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SHELL CORRECTIONS FOR K- AND L-ELECTRONS

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Abstract: Walske's asymptotic stopping power formulae for K- and L-shell electrons are extended to cover the entire periodic table. Extensive use is made of the various existing formulae in numerical calculations.

1. Introduction

When a heavy ion such as a proton or α-particle passes through matter, it may lose its energy to the atomic electrons of the target. The energy loss per unit path length is given by the Bethe [1,2]) formula

$$-\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{4\pi e^4 z^2}{mv^2} NB, \tag{1}$$

where the stopping number B is the sum of contributions from the various atomic shells

$$B = \sum_s B_s \qquad (s = \mathrm{K, L, M}, \ldots). \tag{2}$$

The stopping number B_s for the shell labelled s is defined as

$$B_s(\theta_s, \eta_s) = \int_{W_{\min} = \theta_s/s^2}^{\infty} W \mathrm{d}W I(\eta_s, W). \tag{3}$$

The excitation function I (η_s, W) is defined in terms of the form factor $F_{Ws}(Q)$ by

$$I(\eta_s, W) = \int_{W^2/4\eta_s}^{\infty} \frac{\mathrm{d}Q}{Q^2} |F_{Ws}(Q)|^2. \tag{4}$$

In the above formulae, ez is the charge of the incident particle, v its velocity, m the electron mass and N the number of target atoms per unit volume; η_s is proportional to the energy E of the incident particle and given by $\eta_s = (m/M)E/Z_s^2 R$, where Z_s is the effective nuclear charge for the s-selection, and R is the Rydberg constant; W is the energy transfer in units of $Z_s^2 R$ and θ_s the ratio of the observed ionization potential to $Z_s^2 R/s^2$, s being the principal quantum number of the s-shell.

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TABLE 1
Coefficients of asymptotic stopping number formulae of K electrons

θ_K	S_K	T_K	U_K	V_K
0.64	1.9477	2.5222	1.9999	8.3410
0.65	1.9232	2.5125	2.0134	8.3373
0.66	1.8996	2.5026	2.0258	8.3340
0.68	1.8550	2.4821	2.0478	8.3287
0.70	1.8137	2.4608	2.0662	8.3247
0.72	1.7754	2.4388	2.0817	8.3219
0.74	1.7396	2.4163	2.0945	8.3201
0.75	1.7223	2.4044	2.0999	8.3194
0.76	1.7063	2.3933	2.1049	8.3191
0.78	1.6752	2.3701	2.1132	8.3188
0.80	1.6461	2.3466	2.1197	8.3191
0.82	1.6189	2.3229	2.1246	8.3199
0.84	1.5933	2.2992	2.1280	8.3211
0.85	1.5811	2.2872	2.1292	8.3218
0.86	1.5693	2.2753	2.1301	8.3226
0.88	1.5467	2.2515	2.1310	8.3244
0.90	1.5254	2.2277	2.1310	8.3264
0.92	1.5053	2.2040	2.1300	8.3285
0.94	1.4863	2.1804	2.1283	8.3308
0.95	1.4772	2.1686	2.1271	8.3320

TABLE 2
Coefficients of asymptotic stopping number formulae of L electrons

θ_L	S_L	T_L	U_L
0.24	15.3343	35.0669	0.1215
0.26	13.9389	33.4344	0.5265
0.28	12.7909	32.0073	0.8411
0.30	11.8343	30.7466	1.0878
0.32	11.0283	29.6226	1.2828
0.34	10.3424	28.6128	1.4379
0.35	10.0371	28.1449	1.5032
0.36	9.7537	27.6991	1.5617
0.38	9.2443	26.8674	1.6608
0.40	8.8005	26.1061	1.7401
0.42	8.4114	25.4058	1.8036
0.44	8.0683	24.7587	1.8543
0.45	7.9117	24.4531	1.8756
0.46	7.7641	24.1583	1.8945
0.48	7.4931	23.5992	1.9262
0.50	7.2506	23.0771	1.9508
0.52	7.0327	22.5880	1.9696
0.54	6.8362	22.1285	1.9836
0.55	6.7452	21.9090	1.9890
0.56	6.6584	21.6958	1.9935
0.58	6.4969	21.2872	2.0001
0.60	6.3498	20.9006	2.0039
0.62	6.2154	20.5341	2.0053
0.64	6.0923	20.1859	2.0049
0.65	6.0345	20.0183	2.0040
0.66	5.9792	19.8546	2.0028

An alternative version of eq. (2) which exhibits the main trend of the velocity dependence of the stopping power is

$$B = Z \ln \left(\frac{2mv^2}{I_{\mathrm{av}}}\right) - \sum_s C_s(\theta_s, \eta_s), \tag{5}$$

where Z is the nuclear charge, I_{av} the average ionization potential of the atom and the quantities C_s the binding corrections for K-, L-, M-. . . shells.

The importance of the shell corrections has long been recognized, and a number of calculations and estimates are available [5-11]. However, it seems that these corrections are not available for the entire periodic table and for many incident energies. It is the purpose of the present paper to obtain binding corrections for K- and L-shells to cover the entire periodic table.

The procedure is similar to Walske's calculations for the L-shell. However, when necessary, changes were made for the convenience of the computer. Since it is intended to extend these calculations to higher shells and their subshells, it seemed pertinent to describe the method for the K-shell in sect. 2. Numerical results are listed in tables 1 and 2.

2. Method of calculation

The method consists of casting expression (3) into following form

$$\int_{\theta_{\mathrm{K}}}^{\infty} W \mathrm{d}W I(\eta_{\mathrm{K}}, W) = B_{\mathrm{K}}(0, \eta_{\mathrm{K}}) - [F_{\mathrm{K}}(\eta_{\mathrm{K}}) - D_{\mathrm{K}}(\theta_{\mathrm{K}}, \eta_{\mathrm{K}})], \tag{6}$$

where

$$B_{\mathrm{K}}(0, \eta_{\mathrm{K}}) = \sum_{n=1}^{\infty} \left(1 - \frac{1}{n^2}\right) I(\eta_{\mathrm{K}}, n) + \int_{1}^{\infty} W \mathrm{d}W I(\eta_{\mathrm{K}}, W), \tag{7}$$

$$F_{\mathrm{K}}(\eta_{\mathrm{K}}) = \sum_{n=1}^{\infty} \left(1 - \frac{1}{n^2}\right) I(\eta_{\mathrm{K}}, n), \tag{8}$$

$$D_{\mathrm{K}}(\theta_{\mathrm{K}}, \eta_{\mathrm{K}}) = \int_{\theta_{\mathrm{K}}}^{1} W \mathrm{d}W I(\eta_{\mathrm{K}}, W). \tag{9}$$

