 The correction factor, q, for various screening functions

Z number		Moliere	Kr-C	ZBL	Sommerfeld	Yamamura
1	H	0.516	0.528	0.591	0.455	0.526
2	He	0.402	0.411	0.460	0.354	0.409
3	Li	0.402	0.412	0 461	0.355	0 410
4	Be	0.837	0.857	0.959	0.738	0.853
5	B	0.800	0.819	0.916	0.705	0.815
6	C	0.743	0.760	0.851	0.655	0.756
7	N	0.689	0.705	0.789	0.607	0.702
8	O	0.652	0.667	0.747	0.575	0.664
9	F	0.615	0.630	0.705	0.542	0.626
10	Ne	0.581	0.595	0.666	0.513	0.592
11	Na	0.753	0.771	0.863	0.664	0.767
12	Mg	0.804	0.823	0.921	0.709	0.819
13	Al	0.852	0.872	0.976	0.751	0.868
14	Si	0.857	0.877	0.981	0.755	0.873
15	P	0.846	0.866	0.969	0.746	0.862
16	S	0.838	0.858	0.960	0.739	0.853
17	Cl	0.823	0.842	0 942	0.725	0.838
18	Ar	0.804	0.823	0.921	0.709	0.819
19	K	0.939	0.962	1.076	0.828	0.957
20	Ca	0.992	1.015	1.136	0.874	1.010
21	Sc	0.969	0.992	1.110	0.854	0.987
22	Ti	0.944	0 967	1.082	0.832	0.962
23	V	0.920	0.942	1.054	0.811	0 937
24	Cr	0.942	0.964	1.079	0.830	0.959
25	Mn	0.877	0.898	1 005	0.773	0.893
26	Fe	0.854	0.874	0.978	0.753	0.870
27	Co	0.834	0.854	0.956	0.735	0.850
28	Ni	0.815	0.835	0.934	0 719	0.830
29	Cu	0.759	0.777	0.870	0.669	0.773
30	Zn	0.780	0.799	0.894	0.688	0.794
31	Ga	0.813	0.832	0.931	0.717	0.828
32	Ge	0.825	0.844	0.945	0.727	0.840
33	As	0.828	0.847	0.948	0.730	0.843
34	Se	0.831	0.851	0 952	0.733	0.847
35	Br	0.831	0.851	0.952	0.733	0.846
36	Kr	0.827	0.847	0 948	0.729	0.842
37	Rb	0.923	0.945	1.057	0 813	0 940
38	Sr	0.967	0.990	1 108	0.853	0.985
39	Y	0.965	0.988	1.106	0.851	0.983
40	Zr	0.959	0.982	1.099	0.846	0.977
41	Nb	0.914	0.935	1.046	0.805	0.930
42	Mo	0.904	0.925	1.035	0.797	0.920
43	Tc	0.934	0.956	1.070	0.823	0.951
44	Ru	0.890	0.911	1.020	0.785	0.907
45	Rh	0.882	0.903	1.010	0 778	0.898
46	Pd	0.812	0.832	0.931	0.716	0.827
47	Ag	0.840	0.860	0.963	0.741	0.856
48	Cd	0.883	0.904	1.012	0.779	0.900
49	In	0.911	0.933	1.044	0.803	0.928
50	Sn	0.924	0.946	1.058	0.815	0.941
51	Sb	0.929	0.951	1.065	0 819	0.946
52	Te	0.937	0.959	1.073	0.826	0.954
53	I	0.939	0.962	1.076	0.828	0.957
54	Xe	0.940	0.962	1.077	0.829	0.957
55	Cs	1.022	1.046	1.171	0.901	1.041
56	Ba	1.064	1.089	1.218	0.938	1.083
57	La	1.065	1.091	1.221	0.939	1.085
58	Ce	1.053	1.078	1.206	0.928	1.073
59	Pr	1.041	1.066	1 193	0.918	1.060
60	Nd	1.029	1.054	1 179	0.907	1 048
61	Pm	1.018	1.042	1.166	0.897	1 036
62	Sm	1.006	1.030	1.153	0 887	1 025
63	Eu	0.995	1.019	1.140	0.877	1.014
64	Gd	0.985	1.008	1.128	0.868	1.003
65	Tb	0.975	0.998	1.117	0.859	0.993
66	Dy	0.965	0.988	1.105	0.851	0.983
67	Ho	0.955	0.978	1.094	0.842	0.972
68	Er	0.945	0.967	1.083	0.833	0.962
69	Tm	0.936	0.958	1.072	0.825	0.953
70	Yb	0.926	0.948	1.061	0.817	0.943
71	Lu	0.918	0.939	1.051	0.809	0.934
72	Hf	0.917	0.938	1 050	0.808	0.933
73	Ta	0.914	0.936	1.047	0.806	0.931
74	W	0.911	0.933	1.044	0.804	0.928
75	Re	0.908	0.929	1.040	0.800	0.924
76	Os	0.868	0.888	0.994	0.765	0.884
77	Ir	0.828	0.848	0.949	0.730	0.843
78	Pt	0.851	0.871	0.975	0.750	0.867
79	Au	0.873	0 894	1.000	0.770	0.889
80	Hg	0.888	0.909	1.017	0.783	0.904
81	Tl	0.910	0 932	1.043	0.803	0.927
82	Pb	0 923	0.944	1.057	0.813	0.939
83	Bi	0.930	0.952	1 065	0 820	0.947
84	Po	0.938	0.961	1 075	0 827	0.956
85	At	0.943	0.966	1.081	0 832	0.961
86	Rn	0 947	0.969	1.084	0.835	0 964
87	Fr	1.006	1.030	1.153	0.887	1.025
88	Ra	1.045	1.069	1 197	0.921	1.064
89	Ac	1.051	1.076	1 204	0.926	1.070
90	Th	1.053	1.078	1.207	0.929	1.073
91	Pa	1 039	1.064	1 190	0.916	1.058
92	U	1.033	1.057	1.183	0 911	1 052