Physically, $B_{\mathrm{K}}(0, \eta_{\mathrm{K}})$ is to be understood as twice the stopping number of hydrogen; $F_{\mathrm{K}}(\eta_{\mathrm{K}})$ is the contribution to $B_{\mathrm{K}}(\theta_{\mathrm{K}}, \eta_{\mathrm{K}})$ of the transitions to all the discrete states and $D_{\mathrm{K}}(\theta_{\mathrm{K}}, \eta_{\mathrm{K}})$ the contribution to B_{K} of the part of the continuous spectrum between $W = \theta_{\mathrm{K}}$ and $W = 1$ arising from the outer screening.

Even though $D_{\mathrm{K}}(\theta_{\mathrm{K}}, \eta_{\mathrm{K}})$ involves continuum transitions, we can still use the discrete form factor $F_{n\mathrm{K}}(Q)$ in its evaluation [12]. Thus eqs. (9) and (4) with $W = 1 - 1/n^2$ become

$$D_{\mathrm{K}}(\theta_{\mathrm{K}}, \eta_{\mathrm{K}}) = \int_{(1-\theta_{\mathrm{K}})^{-\frac{1}{2}}}^{\infty} \left(1 - \frac{1}{n^2}\right) I(\eta_{\mathrm{K}}, n) \mathrm{d}n, \tag{10}$$

$$I(\eta_{\mathrm{K}}, n) = \int_{W^2/4\eta_{\mathrm{K}}}^{\infty} \frac{\mathrm{d}Q}{Q^2} |F_{n\mathrm{K}}(Q)|^2. \tag{11}$$

Brown [6]) and Walske [7,8,12]) have expanded $I(\eta_K, n)$ in powers of $1/\eta_K$ and obtained

$$I(\eta_K, n) \approx |X_{nK}|^2 \left\{ H(n) + \ln \eta_K - \frac{1-9/n^2}{4\eta_K} + \frac{5-14/n^2-39/n^4}{32\eta_K^2} \right\}, \tag{12}$$

where

$$|X_{nK}|^2 = \frac{2^8}{3n^3} \frac{\left(1-\frac{1}{n}\right)^{2n-5}}{\left(1+\frac{1}{n}\right)^{2n+5}},$$

$$H(n) = \overline{M}_n + 3[\gamma(\gamma+1)]^{\frac{1}{2}} \overline{L_4^{n-3}}(n) - \gamma \sum_{k=0}^{4} \overline{L_k^{n-3}}(n). \tag{13}$$

The quantities $\overline{M}_n$ and $\overline{L}(n)$ are defined in terms of the following integrals:

$$L_k^m = \int_{z_0}^{1/\gamma} (1-\gamma z)^k (1+z)^m \mathrm{d}z, \tag{14}$$

$$M_n = \int_{z_0}^{1/\gamma} \mathrm{d}z \frac{(1+z)^{n-3}}{z}, \tag{15}$$

with

$$\gamma = \frac{(n-1)^2}{4n}, \qquad z_0 = \frac{W^2/4\eta_K}{\gamma(b+W^2/4\eta_K)}, \qquad b = \left(1+\frac{1}{n}\right)^2.$$

The quantities $\overline{M}_n$ and $\overline{L_k^m}(n)$ in eq. (13) are the constant energy-independent parts of the asymptotic expansions of M_n and L_k^m for large η_K

$$\overline{L_k^m} = -\left[\frac{1}{m+1} + \frac{\gamma k}{(m+1)(m+2)} + \ldots + \frac{\gamma_k^{k-1}(k-1)\ldots 3\cdot 2}{(m+1)(m+2)\ldots(m+k)} + \frac{\gamma^k k! \left[1-\left(1+\frac{1}{\gamma}\right)^{m+k+1}\right]}{(m+1)(m+2)\ldots(m+k+1)}\right].$$

As discussed by Brown, expression (15) can be calculated exactly only for discrete values of n. We have found it convenient to cast this integral in the form

$$M_n \approx \overline{M}_n + \ln \eta_K + \frac{C}{\eta_K}, \tag{16}$$

where

$$C = \frac{-\frac{7}{4}n^2+7n+1}{4n^2}.$$

The integral (15) was numerically evaluated for $\eta_K = 100$. For various discrete values of n, good agreement was found with the exact results. Using the computed values of M_n in eq. (16), $\overline{M}_n$ was obtained. Thus eq. (12) can be evaluated for any value of n for any η.

Following Walske, we can now evaluate $F_K(\eta_K) - D_K(\theta_K, \eta_K)$ in the following way:

$$F_K(\eta_K) - D_K(\theta_K, \eta_K) = \sum_{n=1}^{\infty} \left(1 - \frac{1}{n^2}\right) I(\eta_K, n) - \int_{(1-\theta_K)^{-\frac{1}{2}}}^{\infty} \left(1 - \frac{1}{n^2}\right) I(\eta_K, n)\mathrm{d}n.$$

Using the Euler-Maclaurin summation formula, this can be put as

$$F_K(\eta_K) - D_K(\theta_K, \eta_K) \approx -\int_{(1-\theta_K)^{-\frac{1}{2}}}^{7} \left(1 - \frac{1}{n^2}\right) I(\eta_K, n)\mathrm{d}n$$

$$+ \sum_{n=1}^{6} \left(1 - \frac{1}{n^2}\right) I(\eta_K, n) + \frac{1}{2}\left(1 - \frac{1}{n^2}\right) I(\eta_K, n)\Big|_{n=7} + \tfrac{1}{12}\Delta' - \tfrac{1}{720}\Delta''', \tag{17}$$

where

$$\Delta' = -\frac{\mathrm{d}}{\mathrm{d}n}\left[\left(1 - \frac{1}{n^2}\right) I(\eta_K, n)\right]\Bigg|_{n=7},$$

$$\Delta''' = -\frac{\mathrm{d}^3}{\mathrm{d}n^3}\left[\left(1 - \frac{1}{n^2}\right) I(\eta_K, n)\right]\Bigg|_{n=7}.$$

According to Walske, the expression for $B_K(0, \eta_K)$ is

$$B_K(0, \eta_K) = 2 \ln \eta_K + 2.57861 - 2\eta_K^{-1} - (\tfrac{25}{3})\eta_K^{-2}. \tag{18}$$

Using eqs. (6), (12), (17) and (18), we have the asymptotic expression for the stopping number for any element to second order as

$$B_K(\theta_K, \eta_K) = S_K(\theta_K) \ln \eta_K + T_K(\theta_K) - C_K(\theta_K, \eta_K), \tag{19}$$

with

$$C_K(\theta_K, \eta_K) = U_K(\theta_K)\eta_K^{-1} + V_K(\theta_K)\eta_K^{-2}. \tag{20}$$

Following the above procedure for large η_L, one can put eq. (3) in the form

$$B_L(\theta_L, \eta_L) = S_L(\theta_L) \ln \eta_L + T_L(\theta_L) - C_L(\theta_L, \eta_L),$$

where

$$C_L(\theta_L, \eta_L) = U_L(\theta_L)\eta_L^{-1} + V_L(\theta_L)\eta_L^{-2} + \dots \tag{21}$$

3. Binding corrections for K- and L-shells

A program was written in GAT language for UNIVAC 1105. The program included the evaluation of the constant term (function of n only), coefficients of $\ln \eta_K$, $1/\eta_K$ and $1/\eta_{K^2}$ in $I(\eta_K, n)$, and most of the numerical work needed to evaluate coefficients $S_K(\theta_K)$, $T_K(\theta_K)$ and $V_K(\theta_K)$. A simple program in FORTRAN II for IBM 1620 evaluated † the coefficients $U_K(\theta_K)$. These values were obtained for a large num-

† We thank Dr. M. Pritchard for his help.

TABLE 3

Stopping number contribution of K electrons, $B_K(\theta_K, \eta_K)$

η_K/θ_K	0.95	0.94	0.92	0.90	0.88	0.86	0.85	0.84	0.82	0.80
0.005	1.34782–8[a]	1.46132–8	1.72179–8	2.03521–8	2.41370–8	2.87247–8	3.13778–8	3.43072–8	4.11274–8	4.94946–8
0.007	6.87555–8	7.44373–8	8.74397–8	1.03022–7	1.21760–7	1.44370–7	1.57398–7	1.71747–7	2.05023–7	2.45620–7
0.01	3.78413–7	4.08831–7	4.78154–7	5.60760–7	6.59478–7	7.77847–7	8.45709–7	9.20187–7	1.09192–6	1.29981–6
0.015	2.53200–6	2.72664–6	3.16738–6	3.68791–6	4.30423–6	5.03578–6	5.45200–6	5.90633–6	6.94501–6	8.18757–6
0.02	9.43891–6	1.01339–5	1.16984–5	1.35313–5	1.56829–5	1.82138–5	1.96439–5	2.11973–5	2.47216–5	2.88935–5
0.03	5.67088–5	6.05576–5	6.91311–5	7.90324–5	9.04832–5	1.03744–4	1.11147–4	1.19122–4	1.36980–4	1.57744–4
0.04	1.91576–4	2.03626–4	2.30230–4	2.60584–4	2.95248–4	3.34870–4	3.56771–4	3.80200–4	4.32104–4	4.91584–4
0.05	4.74226–4	5.02006–4	5.62872–4	6.31597–4	7.09244–4	7.97023–4	8.45134–4	8.96410–4	1.00867–3	1.13590–3
0.06	9.67285–4	1.02029–3	1.13566–3	1.26476–3	1.40928–3	1.57113–3	1.65921–3	1.75244–3	1.95562–3	2.18336–3
0.08	2.81537–3	2.95200–3	3.24599–3	3.57027–3	3.92793–3	4.32246–3	4.53473–3	4.75768–3	5.23785–3	5.76765–3
0.1	6.14216–3	6.40864–3	6.97750–3	7.59781–3	8.27424–3	9.01187–3	9.40534–3	9.81623–3	1.06934–2	1.16498–2
0.15	2.23096–2	2.30790–2	2.46978–2	2.64300–2	2.82832–2	3.02661–2	3.13090–2	3.23878–2	3.46580–2	3.70873–2
0.2	5.04022–2	5.18492–2	5.48682–2	5.80617–2	6.14403–2	6.50152–2	6.68798–2	6.87981–2	7.28020–2	7.70407–2
0.3	1.38018–1	1.41026–1	1.47244–1	1.53743–1	1.60536–1	1.67641–1	1.71315–1	1.75074–1	1.82852–1	1.90997–1
0.4	2.56001–1	2.60576–1	2.69992–1	2.79776–1	2.89946–1	3.00525–1	3.05974–1	3.11533–1	3.22994–1	3.34935–1
0.5	3.92181–1	3.98213–1	4.10597–1	4.23427–1	4.36726–1	4.50519–1	4.57610–1	4.64834–1	4.79700–1	4.95148–1
0.6	5.37913–1	5.45268–1	5.60350–1	5.75948–1	5.92092–1	6.08811–1	6.17396–1	6.26136–1	6.44104–1	6.62752–1
0.7	6.87470–1	6.96021–1	7.13543–1	7.31650–1	7.50373–1	7.69748–1	7.79591–1	7.89811–1	8.10602–1	8.32167–1
0.8	8.37159–1	8.46790–1	8.66525–1	8.86910–1	9.07979–1	9.29772–1	9.40953–1	9.52331–1	9.75701–1	9.99934–1
1.0	1.12850	1.14002	1.16362	1.18799	1.21317	1.23921	1.25257	1.26616	1.29408	1.32303
1.2	1.40232	1.41545	1.44232	1.47007	1.49875	1.52842	1.54364	1.55913	1.59095	1.62396
1.4	1.65584	1.67034	1.70004	1.73072	1.76244	1.79526	1.81210	1.82925	1.86448	1.90104
1.5	1.77496	1.79009	1.82107	1.85307	1.88617	1.92042	1.93800	1.95590	1.99269	2.03087
1.7	1.99863	2.01490	2.04822	2.08265	2.11827	2.15555	2.17409	2.19337	2.23302	2.27419
2.0	2.29325	2.31100	2.34738	2.38501	2.42395	2.46429	2.48401	2.50612	2.54955	2.59468
3.0	3.08887	3.11036	3.15445	3.20013	3.24748	3.29664	3.32192	3.34770	3.40081	3.45611
5.0	4.07599	4.10219	4.15606	4.21199	4.27010	4.33056	4.36172	4.39353	4.45918	4.52772
7.0	4.69647	4.72577	4.78608	4.84877	4.91402	4.98200	5.01707	5.05290	5.12695	5.20436
10.0	5.32590	5.35848	5.42560	5.49547	5.56830	5.64429	5.68353	5.72366	5.80666	5.89359

[a]) For 1.34782–8 read 1.34782×10^{-8}.