Table 3 The correction factor, q, for various Z_1 and Z_2 combinations

Z_2		Z_1 = H		He		Li	
		Moliere	Yamamura	Moliere	Yamamura	Moliere	Yamamura
1	H	0.516	0.526	0.441	0.449	0.436	0.445
2	He	0.441	0.449	0.402	0.409	0.402	0.410
3	Li	0.436	0.445	0.402	0.410	0.402	0.410
4	Be	0.683	0.697	0.559	0.569	0.540	0.551
5	B	0.676	0.689	0.562	0.572	0.543	0.553
6	C	0.654	0.666	0.554	0.564	0.537	0.547
7	N	0.628	0.640	0.542	0.552	0.528	0.538
8	O	0.608	0.620	0.532	0.542	0.520	0.530
9	F	0.586	0.597	0.520	0.529	0.509	0.519
10	Ne	0.564	0 574	0.507	0.516	0.498	0.507
11	Na	0.676	0.688	0.583	0.594	0.566	0.576
12	Mg	0.707	0.721	0.606	0.616	0.585	0.597
13	Al	0.737	0.751	0.626	0.637	0.604	0.615
14	Si	0.742	0.756	0.632	0.643	0.609	0.621
15	P	0.739	0.753	0.632	0.643	0.610	0.622
16	S	0.736	0.750	0.633	0.644	0.611	0.622
17	Cl	0.730	0.743	0.630	0.641	0.609	0.621
18	Ar	0.720	0.733	0.626	0.637	0.606	0.617
19	K	0.800	0.815	0.678	0.690	0.651	0.664
20	Ca	0.831	0.846	0.699	0.711	0.670	0.683
21	Sc	0.821	0.837	0.695	0.707	0.667	0.680
22	Ti	0.810	0.825	0.690	0.702	0.663	0.675
23	V	0.798	0.813	0.684	0.696	0.658	0.671
24	Cr	0.812	0.827	0.695	0.707	0.668	0.680
25	Mn	0.775	0.790	0.672	0.684	0.649	0.661
26	Fe	0.763	0.777	0.665	0.677	0.643	0.655
27	Co	0.751	0.765	0.658	0.671	0.637	0.650
28	Ni	0.740	0.753	0.652	0.664	0.632	0.644
29	Cu	0.703	0.716	0.627	0.638	0.610	0.622
30	Zn	0.718	0.731	0.639	0.650	0.621	0.632
31	Ga	0.741	0.755	0.656	0.668	0.636	0.648
32	Ge	0.750	0.764	0.663	0.675	0.643	0.655
33	As	0.753	0.767	0.666	0.678	0.645	0.658
34	Se	0.756	0.770	0.669	0.681	0.648	0.661
35	Br	0.757	0.771	0.670	0.682	0.650	0.662
36	Kr	0.755	0.769	0.670	0.682	0.649	0.662
37	Rb	0.819	0.834	0.715	0.728	0.689	0.703
38	Sr	0.848	0.864	0.735	0.748	0.707	0.721
39	Y	0.848	0.864	0.736	0.749	0.708	0.722
40	Zr	0.845	0.861	0.735	0.748	0.708	0.721
41	Nb	0.817	0.832	0.717	0.730	0.692	0.705
42	Mo	0.811	0.826	0.714	0.726	0.690	0.703
43	Tc	0.832	0.847	0.729	0.742	0.703	0.716
44	Ru	0.804	0.819	0.710	0.723	0.687	0.700
45	Rh	0.799	0.814	0.708	0.720	0.685	0.698
46	Pd	0.751	0.765	0.674	0.686	0.655	0.667
47	Ag	0.771	0.786	0.689	0.702	0.669	0.682
48	Cd	0.802	0.817	0.712	0.725	0.689	0.702
49	In	0.821	0.837	0.726	0.739	0.702	0.716
50	Sn	0.831	0.846	0.733	0.747	0.709	0.722
51	Sb	0.835	0.850	0.737	0.750	0.712	0.726
52	Te	0.841	0.856	0.742	0.755	0.716	0.730
53	I	0.843	0.859	0.744	0.758	0.719	0.733
54	Xe	0.844	0.860	0.746	0.759	0.720	0.734
55	Cs	0.899	0.916	0.784	0.798	0.754	0.768
56	Ba	0.926	0.943	0.803	0.817	0.771	0.785
57	La	0.928	0.945	0.805	0.819	0.773	0.788
58	Ce	0.921	0.939	0.801	0.816	0.770	0.785
59	Pr	0.914	0.931	0.797	0.811	0.766	0.781
60	Nd	0.907	0.924	0.793	0.807	0.763	0.778
61	Pm	0.901	0.917	0.789	0.803	0.760	0.774
62	Sm	0.894	0.911	0.785	0.799	0.757	0.771
63	Eu	0.887	0.904	0.781	0.796	0.753	0.768
64	Gd	0.881	0.897	0.778	0.791	0.750	0.764
65	Tb	0.875	0.891	0.774	0.788	0.747	0.761
66	Dy	0.869	0.885	0.770	0.784	0.744	0.758
67	Ho	0.862	0.878	0.766	0.780	0.740	0.754
68	Er	0.856	0.872	0.762	0.775	0.737	0.751
69	Tm	0.850	0.866	0.758	0.772	0.734	0.748
70	Yb	0.844	0.859	0.754	0.768	0.730	0.744
71	Lu	0.838	0.853	0.751	0.764	0.727	0.741
72	Hf	0.838	0.853	0.751	0.764	0.728	0.741
73	Ta	0.836	0.852	0.750	0.764	0.727	0.741
74	W	0.835	0.850	0.749	0.763	0.727	0.740
75	Re	0.833	0.848	0.748	0.762	0.726	0.739
76	Os	0.804	0.819	0.727	0.741	0.707	0.721
77	Ir	0.774	0.789	0.705	0.718	0.687	0.700
78	Pt	0.792	0.807	0.719	0.732	0.700	0.713
79	Au	0.809	0.824	0.732	0.745	0.712	0.725
80	Hg	0.820	0.835	0.741	0.754	0.720	0.733
81	Tl	0.837	0.852	0.754	0.767	0.731	0.745
82	Pb	0.847	0.862	0.761	0.775	0.738	0.752
83	Bi	0.852	0.868	0.766	0.780	0.742	0.756
84	Po	0.858	0.875	0.771	0.785	0.747	0.761
85	At	0.862	0.879	0.774	0.788	0.750	0.764
86	Rn	0.865	0.881	0.777	0.791	0.753	0.767
87	Fr	0.908	0.925	0.808	0.823	0.780	0.796
88	Ra	0.935	0.952	0.828	0.843	0.798	0.814
89	Ac	0.940	0.957	0.832	0.846	0.802	0.817
90	Th	0.942	0.960	0.833	0.849	0.804	0.819
91	Pa	0.932	0.950	0.827	0.842	0.798	0.813
92	U	0.929	0.946	0.825	0.840	0.796	0.812

Table 3 The corection factor q for various Z_1 and Z_2 combinations (continued)