Table 3 (continued)

η_K/θ_K	0.78	0.76	0.75	0.74	0.72	0.70	0.68	0.66	0.65	0.64
0.005	5.98040–8	7.25636–8	8.00602–8	8.84294–8	1.08253–7	1.33148–7	1.64573–7	2.04459–7	2.28346–7	2.55370–7
0.007	2.95345–7	3.56497–7	3.92247–7	4.32017–7	5.25688–7	6.42391–7	7.88464–7	9.72171–7	1.08140–6	1.20435–6
0.01	1.55232–6	1.86011–6	2.03881–6	2.23662–6	2.69889–6	3.26860–6	3.26860–6	4.84882–6	5.36428–6	5.94048–6
0.015	9.67802–6	1.14707–5	1.25008–5	1.36329–5	1.62480–5	1.94200–5	2.32783–5	2.79850–5	3.07181–5	3.37432–5
0.02	3.38425–5	3.97259–5	4.30763–5	4.67351–5	5.51033–5	6.51154–5	7.71154–5	9.15431–5	9.98212–5	1.08909–4
0.03	1.81920–4	2.10106–4	2.25918–4	2.43007–4	2.81460–4	3.26458–4	3.79175–4	4.41006–4	4.75845–4	5.13606–4
0.04	5.59802–4	6.38103–4	6.81511–4	7.28042–4	8.31425–4	9.50341–4	1.08721–3	1.24485–3	1.33245–3	1.42650–3
0.05	1.28002–3	1.44336–3	1.53305–3	1.62855–3	1.83861–3	2.07396–3	2.34750–3	2.65469–3	2.82358–3	3.00358–3
0.06	2.42872–3	2.72510–3	2.88111–3	3.04636–3	3.40681–3	3.81132–3	4.26536–3	4.77507–3	5.05294–3	5.34739–3
0.08	6.35222–3	6.99730–3	7.34446–3	7.70916–3	8.49478–3	9.36187–3	1.03189–2	1.13754–2	1.19441–2	1.25417–2
0.1	1.26929–2	1.38803–2	1.44371–2	1.50707–2	1.64235–2	1.78989–2	1.95083–2	2.12640–2	2.22009–2	2.31795–2
0.15	3.96872–2	4.24699–2	4.39340–2	4.54488–2	4.86383–2	5.20542–2	5.57135–2	5.96350–2	6.17003–2	6.38389–2
0.2	8.15290–2	8.62830–2	8.87650–2	9.13200–2	9.66589–2	1.02320–1	1.08326–1	1.14701–1	1.18035–1	1.21472–1
0.3	1.99528–1	2.08471–1	2.13103–1	2.17848–1	2.27689–1	2.38022–1	2.48882–1	2.60304–1	2.66239–1	2.72329–1
0.4	3.47383–1	3.60369–1	3.67073–1	3.73925–1	3.88089–1	4.02900–1	4.18404–1	4.34647–1	4.43063–1	4.51685–1
0.5	5.11214–1	5.27935–1	5.36554–1	5.45354–1	5.63515–1	5.82470–1	6.02273–1	6.22986–1	6.33705–1	6.44677–1
0.6	6.82122–1	7.02260–1	7.12631–1	7.23214–1	7.45041–1	7.67800–1	7.91559–1	8.16391–1	8.29235–1	8.42380–1
0.7	8.54544–1	8.77814–1	8.89791–1	9.02008–1	9.27198–1	9.53454–1	9.80856–1	1.00949	1.02430	1.03945
0.8	1.02508	1.05121	1.06466	1.07838	1.10667	1.13615	1.16692	1.19907	1.21570	1.23272
1.0	1.35307	1.38429	1.40036	1.41676	1.45057	1.48582	1.52263	1.56111	1.58102	1.60140
1.2	1.65823	1.69385	1.71220	1.73092	1.76954	1.80983	1.85192	1.89596	1.91876	1.94211
1.4	1.93902	1.97852	1.99887	2.01964	2.06251	2.10727	2.15406	2.20304	2.22842	2.25442
1.5	2.07055	2.11182	2.13309	2.15480	2.19963	2.24644	2.29539	2.34666	2.37323	2.40045
1.7	2.31700	2.36154	2.38451	2.40798	2.45641	2.50703	2.56000	2.61552	2.64430	2.67381
2.0	2.64162	2.69053	2.71576	2.74154	2.79481	2.85052	2.90887	2.97009	3.00185	3.03442
3.0	3.51376	3.57394	3.60503	3.63684	3.70268	3.77170	3.84418	3.92040	3.96003	4.00073
5.0	4.59935	4.67433	4.71316	4.75293	4.83543	4.92217	5.01353	5.10992	5.16014	5.21181
7.0	5.28542	5.37040	5.41445	5.45962	5.55344	5.65226	5.79496	5.90517	5.96269	6.02191
10.0	5.98474	6.08046	6.13015	6.18112	6.28715	6.39903	6.51728	6.64249	6.70792	6.77535

TABLE 4

Stopping number contribution of L_I electrons, $B_{L_I}(\theta_{L_I}, \eta_{L_I})$

η_{L_I}/θ_{L_I}	0.66	0.65	0.64	0.62	0.60	0.58	0.56	0.55	0.54
0.005	2.4111–4	2.5612–4	2.7202–4	3.0658–4	3.4511–4	3.8795–4	4.3542–4	4.6100–4	4.8786–4
0.007	6.3947–4	6.7058–4	7.0295–4	7.7167–4	8.4592–4	9.2605–4	1.0125–3	1.0583–3	1.1058–3
0.01	1.5469–3	1.6036–3	1.6622–3	1.7856–3	1.9181–3	2.1615–3	2.3178–3	2.4019–3	2.4904–3
0.015	3.7221–3	3.8404–3	3.9650–3	4.2354–3	4.5396–3	4.8853–3	5.2820–3	5.5031–3	5.7414–3
0.02	6.9449–3	7.1910–3	7.4535–3	8.0336–3	8.6984–3	9.4638–3	1.0348–2	1.0841–2	1.1372–2
0.03	1.7411–2	1.8180–2	1.8997–2	2.0784–2	2.2797–2	2.5066–2	2.7622–2	2.9020–2	3.0503–2
0.04	3.8474–2	4.0056–2	4.1718–2	4.5300–2	4.9254–2	5.3619–2	5.8436–2	6.1028–2	6.3752–2
0.05	6.7371–2	6.9928–2	7.2596–2	7.8282–2	8.4470–2	9.1206–2	9.8538–2	1.0244–1	1.0652–1
0.06	1.0418–1	1.0778–1	1.1152–1	1.1943–1	1.2796–1	1.3715–1	1.4706–1	1.5231–1	1.5776–1
0.08	1.9647–1	2.0217–1	2.0805–1	2.2038–1	2.3351–1	2.4751–1	2.6244–1	2.7027–1	2.7837–1
0.1	3.0594–1	3.1361–1	3.2150–1	3.3796–1	3.5537–1	3.7381–1	3.9336–1	4.0357–1	4.1410–1
0.15	6.1411–1	6.2597–1	6.3811–1	6.6330–1	6.8974–1	7.1753–1	7.4678–1	7.6199–1	7.7761–1
0.2	9.3100–1	9.5614–1	9.7162–1	1.0037	1.0372	1.0723	1.1092	1.1284	1.1480
0.3	1.5172	1.5372	1.5576	1.5998	1.6438	1.6899	1.7382	1.7632	1.7889
0.4	2.0173	2.0408	2.0647	2.1142	2.1659	2.2199	2.2765	2.3059	2.3360
0.5	2.3932	2.4193	2.4460	2.5011	2.5587	2.6190	2.6821	2.7148	2.7484
0.6	2.7091	2.7374	2.7663	2.8260	2.8884	2.9538	3.0222	3.0577	3.0941
0.7	2.9742	3.0044	3.0352	3.0988	3.1652	3.2349	3.3079	3.3457	3.3845
0.8	3.2222	3.2539	3.2863	3.3532	3.4232	3.4965	3.5734	3.6133	3.6542
1.0	3.6690	3.7033	3.7384	3.8108	3.8866	3.9661	4.0495	4.0928	4.1371
1.2	3.9819	4.0183	4.0555	4.1324	4.2130	4.2974	4.3861	4.4321	4.4794
1.4	4.2745	4.3127	4.3517	4.4324	4.5170	4.6056	4.6988	4.7471	4.7968
1.5	4.4047	4.4436	4.4834	4.5658	4.6521	4.7426	4.8378	4.8872	4.9379
1.7	4.6383	4.6787	4.7200	4.8054	4.8949	4.9888	5.0876	5.1388	5.1915
2.0	4.9369	4.9791	5.0223	5.1116	5.2053	5.3036	5.4070	5.4607	5.5159
3.0	5.6514	5.6981	5.7459	5.8450	5.9489	6.0581	6.1730	6.2328	6.2943
5.0	6.4665	6.5189	6.5724	6.6835	6.8003	6.9231	7.0525	7.1199	7.1892
7.0	6.8634	6.9194	6.9767	7.0957	7.2208	7.3526	7.4915	7.5639	7.6384

TABLE 4 (continued)

η_{L_I}/θ_{L_I}	0.52	0.50	0.48	0.46	0.45	0.44	0.42	0.40	0.38
0.005	5.4561–4	6.0905–4	6.7863–4	7.5494–4	7.9587–4	8.3883–4	9.3160–4	1.0352–3	1.1529–3
0.007	1.2068–3	1.3170–3	1.4377–3	1.5719–3	1.6451–3	1.7231–3	1.8969–3	2.1009–3	2.3459–3
0.01	2.6832–3	2.9017–3	3.1534–3	3.4479–3	3.6149–3	3.7976–3	4.2187–3	4.7320–3	5.3636–3
0.015	6.2775–3	6.9077–3	7.6525–3	8.5370–2	9.0407–3	9.5910–3	1.0850–2	1.2358–2	1.4165–2
0.02	1.2561–2	1.3943–2	1.5553–2	1.7327–2	1.8478–2	1.9612–2	2.2160–2	2.5130–2	2.8594–2
0.03	3.3750–2	3.7470–2	4.1528–2	4.6170–2	4.8708–2	5.1401–2	5.7297–2	6.3943–2	7.1441–2
0.04	6.9619–2	7.6098–2	8.3249–2	9.1150–2	9.5406–2	9.9881–2	1.0954–1	1.2023–1	1.3208–1
0.05	1.1522–1	1.2470–1	1.3504–1	1.4632–1	1.5234–1	1.5864–1	1.7211–1	1.8686–1	2.0304–1
0.06	1.6931–1	1.8179–1	1.9530–1	2.0991–1	2.1767–1	2.2576–1	2.4295–1	2.6165–1	2.8201–1
0.08	2.9540–1	3.1361–1	3.3312–1	3.5403–1	3.6506–1	3.7650–1	4.0067–1	4.2673–1	4.5488–1
0.1	4.3613–1	4.5956–1	4.852 –1	5.1115–1	5.2514–1	5.3961–1	5.7008–1	6.0277–1	6.3793–1
0.15	8.1014–1	8.4453–1	8.8093–1	9.1954–1	9.3973–1	9.6056–1	1.0043	1.0509	1.1008
0.2	1.1888	1.2319	1.2774	1.3255	1.3506	1.3765	1.4308	1.4886	1.5504
0.3	1.8422	1.8983	1.9575	2.0201	2.0528	2.0864	2.1569	2.2319	2.3120
0.4	2.3984	2.4642	2.5336	2.6070	2.6452	2.6847	2.7674	2.8554	2.9494
0.5	2.8181	2.8915	2.9690	3.0509	3.0937	3.1378	3.2301	3.3285	3.4337
0.6	3.1698	3.2494	3.3336	3.4226	3.4691	3.5171	3.6175	3.7246	3.8391
0.7	3.4652	3.5502	3.6400	3.7351	3.7848	3.8360	3.9433	4.0578	4.1804
0.8	3.7392	3.8289	3.9236	4.0239	4.0764	4.1304	4.2438	4.3648	4.4944
1.0	4.2295	4.3269	4.4299	4.5391	4.5962	4.6551	4.7786	4.9106	5.0520
1.2	4.5777	4.6814	4.7912	4.9076	4.9685	5.0314	5.1633	5.3043	5.4555
1.4	4.9001	5.0092	5.1247	5.2473	5.3114	5.3776	5.5166	5.6653	5.8249
1.5	5.0434	5.1550	5.2731	5.3984	5.4640	5.5317	5.6739	5.8260	5.9893
1.7	5.3011	5.4170	5.5398	5.6701	5.7373	5.8088	5.9568	6.1152	6.2853
2.0	5.6308	5.7523	5.8811	6.0174	6.0896	6.1636	6.3192	6.4857	6.6647
3.0	6.4224	6.5580	6.7019	6.8549	6.9351	7.0180	7.1925	7.3795	7.5808
5.0	7.3338	7.4872	7.6500	7.8235	7.9146	8.0087	8.2071	8.4200	8.6496
7.0	7.7938	7.9588	8.1342	8.3211	8.4193	8.5209	8.7350	8.9651	9.2133