Z_2 \ Z_1		Be		C		O	
		Moliere	Yamamura	Moliere	Yamamura	Moliere	Yamamura
1	H	0.683	0.697	0.654	0.666	0 608	0.620
2	He	0.559	0.569	0.554	0.564	0.532	0 542
3	Li	0.540	0.551	0.537	0.547	0.520	0.530
4	Be	0.837	0.853	0.782	0 796	0.715	0.728
5	B	0.817	0.832	0.769	0 783	0.708	0.721
6	C	0.782	0.796	0.743	0.756	0.691	0.703
7	N	0.744	0.758	0 714	0.727	0.669	0.682
8	O	0.715	0.728	0 691	0.703	0.652	0.664
9	F	0.684	0.697	0.665	0.677	0.632	0.644
10	Ne	0.654	0.667	0.640	0.652	0.612	0.623
11	Na	0.782	0.797	0.749	0 762	0.702	0.715
12	Mg	0.816	0.831	0.777	0 791	0.726	0.739
13	Al	0.847	0.863	0.803	0.818	0.747	0.761
14	Si	0.850	0.866	0 807	0.822	0.751	0 765
15	P	0.843	0.859	0.802	0.817	0 748	0.762
16	S	0.838	0.853	0.798	0.813	0.747	0.760
17	Cl	0.828	0.843	0.791	0.805	0.741	0 755
18	Ar	0.814	0.830	0.780	0.794	0 733	0.747
19	K	0.904	0.921	0.855	0.871	0.794	0.809
20	Ca	0.937	0.954	0.882	0.898	0.816	0.831
21	Sc	0.924	0.941	0.872	0.888	0.809	0.824
22	Ti	0.909	0.926	0.861	0.877	0.801	0.816
23	V	0.893	0.910	0.849	0.864	0.792	0.807
24	Cr	0.908	0.925	0.862	0.877	0.803	0.818
25	Mn	0.865	0.881	0.827	0.841	0.776	0.790
26	Fe	0.849	0.865	0.814	0.828	0.766	0 780
27	Co	0.835	0.851	0.802	0.817	0.757	0 771
28	Ni	0.821	0.836	0.790	0.805	0.747	0 761
29	Cu	0.778	0.793	0.754	0.768	0.717	0.731
30	Zn	0.794	0.809	0.768	0.782	0.730	0.743
31	Ga	0.819	0.834	0.790	0.804	0.748	0.762
32	Ge	0.828	0.843	0.798	0.812	0.756	0.769
33	As	0.830	0.846	0.800	0.814	0 758	0 772
34	Se	0.833	0.849	0.802	0.817	0.760	0.774
35	Br	0.833	0.848	0.803	0.817	0.761	0 774
36	Kr	0.829	0.845	0.800	0.815	0.759	0.773
37	Rb	0.900	0.916	0.861	0.876	0.810	0.825
38	Sr	0.931	0.948	0.887	0.903	0.832	0 847
39	Y	0.930	0.947	0 887	0.903	0.832	0.847
40	Zr	0.926	0.943	0 884	0.900	0.830	0.845
41	Nb	0.894	0.910	0.857	0.872	0 808	0.823
42	Mo	0.887	0.903	0.852	0.867	0.804	0.818
43	Tc	0.909	0.926	0.871	0.886	0.820	0.835
44	Ru	0.877	0.894	0.843	0.859	0.798	0.813
45	Rh	0.871	0.887	0.839	0.854	0.794	0.809
46	Pd	0.818	0.833	0.792	0.807	0.755	0.769
47	Ag	0.839	0.855	0.811	0.827	0.772	0.786
48	Cd	0.872	0.889	0.840	0.856	0.797	0.812
49	In	0.893	0.910	0.859	0.874	0.812	0.827
50	Sn	0.903	0.920	0.867	0.883	0.820	0.835
51	Sb	0.907	0.924	0.871	0.887	0.823	0.838
52	Te	0.913	0.930	0.876	0.892	0.828	0.843
53	I	0.914	0.932	0.878	0.894	0.830	0.845
54	Xe	0.915	0.932	0.879	0.895	0.831	0.846
55	Cs	0.974	0.993	0.930	0.947	0.873	0.890
56	Ba	1.004	1.022	0.955	0.972	0.894	0.911
57	La	1.005	1.024	0.956	0.974	0.896	0.912
58	Ce	0.997	1.016	0.950	0.967	0.891	0.908
59	Pr	0.989	1.007	0.943	0.960	0.886	0.902
60	Nd	0.981	0.999	0.937	0.954	0.881	0 897
61	Pm	0.973	0.991	0.931	0.947	0.876	0.892
62	Sm	0.965	0.983	0.924	0.941	0.871	0.887
63	Eu	0.957	0.976	0.917	0.934	0.866	0.882
64	Gd	0.950	0.968	0.911	0.928	0.861	0.877
65	Tb	0.943	0.961	0.906	0.922	0.856	0.872
66	Dy	0.936	0.953	0.899	0.916	0.851	0.867
67	Ho	0.929	0.945	0.893	0.909	0.846	0.862
68	Er	0.921	0.938	0.887	0.903	0.841	0.857
69	Tm	0.915	0.931	0.881	0.897	0.837	0.852
70	Yb	0.907	0.924	0.875	0.891	0.832	0.847
71	Lu	0.901	0.917	0.870	0.885	0.827	0.842
72	Hf	0.900	0.916	0.869	0.885	0.827	0.842
73	Ta	0.898	0.915	0.868	0.884	0.826	0.841
74	W	0.896	0.913	0.866	0.882	0.825	0.840
75	Re	0.894	0.910	0.864	0.879	0.823	0.838
76	Os	0.862	0.878	0.836	0.851	0.799	0.814
77	Ir	0.830	0.845	0.807	0 822	0.775	0 789
78	Pt	0.848	0.864	0.824	0.840	0.789	0 804
79	Au	0.866	0.882	0.840	0.855	0.803	0.818
80	Hg	0.878	0.894	0.851	0.866	0.813	0.828
81	Tl	0.896	0.912	0.867	0.883	0.827	0.842
82	Pb	0.906	0.922	0.876	0.891	0.835	0.849
83	Bi	0.911	0.928	0.881	0.897	0.839	0.855
84	Po	0.918	0.935	0.887	0.903	0.844	0.860
85	At	0.922	0.939	0.890	0.907	0.848	0.864
86	Rn	0.925	0.942	0.893	0.909	0.850	0.866
87	Fr	0.970	0.988	0.933	0.950	0.884	0.901
88	Ra	0.999	1.018	0.959	0.976	0.906	0 923
89	Ac	1.004	1.022	0.963	0.980	0.910	0.926
90	Th	1.006	1.025	0.964	0.982	0.911	0.929
91	Pa	0.995	1.014	0.956	0.973	0.904	0.921
92	U	0.991	1.010	0.952	0.969	0.902	0.918

Table 3 The corection factor q for various Z_1 and Z_2 combinations (continued)