TABLE 4 (continued)

η_{L_I}/θ_{L_I}	0.36	0.35	0.34	0.32	0.30	0.28	0.26	0.24
0.005	1.2895–3	1.3670–3	1.4524–3	1.6524–3	1.9078–3	2.2414–3	2.6889–3	3.3006–3
0.007	2.6467–3	2.8242–3	3.0238–3	3.5045–3	4.1260–3	4.9376–3	6.0050–3	7.4152–3
0.01	6.1472–3	6.6086–3	7.1246–3	8.3491–3	9.8871–3	1.1822–2	1.4261–2	1.7335–2
0.015	1.63316–2	1.7572–2	1.8932–2	2.2053–2	2.5803–2	3.0308–2	3.5728–2	4.2258–2
0.02	3.2634–2	3.4900–2	3.7348–2	4.2850–2	4.9278–2	5.6798–2	6.5610–2	7.5963–2
0.03	7.9907–2	8.4544–2	8.9486–2	1.0032–1	1.1260–1	1.2656–1	1.4248–1	1.6071–1
0.04	1.4523–1	1.5237–1	1.5985–1	1.7614–1	1.9434–1	2.1473–1	2.3766–1	2.6357–1
0.05	2.2082–1	2.3036–1	2.4038–1	2.6199–1	2.8590–1	3.1248–1	3.4212–1	3.7536–1
0.06	3.0423–1	3.1611–1	3.2854–1	3.5522–1	3.8459–1	4.1704–1	4.5306–1	4.9326–1
0.08	4.8536–1	5.0156–1	5.1846–1	5.5453–1	5.9397–1	6.3728–1	6.8507–1	7.3810–1
0.1	6.7586–1	6.9596–1	7.1688–1	7.6141–1	8.0992–1	8.6301–1	9.2142–1	9.8604–1
0.15	1.1544	1.1828	1.2122	1.2746	1.3424	1.4163	1.4974	1.5868
0.2	1.6167	1.6517	1.6880	1.7650	1.8484	1.9394	2.0390	2.1489
0.3	2.3979	2.4432	2.4902	2.5899	2.6980	2.8159	2.9451	3.0876
0.4	3.0502	3.1034	3.1586	3.2758	3.4030	3.5416	3.6938	3.8620
0.5	3.5466	3.6062	3.6681	3.7994	3.9421	4.0978	4.2688	4.4580
0.6	3.9620	4.0270	4.0945	4.2378	4.3935	4.5636	4.7506	4.9576
0.7	4.3020	4.3715	4.4438	4.5974	4.7644	4.9470	5.1478	5.3703
0.8	4.6336	4.7072	4.7837	4.9463	5.1233	5.3169	5.5300	5.7661
1.0	5.2041	5.2845	5.3682	5.5462	5.7400	5.9523	6.1863	6.4458
1.2	5.6182	5.7044	5.7940	5.9848	6.1927	6.4206	6.6719	6.9510
1.4	5.9967	6.0876	6.1823	6.3839	6.6038	6.8451	7.1113	7.4071
1.5	6.1652	6.2583	6.3553	6.5618	6.7871	7.0344	7.3073	7.6107
1.7	6.4686	6.5657	6.6668	6.8823	7.1175	7.3757	7.6609	7.9782
2.0	6.8577	6.9600	7.0666	7.2937	7.5418	7.8143	8.1156	8.4510
3.0	7.7981	7.9134	8.0336	8.2901	8.5708	8.8796	9.2214	9.6027
5.0	8.8978	9.0297	9.1673	9.4612	9.7834	10.1384	10.5323	10.9722
7.0	9.4819	9.6248	9.7739	10.0926	10.4423	10.8282	11.2565	11.7356

TABLE 5

Stopping number contribution of L_{II} electrons, $B_{L_{II}}(\theta_{L_{II}}, \eta_{L_{II}})$

$\eta_{L_{II}}/\theta_{L_{II}}$	0.66	0.65	0.64	0.62	0.60	0.58	0.56	0.55	0.54
0.005	3.6324–5	4.0609–5	4.5430–5	5.6969–5	7.1625–5	9.0279–5	1.1407–4	1.2834–4	1.4447–4
0.007	1.8110–4	2.0001–4	2.2099–4	2.7006–4	3.3049–4	4.0498–4	4.9688–4	5.5061–4	6.1032–4
0.01	8.6524–4	9.4223–4	1.0262–3	1.2178–3	1.4459–3	1.7174–3	2.0405–3	2.2245–3	2.4252–3
0.015	4.2293–3	4.5314–3	4.8551–3	5.5731–3	6.3968–3	7.3414–3	8.4242–3	9.0236–3	9.6652–3
0.02	1.1485–2	1.2172–2	1.2900–2	1.4486–2	1.6264–2	1.8256–2	2.0487–2	2.1702–2	2.2989–2
0.03	3.9471–2	4.1270–2	4.3149–2	4.7163–2	5.1543–2	5.6423–2	6.1540–2	6.4326–2	6.7237–2
0.04	8.4454–2	8.7599–2	9.0860–2	9.7747–2	1.0516–1	1.1313–1	1.2171–1	1.2625–1	1.3096–1
0.05	1.4339–1	1.4795–1	1.5266–1	1.6253–1	1.7306–1	1.8430–1	1.9630–1	2.0261–1	2.0924–1
0.06	2.1304–1	2.1899–1	2.2512–1	2.3794–1	2.5153–1	2.6596–1	2.8130–1	2.8934–1	2.9763–1
0.08	3.7382–1	3.8241–1	3.9122–1	4.0955–1	4.2888–1	4.4928–1	4.7086–1	4.8212–1	4.9371–1
0.1	5.5056–1	5.6151–1	5.7273–1	5.9601–1	6.2049–1	6.4627–1	6.7346–1	6.8762–1	7.0218–1
0.15	1.0066	1.0224	1.0386	1.0721	1.1073	1.1443	1.1832	1.2035	1.2243
0.2	1.4376	1.4572	1.4773	1.5188	1.5624	1.6083	1.6566	1.6817	1.7076
0.3	2.1712	2.1964	2.2223	2.2758	2.3322	2.3915	2.4542	2.4869	2.5205
0.4	2.7500	2.7793	2.8094	2.8719	2.9377	3.0072	3.0807	3.1192	3.1587
0.5	3.2033	3.2359	3.2693	3.3389	3.4122	3.4898	3.5721	3.6151	3.6595
0.6	3.6038	3.6391	3.6753	3.7506	3.8303	3.9146	4.0042	4.0511	4.0995
0.7	3.9106	3.9482	3.9867	4.0670	4.1520	4.2421	4.3380	4.3882	4.4401
0.8	4.1790	4.2185	4.2590	4.3437	4.4333	4.5285	4.6298	4.6830	4.7380
1.0	4.6344	4.6772	4.7212	4.8131	4.9106	5.0144	5.1250	5.1831	5.2432
1.2	4.9787	5.0242	5.0711	5.1689	5.2729	5.3837	5.5050	5.5642	5.6287
1.4	5.2688	5.3166	5.3658	5.4687	5.5782	5.6950	5.8198	5.8855	5.9554
1.5	5.3966	5.4454	5.4957	5.6009	5.7128	5.8323	5.9601	6.0274	6.0972
1.7	5.6255	5.6762	5.7284	5.8377	5.9541	6.0785	6.2116	6.2818	6.3546
2.0	5.9170	5.9701	6.0248	6.1395	6.2618	6.3925	6.5327	6.6066	6.6833
3.0	6.6210	6.6801	6.7411	6.8692	7.0062	7.1529	7.3107	7.3941	7.4807
5.0	7.4620	7.5288	7.5977	7.7428	7.8982	8.0653	8.2454	8.3409	8.4402
7.0	7.7362	7.8079	7.8821	8.0383	8.2061	8.3866	8.5816	8.6850	8.7927

TABLE 5 (continued)

$\eta_{L_{II}}/\theta_{L_{II}}$	0.52	0.50	0.48	0.46	0.45	0.44	0.42	0.40	0.38
0.005	1.8339–4	2.3330–4	2.9738–4	3.7977–4	4.2945–4	4.8582–4	6.2244–4	7.9858–4	1.0258–3
0.007	7.5042–4	9.2355–4	1.1375–3	1.4021–3	1.5570–3	1.7292–3	2.1335–3	2.6335–3	3.2515–3
0.01	2.8829–3	3.4275–3	4.0758–3	4.8457–3	5.2839–3	5.7617–3	6.8504–3	8.1442–3	9.6816–3
0.015	1.1087–2	1.2716–2	1.4581–2	1.6717–2	1.7898–2	1.9163–2	2.1964–2	2.5173–2	2.8851–2
0.02	2.5786–2	2.8922–2	3.2435–2	3.6371–2	3.8514–2	4.0784–2	4.5733–2	5.1288–2	5.7531–2
0.03	7.3461–2	8.0264–2	8.7705–2	9.5852–2	1.0021–1	1.0478–1	1.1458–1	1.2535–1	1.3721–1
0.04	1.4094–1	1.5172–1	1.6336–1	1.7596–1	1.8265–1	1.8962–1	2.0445–1	2.2058–1	2.3818–1
0.05	2.2289–1	2.3762–1	2.5344–1	2.7045–1	2.7944–1	2.8877–1	3.0855–1	3.2995–1	3.5318–1
0.06	3.1503–1	3.3361–1	3.5346–1	3.7473–1	3.8594–1	3.9756–1	4.2212–1	4.4861–1	4.7727–1
0.08	5.1793–1	5.4368–1	5.7109–1	6.0032–1	6.1569–1	6.3159–1	6.6512–1	7.0119–1	7.4012–1
0.1	7.3258–1	7.6481–1	7.9907–1	8.3556–1	8.5472–1	8.7454–1	9.1630–1	9.6119–1	1.0096
0.15	1.2677	1.3137	1.3626	1.4147	1.4421	1.4703	1.5300	1.5942	1.6636
0.2	1.7615	1.8188	1.8797	1.9446	1.9788	2.0142	2.0889	2.1694	2.2567
0.3	2.5909	2.6658	2.7457	2.8312	2.8762	2.9231	3.0222	3.1295	3.2463
0.4	3.2417	3.3302	3.4249	3.5266	3.5803	3.6361	3.7546	3.8835	4.0242
0.5	3.7527	3.8523	3.9591	4.0741	4.1350	4.1983	4.3330	4.4799	4.6408
0.6	4.2013	4.3103	4.4274	4.5537	4.6206	4.6904	4.8390	5.0013	5.1796
0.7	4.5493	4.6664	4.7925	4.9286	5.0009	5.0762	5.2370	5.4129	5.6066
0.8	4.8537	4.9780	5.1119	5.2568	5.3338	5.4141	5.5857	5.7738	5.9811
1.0	5.3701	5.5066	5.6540	5.8138	5.8989	5.9878	6.1780	6.3870	6.6179
1.2	5.7648	5.9114	6.0701	6.2424	6.3343	6.4303	6.6361	6.8626	7.1137
1.4	6.0976	6.2530	6.4214	6.6044	6.7021	6.8043	7.0237	7.2655	7.5338
1.5	6.2447	6.4041	6.5768	6.7647	6.8650	6.9700	7.1954	7.4442	7.7203
1.7	6.5087	6.6752	6.8558	7.0526	7.1578	7.2679	7.5045	7.7660	8.0565
2.0	6.8458	7.0218	7.2129	7.4213	7.5328	7.6496	7.9010	8.1791	8.4886
3.0	7.6647	7.8644	8.0819	8.3189	8.4475	8.5814	8.8702	9.1908	9.5488
5.0	8.6515	8.8816	9.1330	9.4090	9.5572	9.7132	10.0504	10.4259	10.8466
7.0	9.0221	9.2724	9.5464	9.8477	10.0099	10.1805	10.5499	10.9622	11.4250