Z_2 \ Z_1		Ne		Na		Si	
		Moliere	Yamamura	Moliere	Yamamura	Moliere	Yamamura
1	H	0.564	0.574	0.676	0.688	0.742	0.756
2	He	0.507	0.516	0.583	0.594	0.632	0.643
3	Li	0.498	0.507	0.566	0.576	0.609	0.621
4	Be	0.654	0.667	0.782	0.797	0.850	0.866
5	B	0.652	0.664	0.771	0.785	0.835	0.850
6	C	0.640	0.652	0.749	0.762	0.807	0.822
7	N	0.625	0.636	0.723	0.736	0.776	0.791
8	O	0.612	0.623	0.702	0.715	0.751	0.765
9	F	0.597	0.608	0.679	0.691	0.724	0.738
10	Ne	0.581	0.592	0.655	0.668	0.697	0.710
11	Na	0.655	0.668	0.753	0.767	0.804	0.819
12	Mg	0.675	0.688	0.778	0.792	0.830	0.846
13	Al	0.693	0.706	0.801	0.816	0.855	0.871
14	Si	0.697	0.710	0.804	0.819	0.857	0.873
15	P	0.696	0.709	0.800	0.815	0.851	0.867
16	S	0.695	0.708	0.797	0.811	0.847	0.863
17	Cl	0.692	0.705	0.790	0.804	0.839	0.854
18	Ar	0.686	0.699	0.781	0.795	0.828	0.843
19	K	0.735	0.749	0.846	0.862	0.899	0.916
20	Ca	0.754	0.768	0.870	0.886	0.924	0.941
21	Sc	0.749	0.763	0.861	0.877	0.914	0.931
22	Ti	0.743	0.757	0.852	0.868	0.903	0.920
23	V	0.737	0.751	0.841	0.857	0.891	0.908
24	Cr	0.746	0.760	0.853	0.868	0.903	0.919
25	Mn	0.725	0.738	0.822	0.837	0.868	0.884
26	Fe	0.717	0.731	0.810	0.825	0.855	0.871
27	Co	0.710	0.724	0.800	0.815	0.843	0.859
28	Ni	0.703	0.716	0.790	0.804	0.832	0.847
29	Cu	0.679	0.691	0.757	0.771	0.796	0.810
30	Zn	0.689	0.702	0.770	0.784	0.809	0.824
31	Ga	0.705	0.719	0.789	0.804	0.830	0.845
32	Ge	0.712	0.725	0.796	0.811	0.837	0.853
33	As	0.714	0.727	0.798	0.813	0.839	0.855
34	Se	0.716	0.730	0.800	0.816	0.841	0.857
35	Br	0.717	0.730	0.801	0.815	0.841	0.856
36	Kr	0.716	0.729	0.799	0.813	0.838	0 854
37	Rb	0.758	0 772	0.853	0.869	0.896	0.913
38	Sr	0.777	0.791	0.876	0.893	0.921	0.939
39	Y	0.777	0.792	0.876	0.892	0.921	0.938
40	Zr	0.776	0.791	0.873	0.890	0.918	0.935
41	Nb	0.759	0.773	0.850	0.865	0.892	0.908
42	Mo	0.756	0.769	0.845	0.860	0.886	0.902
43	Tc	0.769	0.784	0.862	0.878	0.904	0.921
44	Ru	0.751	0 766	0.838	0.854	0.878	0.894
45	Rh	0.749	0.762	0.833	0.849	0.873	0.889
46	Pd	0.716	0.729	0.791	0.806	0.827	0.843
47	Ag	0.730	0.744	0.809	0.824	0.846	0.862
48	Cd	0.751	0.766	0.835	0.851	0.874	0.890
49	In	0.765	0.779	0.852	0.868	0.891	0.908
50	Sn	0.771	0.786	0.859	0.875	0 899	0.916
51	Sb	0.775	0.789	0.863	0.879	0.903	0.919
52	Te	0.779	0.793	0.868	0.884	0 908	0.924
53	I	0.781	0.795	0.869	0.886	0.909	0.926
54	Xe	0.782	0.796	0.870	0.886	0.910	0.926
55	Cs	0.817	0.833	0.915	0.932	0.958	0.976
56	Ba	0.835	0.850	0.938	0.955	0.982	1.000
57	La	0.836	0 852	0.939	0.956	0.983	1.001
58	Ce	0.833	0.848	0.933	0.951	0.977	0.995
59	Pr	0.829	0.844	0.928	0.945	0.970	0.988
60	Nd	0.825	0.840	0.922	0.939	0.964	0.982
61	Pm	0.821	0.836	0.917	0.933	0.958	0.975
62	Sm	0.817	0.832	0.911	0.928	0.951	0.969
63	Eu	0.813	0.829	0.905	0.922	0.945	0.963
64	Gd	0.810	0.825	0 900	0.916	0.939	0.957
65	Tb	0.806	0.821	0.895	0.911	0.933	0.951
66	Dy	0.802	0.817	0.889	0.906	0.927	0.945
67	Ho	0.798	0.813	0.884	0.900	0.921	0.938
68	Er	0.794	0.809	0.878	0.894	0.915	0.932
69	Tm	0.791	0.805	0.873	0.889	0.910	0.926
70	Yb	0.786	0.801	0.867	0.883	0.903	0.920
71	Lu	0.783	0.797	0.863	0.878	0.898	0.914
72	Hf	0.783	0.797	0.862	0.878	0.898	0.914
73	Ta	0.782	0.797	0.861	0.877	0.896	0.912
74	W	0.781	0.796	0.859	0.875	0.894	0.910
75	Re	0.780	0.795	0.857	0.873	0.892	0.908
76	Os	0.760	0.774	0.832	0.847	0.865	0.881
77	Ir	0.739	0.753	0.806	0.820	0.836	0.852
78	Pt	0.752	0.766	0.821	0.837	0.853	0.869
79	Au	0.764	0 778	0.836	0.851	0.868	0.884
80	Hg	0.773	0.787	0.846	0.861	0.879	0.895
81	Tl	0.784	0.799	0.860	0.876	0.894	0.910
82	Pb	0.791	0.806	0.868	0.884	0.902	0.918
83	Bi	0.795	0.810	0.873	0.889	0.907	0.924
84	Po	0.800	0.815	0.878	0.895	0.913	0.930
85	At	0.803	0.818	0.882	0.898	0.916	0.933
86	Rn	0.805	0.820	0.884	0.900	0.919	0.935
87	Fr	0.834	0.850	0.920	0.938	0.957	0.975
88	Ra	0.853	0.869	0.943	0.961	0.981	0.999
89	Ac	0.856	0.872	0.947	0.965	0.985	1.003
90	Th	0.858	0.874	0.949	0.967	0.987	1.005
91	Pa	0.852	0.868	0.941	0.958	0.978	0.996
92	U	0.850	0.866	0.938	0.955	0.975	0.993

Table 3 The corection factor q for various Z_1 and Z_2 combinations (continued)

Z_2 \ Z_1		Ar		K		Ni	
		Moliere	Yamamura	Moliere	Yamamura	Moliere	Yamamura
1	H	0.720	0.733	0 800	0.815	0.740	0.753
2	He	0.626	0.637	0 678	0.690	0.652	0.664
3	Li	0.606	0.617	0.651	0.664	0.632	0.644
4	Be	0.814	0.830	0.904	0.921	0.821	0.836
5	B	0.803	0.818	0.885	0.902	0.810	0.825
6	C	0.780	0.794	0.855	0.871	0.790	0.805
7	N	0.754	0.769	0.821	0.837	0.767	0.781
8	O	0.733	0.747	0.794	0.809	0.747	0.761
9	F	0.710	0.723	0.764	0.779	0.726	0.739
10	Ne	0.686	0.699	0.735	0.749	0.703	0.716
11	Na	0.781	0.795	0.846	0.862	0.790	0.804
12	Mg	0.804	0.819	0.873	0.889	0.811	0.826
13	Al	0.825	0.841	0.897	0.914	0.830	0.845
14	Si	0.828	0.843	0.899	0.916	0.832	0.847
15	P	0.823	0.839	0.892	0.909	0.828	0.843
16	S	0.820	0.835	0.887	0.903	0.825	0.840
17	Cl	0.813	0.828	0.878	0.894	0.818	0.833
18	Ar	0.804	0.819	0.866	0.882	0.810	0.825
19	K	0.866	0.882	0.939	0.957	0.866	0.882
20	Ca	0.888	0.905	0.965	0.983	0.885	0.902
21	Sc	0.880	0.896	0.954	0.972	0.878	0.895
22	Ti	0.870	0.887	0.942	0.960	0.870	0.886
23	V	0.861	0.877	0.929	0.946	0.861	0.877
24	Cr	0.871	0.887	0.941	0.958	0.870	0.886
25	Mn	0.842	0.857	0.905	0.921	0.844	0.859
26	Fe	0.830	0.846	0.891	0.908	0.834	0.849
27	Co	0.820	0.836	0.878	0.895	0.824	0.840
28	Ni	0.810	0.825	0.866	0.882	0.815	0.830
29	Cu	0.778	0.792	0.828	0.843	0.786	0.800
30	Zn	0.790	0.805	0.842	0.857	0.797	0.811
31	Ga	0.809	0.824	0.863	0.879	0.814	0.829
32	Ge	0.816	0.831	0.870	0.886	0.820	0.835
33	As	0.818	0.833	0.872	0.888	0.822	0.837
34	Se	0.819	0.835	0.873	0.890	0.823	0.839
35	Br	0.819	0.834	0.873	0.889	0.823	0.838
36	Kr	0.817	0.832	0.870	0.886	0.821	0.836
37	Rb	0.869	0.885	0.930	0.947	0.869	0.885
38	Sr	0.891	0.908	0.955	0.973	0.889	0.905
39	Y	0.891	0.907	0.954	0.972	0.888	0.905
40	Zr	0.888	0.905	0.951	0.969	0.886	0.903
41	Nb	0.866	0.881	0.924	0.941	0.866	0.881
42	Mo	0.861	0.876	0.918	0.934	0.861	0.877
43	Tc	0.877	0.893	0.936	0.953	0.876	0.892
44	Ru	0.854	0.870	0.909	0.926	0.855	0.871
45	Rh	0.850	0.865	0.903	0.920	0.851	0.866
46	Pd	0.809	0.824	0.856	0.872	0.813	0.828
47	Ag	0.826	0.841	0.875	0.892	0.829	0.844
48	Cd	0.851	0.867	0.904	0.921	0.852	0.868
49	In	0.867	0.883	0.921	0.939	0.866	0.882
50	Sn	0.874	0.890	0.930	0.947	0.873	0.889
51	Sb	0.877	0.893	0.933	0.950	0.876	0.892
52	Te	0.882	0.898	0.938	0.955	0.880	0.896
53	I	0.883	0.900	0.939	0.957	0.881	0.898
54	Xe	0.884	0.900	0.940	0.957	0.882	0.898
55	Cs	0.927	0.944	0.989	1.008	0.921	0.938
56	Ba	0.948	0.965	1.013	1.032	0.940	0.957
57	La	0.949	0.967	1.014	1.033	0.941	0.959
58	Ce	0.944	0.962	1.008	1.027	0.937	0.954
59	Pr	0.938	0.956	1.001	1.020	0.932	0.949
60	Nd	0.933	0.950	0.994	1.013	0.927	0.944
61	Pm	0.928	0.944	0.988	1.006	0.922	0.939
62	Sm	0.922	0.939	0.981	0.999	0.917	0.934
63	Eu	0.916	0.934	0.974	0.993	0.912	0.929
64	Gd	0.911	0.928	0.968	0.986	0.907	0.924
65	Tb	0.906	0.923	0.962	0.980	0.903	0.919
66	Dy	0.901	0.918	0.956	0.974	0.898	0.915
67	Ho	0.896	0.912	0.949	0.967	0.893	0.909
68	Er	0.891	0.907	0.943	0.960	0.888	0.904
69	Tm	0.886	0.902	0.937	0.954	0.884	0.900
70	Yb	0.880	0.896	0.930	0.948	0.879	0.895
71	Lu	0.875	0.891	0.925	0.942	0.875	0.890
72	Hf	0.875	0.891	0.924	0.941	0.874	0.890
73	Ta	0.873	0.890	0.922	0.940	0.873	0.889
74	W	0.872	0.888	0.920	0.938	0.871	0.887
75	Re	0.870	0.886	0.918	0.935	0.870	0.885
76	Os	0.846	0.861	0.890	0.907	0.847	0.863
77	Ir	0.820	0.835	0.861	0.877	0.823	0.838
78	Pt	0.835	0.851	0.878	0.894	0.837	0.853
79	Au	0.849	0.865	0.893	0.910	0.850	0.866
80	Hg	0.859	0.874	0.904	0.921	0.859	0.875
81	Tl	0 872	0.889	0.919	0.937	0.872	0.888
82	Pb	0.880	0.896	0.928	0.945	0.879	0.895
83	Bi	0.885	0.901	0.933	0.950	0.883	0.899
84	Po	0.890	0.907	0.938	0.956	0.888	0.905
85	At	0.893	0.910	0.942	0.960	0.891	0.908
86	Rn	0.896	0.912	0.944	0.962	0.893	0.909
87	Fr	0.930	0.948	0.983	1.002	0.925	0 942
88	Ra	0.952	0.969	1.008	1.027	0.945	0.962
89	Ac	0.956	0.973	1.012	1.031	0.948	0.966
90	Th	0.957	0.975	1.013	1.033	0.950	0.967
91	Pa	0.950	0.967	1.005	1.024	0.943	0.960
92	U	0.947	0.964	1.001	1.020	0 940	0.957

Table 3 The corection factor q for various Z_1 and Z_2 combinations (continued)