TABLE 5 (continued)

$\eta_{L_{II}}/\theta_{L_{II}}$	0.36	0.35	0.34	0.32	0.30	0.28	0.26	0.24
0.005	1.3190–3	1.4961–3	1.6974–3	2.1858–3	2.8163–3	3.6302–3	4.6814–3	6.0395–3
0.007	4.0158–3	4.4623–3	4.9592–3	6.1257–3	7.5675–3	9.3502–3	1.1556–2	1.4290–2
0.01	1.1509–2	1.2548–2	1.3681–2	1.6263–2	1.9336–2	2.2999–2	2.7370–2	3.2603–2
0.015	3.3070–2	3.5408–2	3.7914–2	4.3483–2	4.9898–2	5.7304–2	6.5884–2	7.5861–2
0.02	6.4555–2	6.8394–2	7.2472–2	8.1413–2	9.1539–2	1.0304–1	1.1617–1	1.3121–1
0.03	1.5030–1	1.5101–1	1.5844–1	1.7451–1	1.9244–1	2.1244–1	2.3496–1	2.6044–1
0.04	2.5743–1	2.6774–1	2.7855–1	3.0180–1	3.2751–1	3.5608–1	3.8803–1	4.2401–1
0.05	3.7846–1	3.9195–1	4.0607–1	4.3635–1	4.6973–1	5.0672–1	5.4798–1	5.9436–1
0.06	5.0839–1	5.2497–1	5.4230–1	5.7943–1	6.2028–1	6.6549–1	7.1589–1	7.7252–1
0.08	7.8230–1	8.0474–1	8.2818–1	8.7836–1	9.3355–1	9.9462–1	1.0627	1.1394
0.1	1.0621	1.0900	1.1192	1.1816	1.2503	1.3265	1.4116	1.5076
0.15	1.7389	1.7790	1.8210	1.9112	2.0108	2.1217	2.2462	2.3876
0.2	2.3516	2.4024	2.4556	2.5701	2.6971	2.8391	2.9994	3.1822
0.3	3.3741	3.4427	3.5148	3.6706	3.8445	4.0404	4.2631	4.5193
0.4	4.1788	4.2620	4.3496	4.5398	4.7530	4.9944	5.2703	5.5895
0.5	4.8180	4.9137	5.0146	5.2341	5.4811	5.7618	6.0840	6.4583
0.6	5.3765	5.4830	5.5954	5.8406	6.1173	6.4326	6.7958	7.2191
0.7	5.8208	5.9369	6.0596	6.3275	6.6306	6.9769	7.3767	7.8440
0.8	6.2109	6.3355	6.4674	6.7558	7.0827	7.4570	7.8900	8.3972
1.0	6.8747	7.0142	7.1621	7.4861	7.8546	8.2778	8.7690	9.3464
1.2	7.3933	7.5454	7.7068	8.0612	8.4652	8.9302	9.4713	10.1090
1.4	7.8331	7.9967	8.1694	8.5502	8.9851	9.4866	10.0713	10.7619
1.5	8.0286	8.1967	8.3753	8.7681	9.2181	9.7352	10.3399	11.0546
1.7	8.3813	8.5585	8.7469	9.1618	9.6367	10.1856	10.8270	11.5863
2.0	8.8352	9.0245	9.2260	9.6701	10.1793	10.7688	11.4590	12.2775
3.0	9.9511	10.1714	10.4062	10.9254	11.5229	12.2172	13.0332	14.0048
5.0	11.3211	11.5818	11.8601	12.4771	13.1898	14.0213	15.0024	16.1752
7.0	11.9480	12.2357	12.5432	13.2260	14.0164	14.9404	16.0330	17.3420

ber of screening parameters and are listed in table 1. Another computer program made the necessary numerical calculations for the evaluation of coefficients $S_L(\theta_L)$, $T_L(\theta_L)$ and $U_L(\theta_L)$. The coefficients are obtained for θ_L ranging from 0.24 to 0.66. No attempt was made to evaluate coefficients V_L etc. Results are exhibited in table 2.

Since the main aim of this paper is to evaluate inner shell corrections, this can now be accomplished for any θ and large η from eqs. (20) and (21). In order to get corrections for low energies, we have also numerically evaluated stopping numbers [13] for an extensive range of energies ($\eta_K = 0.005-10$ and $\eta_L = 0.005-7.0$) and for screening parameters used in this paper. Table 3 lists stopping numbers for K-electrons as a function of η_K and θ_K. Tables 4 and 5 list stopping numbers for L_I and L_{II} subshells of the L-shell. The stopping number B_L for the L-electron, can be obtained by the relation $B_L = B_{L_I}+3B_{L_{II}}$. Following Bethe, we write corrections C_K and C_L for low incident energy as

$$C_K(\theta_K, \eta_K) = S_K(\theta_K) \ln \eta_K + T_K(\theta_K) - B_K(\theta_K, \eta_K),$$
$$C_L(\theta_L, \eta_L) = S_L(\theta_L) \ln \eta_L + T_L(\theta_L) - B_L(\theta_L, \eta_L),$$

where S_K, T_K, B_K and S_L, T_L, B_L can be read from tables 1-5. Tables 4 and 5 contain stopping numbers to four figures. Even though stopping numbers B_K are presented with five figures, they should be good to four figures only.

It should be pointed out that the theory itself might be in relatively larger error than the accuracy with which results are presented here. However, it is desirable to remove, as much as possible, inaccuracies arising from interpolation, extrapolation and the numerical evaluation of stopping numbers. The present work is an attempt in this direction. More accurate calculations using Hartree wave functions may perhaps be available in the future [14, 15]. In the meantime, it is hoped that the present calculations may be useful in interpreting binding corrections.

As expected, there is very good agreement in coefficients with Walske's results for $\theta_K = 0.7$, 0.8, 0.85 and 0.9 and for $\theta_L = 0.35$, 0.45, 0.55 and 0.65. The advantage of the present procedure is that it is computer oriented and could easily be carried over to form factors of the M-shell [16] and subshells of L- and M-shells [17], which are otherwise unmanageably complicated. It is planned to extend this program to them.

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