Z_2 \ Z_1		Cu		Kr		Ag	
		Moliere	Yamamura	Moliere	Yamamura	Moliere	Yamamura
1	H	0.703	0.716	0.755	0.769	0.771	0.786
2	He	0.627	0.638	0.670	0.682	0.689	0.702
3	Li	0.610	0.622	0.649	0.662	0.669	0.682
4	Be	0.778	0.793	0.829	0.845	0.839	0.855
5	B	0.770	0.785	0.819	0.834	0.830	0.845
6	C	0.754	0.768	0.800	0.815	0.811	0.827
7	N	0.734	0.748	0.778	0.792	0.790	0.805
8	O	0.717	0.731	0.759	0.773	0.772	0.786
9	F	0.698	0.711	0.738	0.751	0.752	0.766
10	Ne	0.679	0.691	0.716	0.729	0.730	0.744
11	Na	0.757	0.771	0.799	0.813	0.809	0.824
12	Mg	0.776	0.790	0.818	0.833	0.827	0.843
13	Al	0.793	0.808	0.836	0.852	0.844	0.860
14	Si	0.796	0.810	0.838	0.854	0.846	0.862
15	P	0.793	0.807	0.834	0.850	0.842	0.858
16	S	0.790	0.805	0.831	0.846	0.839	0.855
17	Cl	0.785	0.800	0.825	0.840	0.834	0 849
18	Ar	0.778	0.792	0.817	0.832	0.826	0.841
19	K	0.828	0.843	0.870	0.886	0.875	0.892
20	Ca	0.846	0.861	0.888	0.905	0.893	0.909
21	Sc	0.840	0.855	0.882	0.898	0.886	0.903
22	Ti	0.833	0.848	0.874	0.890	0.879	0.895
23	V	0.825	0.841	0.865	0.881	0.871	0.887
24	Cr	0.834	0.849	0.874	0.890	0.879	0.895
25	Mn	0.811	0.825	0.849	0.864	0.855	0.871
26	Fe	0.802	0.817	0.839	0.855	0.846	0.862
27	Co	0.794	0.809	0.830	0.846	0.837	0.853
28	Ni	0.786	0.800	0.821	0.836	0.829	0.844
29	Cu	0.759	0.773	0.793	0.808	0.802	0.817
30	Zn	0.769	0.783	0.804	0.818	0.812	0.827
31	Ga	0.785	0.800	0.820	0.835	0.828	0.843
32	Ge	0.791	0.806	0.826	0.841	0.833	0.849
33	As	0.793	0.807	0.827	0.842	0.834	0.850
34	Se	0.794	0.809	0.829	0.844	0.836	0.852
35	Br	0.795	0.809	0.829	0.844	0.836	0.851
36	Kr	0.793	0.808	0.827	0.842	0.834	0.849
37	Rb	0.836	0.851	0.872	0.888	0.877	0.893
38	Sr	0.854	0.870	0.891	0.907	0.895	0.911
39	Y	0.854	0.870	0.891	0.907	0.894	0.911
40	Zr	0.852	0.868	0.889	0.905	0.892	0.909
41	Nb	0.834	0.849	0.869	0.885	0.874	0.890
42	Mo	0.830	0.845	0.865	0.880	0.870	0.886
43	Tc	0.844	0.859	0.879	0.895	0.883	0.899
44	Ru	0.825	0.840	0.859	0.875	0.864	0.880
45	Rh	0.821	0.837	0.855	0.870	0.860	0.876
46	Pd	0.787	0.802	0.819	0.834	0.826	0.841
47	Ag	0.802	0.817	0.834	0.849	0.840	0.856
48	Cd	0.823	0.838	0.856	0.872	0.861	0.877
49	In	0.836	0.852	0.870	0.886	0.874	0.891
50	Sn	0.843	0.858	0.876	0.892	0.880	0.897
51	Sb	0.845	0.861	0.879	0.895	0.883	0.899
52	Te	0.849	0.865	0.883	0.899	0.886	0.903
53	I	0.851	0.867	0.884	0.900	0.888	0.904
54	Xe	0.851	0.867	0.885	0.901	0.888	0.905
55	Cs	0.887	0.903	0.922	0.939	0.923	0.941
56	Ba	0.904	0.921	0.940	0.957	0.940	0.958
57	La	0.905	0.922	0.941	0.958	0.941	0.959
58	Ce	0.901	0.918	0.936	0.954	0.937	0.955
59	Pr	0.897	0.914	0.932	0.949	0.933	0.950
60	Nd	0.893	0.909	0.927	0.944	0.928	0.946
61	Pm	0.889	0.905	0.923	0.939	0.924	0.941
62	Sm	0.884	0.901	0.918	0.935	0.919	0.937
63	Eu	0.880	0.896	0.913	0.930	0.915	0.932
64	Gd	0.876	0.892	0.909	0.925	0.911	0.928
65	Tb	0.872	0.888	0.904	0.921	0.907	0.924
66	Dy	0.868	0.884	0.900	0.916	0.902	0.919
67	Ho	0.863	0.879	0.895	0.911	0.898	0.915
68	Er	0.859	0.875	0.890	0.907	0.893	0.910
69	Tm	0.855	0.871	0.886	0.902	0.889	0.906
70	Yb	0.850	0.866	0.881	0.897	0.885	0.901
71	Lu	0.847	0.862	0.877	0.893	0.881	0.897
72	Hf	0.847	0.862	0.877	0.892	0.880	0.897
73	Ta	0.845	0.861	0.875	0.892	0.879	0.896
74	W	0.844	0.860	0.874	0.890	0.878	0.894
75	Re	0.843	0.858	0.873	0.888	0.876	0.892
76	Os	0.822	0.837	0.851	0.866	0.855	0.871
77	Ir	0.800	0.815	0.828	0.843	0.833	0.849
78	Pt	0.813	0.828	0.841	0.857	0.846	0.862
79	Au	0.825	0.840	0.854	0.869	0.858	0.874
80	Hg	0.833	0.849	0.862	0.878	0.866	0.882
81	Tl	0.845	0.861	0.874	0.891	0.878	0.895
82	Pb	0.852	0.867	0.882	0.897	0.885	0.901
83	Bi	0.856	0.872	0.885	0.902	0.889	0.905
84	Po	0.860	0.877	0.890	0.907	0.893	0.910
85	At	0.863	0.879	0.893	0.909	0.895	0.912
86	Rn	0.865	0.881	0.895	0.911	0.898	0.914
87	Fr	0.895	0.911	0.925	0.942	0.926	0.944
88	Ra	0.913	0.930	0.944	0.962	0.945	0.962
89	Ac	0.916	0.933	0.948	0.965	0.948	0.965
90	Th	0.917	0.935	0.949	0.966	0.949	0.967
91	Pa	0.911	0.928	0.942	0.960	0.943	0.960
92	U	0.909	0.926	0.940	0.957	0.940	0.958

Table 3 The corection factor q for various Z_1 and Z_2 combinations (continued)

Z_2 \ Z_1		Xe		W		Au	
		Moliere	Yamamura	Moliere	Yamamura	Moliere	Yamamura
1	H	0.844	0.860	0.835	0.850	0.809	0 824
2	He	0.746	0.759	0.749	0 763	0.732	0 745
3	Li	0.720	0.734	0.727	0 740	0.712	0.725
4	Be	0.915	0.932	0.896	0.913	0.866	0.882
5	B	0.902	0.918	0.885	0.902	0.857	0.873
6	C	0.879	0.895	0.866	0.882	0.840	0.855
7	N	0.853	0.869	0.844	0.859	0.820	0.836
8	O	0.831	0.846	0.825	0.840	0.803	0.818
9	F	0.807	0.821	0.803	0.818	0.784	0.799
10	Ne	0.782	0.796	0.781	0.796	0 764	0.778
11	Na	0.870	0.886	0.859	0.875	0.836	0.851
12	Mg	0.890	0 907	0.877	0.893	0.852	0.868
13	Al	0.909	0.925	0.893	0.909	0.867	0.883
14	Si	0.910	0.926	0.894	0.910	0.868	0.884
15	P	0.905	0.921	0.890	0.906	0.865	0.881
16	S	0.901	0.917	0.886	0.902	0.862	0.877
17	Cl	0.893	0.910	0.880	0.896	0.856	0.872
18	Ar	0.884	0.900	0.872	0.888	0.849	0.865
19	K	0.940	0.957	0.920	0.938	0.893	0.910
20	Ca	0.959	0.976	0.937	0.954	0.909	0.925
21	Sc	0.951	0.968	0.930	0.947	0.903	0.920
22	Ti	0.942	0.959	0.922	0.940	0.896	0.913
23	V	0.932	0.949	0.914	0.931	0.889	0.905
24	Cr	0.941	0.958	0.922	0.939	0.896	0 912
25	Mn	0.913	0.930	0.898	0.915	0.874	0.890
26	Fe	0.902	0.919	0.889	0.905	0.866	0.882
27	Co	0.892	0.909	0.880	0.897	0.858	0.874
28	Ni	0.882	0.898	0.871	0.887	0.850	0.866
29	Cu	0.851	0.867	0.844	0.860	0.825	0.840
30	Zn	0.862	0.878	0.854	0.870	0.834	0.850
31	Ga	0.880	0.896	0.869	0.885	0.849	0.864
32	Ge	0.885	0.901	0.874	0.890	0.854	0.869
33	As	0.886	0.902	0.875	0.891	0.855	0.870
34	Se	0.888	0.904	0.876	0.893	0.856	0.872
35	Br	0.887	0.903	0.876	0 892	0.856	0.871
36	Kr	0.885	0.901	0.874	0.890	0.854	0.869
37	Rb	0.932	0.949	0.916	0.933	0.892	0.909
38	Sr	0.952	0.970	0.933	0.951	0.909	0.925
39	Y	0.951	0.969	0.933	0.950	0.908	0.925
40	Zr	0.949	0.966	0.931	0.948	0.906	0.923
41	Nb	0.928	0.944	0.912	0.929	0.890	0.906
42	Mo	0.923	0.939	0.908	0.925	0.886	0.902
43	Tc	0.937	0.954	0.921	0.938	0.898	0.914
44	Ru	0.915	0.932	0.902	0.919	0.880	0.897
45	Rh	0.911	0.928	0.898	0.915	0.877	0.893
46	Pd	0.873	0.889	0.864	0.880	0.845	0.861
47	Ag	0.888	0.905	0.878	0.894	0.858	0.874
48	Cd	0.911	0.928	0.898	0.915	0.877	0.894
49	In	0.926	0.943	0.911	0.928	0.889	0.906
50	Sn	0.932	0.949	0.917	0.934	0.895	0.911
51	Sb	0.935	0.952	0.919	0.936	0.897	0 913
52	Te	0.939	0.956	0.923	0.940	0.900	0.917
53	I	0.940	0.957	0.924	0.941	0.901	0.918
54	Xe	0.940	0.957	0.924	0.941	0.902	0.918
55	Cs	0.979	0.997	0.958	0.976	0.934	0 951
56	Ba	0.998	1.016	0.975	0.993	0.949	0.966
57	La	0.998	1.017	0.976	0.994	0.950	0.967
58	Ce	0.994	1 012	0.971	0.990	0.946	0.963
59	Pr	0.988	1.006	0.967	0.985	0.942	0.959
60	Nd	0.983	1.001	0.962	0.980	0.938	0.955
61	Pm	0.978	0.996	0.958	0.976	0.934	0.951
62	Sm	0.973	0.991	0.953	0.971	0.930	0.947
63	Eu	0.968	0.986	0.949	0.967	0.926	0.943
64	Gd	0.963	0.980	0.945	0.962	0.922	0.939
65	Tb	0.958	0.975	0.941	0.958	0.918	0.935
66	Dy	0.953	0.970	0.936	0.954	0.914	0.931
67	Ho	0.948	0.965	0.932	0.949	0.910	0.926
68	Er	0.943	0.960	0.927	0.944	0.906	0.922
69	Tm	0.938	0.955	0.923	0.940	0.902	0.919
70	Yb	0.932	0.949	0.918	0 935	0.898	0.914
71	Lu	0.928	0.945	0.914	0.931	0.894	0.910
72	Hf	0.927	0.944	0.914	0.930	0.894	0 910
73	Ta	0.926	0.943	0.912	0.929	0.893	0.909
74	W	0.924	0.941	0.911	0.928	0.891	0.908
75	Re	0.922	0.939	0.909	0.926	0.890	0.906
76	Os	0.899	0.916	0.889	0.905	0.871	0.887
77	Ir	0.875	0.891	0.867	0.883	0.850	0.865
78	Pt	0.889	0.905	0.879	0.896	0.862	0.878
79	Au	0.902	0.918	0.891	0.908	0.873	0.889
80	Hg	0.911	0.927	0.899	0.916	0.880	0.896
81	Tl	0.923	0.940	0.910	0.927	0.891	0.908
82	Pb	0.931	0.947	0.917	0.934	0.897	0.913
83	Bi	0.934	0.951	0.921	0.938	0.901	0.917
84	Po	0.939	0.956	0.925	0.942	0.905	0 921
85	At	0.942	0.959	0.927	0.945	0.907	0.924
86	Rn	0.944	0.961	0.929	0.946	0.909	0.925
87	Fr	0.976	0.994	0.957	0.975	0.935	0.953
88	Ra	0.995	1.013	0.975	0.993	0.952	0.969
89	Ac	0.999	1.017	0.978	0.996	0.954	0.972
90	Th	1.000	1.018	0.979	0.997	0.955	0 973
91	Pa	0.993	1.011	0.973	0.991	0.950	0.967
92	U	0.990	1.008	0.971	0.989	0.948	0.965

Table 4 The comparison between the q-values determined by the ICISS computer analysis and the present q-values

Ion	Energy (keV)	Target	ICISS-q	q (theory)	Ref.
He^+	0.5	Ni(001)	0.7	0.65	[15]
	1.5	Ni(110)	0.6	0.65	[16]
	1.5	Ni(110)	0.7	0.65	[17]
	1.5	Cu(110)	0.7	0.63	[18]
	0.6	Cu(110)	0.67	0.63	[19]
	5.0	Au	0.60	0.73	[20]
	2.0	NiAl(111)	0.60 (Ni)	0.65	[11]
			0.60 (Al)	0.63	
	3.0	NiAl(001)	0.7 (Ni)	0.65	[21]
			0.7 (Al)	0.63	
	1.0	TiC	0.90 (Ti)	0.79	[22]
Li^+	5.0	Si	0.735	0.61	[23]
	1.0	Ag	0.70	0.67	[24]
	5.0	Cu(110)	0.6	0.61	[25]
	1.0	NbC(111)	0.85 (Nb)	0.69	[26]
	0.5 and 1.0	Sn/Pt(110)	0.76 (Sn)	0.71	[27]
			0.80 (Pt)	0.70	
	5.0	Au	0.70	0.71	[20]
	5.0	Au	0.735	0.71	[23]
	5.0	$NiSi_2$(001)	0.6 (Si)	0.61	[28]
			0.6 (Ni)	0.63	
	1.0	HfC(111)	0.70 (C)	0.54	[29]
Ne^+	2.5	Ni(001)	0.7	0.70	[15]
	2.5	Ni	0.7	0.70	[30]
	3.0	Ni(111)	0.7	0.70	[31]
	5.0	Cu(110)	0.77	0.68	[19]
	5.0	S/Ni(001)	0.63 (Ni)	0.70	[32]
			0.72 (S)	0.70	
	5.0	Ag(001)	0.69	0.73	[33]
	3.0	Ag(111)	0.62	0.73	[34]
	2.0	Pt(111)	0.85	0.75	[35]
	2.0	Au(110)	0.8	0.76	[36]
	3.0	Pb	0.9	0.75	[31]
Na^+	2.0	Cu(110)	0.65	0.76	[37]
	2.0	Pt	0.65	0.82	[37]
	1.45	NiAl(100)	0.8 (Ni)	0.79	[38]
			0.8 (Al)	0.80	

Recent Issues of NIFS-DATA Series

NIFS-DATA-11 T. Kaneko, T. Nishihara, T. Taguchi, K. Nakagawa, M. Murakami, M Hosono, S Matsushita, K. Hayase, M.Moriya, Y.Matsukuma, K.Miura and Hiro Tawara,
Partial and Total Electronic StoppingCross Sections of Atoms for a Singly Charged Helium Ion: Part 1; Mar. 1991

NIFS-DATA-12 Hiro Tawara,
Total and Partial Cross Sections of Electron Transfer Processes for Be^{q+} and B^{q+} Ions in Collisions with H, H_2 and He Gas Targets -Status in 1991-; June 1991

NIFS-DATA-13 T. Kaneko, M. Nishikori, N. Yamato, T. Fukushima, T. Fujikawa, S. Fujita, K. Miki, Y. Mitsunobu, K. Yasuhara, H. Yoshida and Hiro Tawara,
Partial and Total Electronic Stopping Cross Sections of Atoms for a Singly Charged Helium Ion : Part II; Aug. 1991

NIFS-DATA-14 T. Kato, K. Masai and M. Arnaud,
Comparison of Ionization Rate Coefficients of Ions from Hydrogen through Nickel ; Sep. 1991

NIFS-DATA-15 T. Kato, Y. Itikawa and K. Sakimoto,
Compilation of Excitation Cross Sections for He Atoms by Electron Impact; Mar. 1992

NIFS-DATA-16 T. Fujimoto, F. Koike, K. Sakimoto, R. Okasaka, K. Kawasaki, K. Takiyama, T. Oda and T. Kato,
Atomic Processes Relevant to Polarization Plasma Spectroscopy ; Apr. 1992

NIFS-DATA-17 H Tawara,
Electron Stripping Cross Sections for Light Impurity Ions in Colliding with Atomic Hydrogens Relevant to Fusion Research; Apr. 1992

NIFS-DATA-18 T. Kato,
Electron Impact Excitation Cross Sections and Effective Collision Strengths of N Atom and N-Like Ions -A Review of Available Data and Recommendations- ; Sep. 1992

NIFS-DATA-19 Hiro Tawara,
Atomic and Molecular Data for H_2O, CO & CO_2 Relevant to Edge Plasma Impurities, Oct. 1992

NIFS-DATA-20 Hiro. Tawara,
Bibliography on Electron Transfer Processes in Ion-Ion/Atom/Molecule Collisions -Updated 1993-; Apr. 1993

NIFS-DATA-21 J. Dubau and T. Kato,
Dielectronic Recombination Rate Coefficients to the Excited States of C I from C II; Aug. 1994

NIFS-DATA-22 T. Kawamura, T. Ono, Y. Yamamura,
Simulation Calculations of Physical Sputtering and Reflection Coefficient of Plasma-Irradiated Carbon Surface; Aug. 1994

NIFS-DATA-23 Y. Yamamura and H. Tawara,
Energy Dependence of Ion-Induced Sputtering Yields from Monoatomic Solids at Normal Incidence; Mar. 1995

NIFS-DATA-24 T. Kato, U. Safronova, A. Shlyaptseva, M. Cornille, J. Dubau,
Comparison of the Satellite Lines of H-like and He-like Spectra; Apr. 1995

NIFS-DATA-25 H. Tawara,
Roles of Atomic and Molecular Processes in Fusion Plasma Researches - from the cradle (plasma production) to the grave (after-burning) -; May 1995

NIFS-DATA-26 N. Toshima and H. Tawara
Excitation, Ionization, and Electron Capture Cross Sections of Atomic Hydrogen in Collisions with Multiply Charged Ions; July 1995

NIFS-DATA-27 V.P. Shevelko, H. Tawara and E.Salzborn,
Multiple-Ionization Cross Sections of Atoms and Positive Ions by Electron Impact; July 1995

NIFS-DATA-28 V.P. Shevelko and H. Tawara,
Cross Sections for Electron-Impact Induced Transitions Between Excited States in He: n, n'=2,3 and 4; Aug. 1995

NIFS-DATA-29 U.I. Safronova, M.S. Safronova and T. Kato,
Cross Sections and Rate Coefficients for Excitation of Δn = 1 Transitions in Li-like Ions with 6<Z<42; Sep. 1995

NIFS-DATA-30 T. Nishikawa, T. Kawachi, K. Nishihara and T. Fujimoto,
Recommended Atomic Data for Collisional-Radiative Model of Li-like Ions and Gain Calculation for Li-like Al Ions in the Recombining Plasma; Sep. 1995

NIFS-DATA-31 Y. Yamamura, K. Sakaoka and H. Tawara,
Computer Simulation and Data Compilation of Sputtering Yield by Hydrogen Isotopes ($^1H^+$, $^2D^+$, $^3T^+$) and Helium ($^4He^+$) Ion Impact from Monatomic Solids at Normal Incidence; Oct. 1995

NIFS-DATA-32 T. Kato, U. Safronova and M. Ohira,
Dielectronic Recombination Rate Coefficients to the Excited States of CII from CIII; Feb. 1996

NIFS-DATA-33 K.J. Snowdon and H. Tawara,
Low Energy Molecule-Surface Interaction Processes of Relevance to Next-Generation Fusion Devices; Mar. 1996

NIFS-DATA-34 T. Ono, T. Kawamura, K. Ishii and Y. Yamamura,
Sputtering Yield Formula for B_4C Irradiated with Monoenergetic Ions at Normal Incidence; Apr. 1996

NIFS-DATA-35 I. Murakami, T. Kato and J. Dubau.
UV and X-Ray Spectral Lines of Be-Like Fe Ion for Plasma Diagnostics; Apr. 1996

NIFS-DATA-36 K. Moribayashi and T. Kato,
Dielectronic Recombination of Be-like Fe Ion; Apr. 1996

NIFS-DATA-37 U. Safronova, T. Kato and M. Ohira,
Dielectronic Recombination Rate Coefficients to the Excited States of CIII from CIV; July 1996

NIFS-DATA-38 T. Fujimoto, H. Sahara, G. Csanak and S. Grabbe,
Atomic States and Collisional Relaxation in Plasma Polarization Spectroscopy: Axially Symmetric Case; Oct. 1996

NIFS-DATA-39 H. Tawara (Ed.)
Present Status on Atomic and Molecular Data Relevant to Fusion Plasma Diagnostics and Modeling; Jan. 1997

NIFS-DATA-40 Inga Yu. Tolstikhina,
LS-Averaged 1/Z Method as a Tool of Studying the Interactions of Highly Charged Ions with a Metal Surface; Jan. 1997

NIFS-DATA-41 K. Moribayashi and T. Kato,
Atomic Nuclear Charge Scaling for Dielectronic Recombination to Be-like Ions; Apr. 1997

NIFS-DATA-42 H. Tawara,
Bibliography on Electron Transfer Processes in Ion-ion / Atom / Molecule Collisions -Updated 1997 -; May 1997

NIFS-DATA-43 M. Goto and T. Fujimoto,
Collisional-radiative Model for Neutral Helium in Plasma: Excitation Cross Section and Singlet-triplet Wavefunction Mixing; Oct. 1997

NIFS-DATA-44 J. Dubau, T. Kato and U.I. Safronova,
Dielectronic Recombination Rate Coefficients to the Excited States of CI From CII; Jan. 1998

NIFS-DATA-45 Y. Yamamura, W. Takeuchi and T. Kawamura,
The Screening Length of Interatomic Potential in Atomic Collisions; Mar. 1998