Relativistic study of K-shell x-ray and Auger-electron energy shifts for additional atomic vacancies

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The hydrogenic model of Burch *et al.* for calculating the energy shifts of the K x ray and Auger electrons for a vacancy in the L shell is extended to incorporate the effect of relativity. Numerical results are presented for 18 values of Z (from 10 to 95 in steps of 5). The computations are based on two different choices of the screening parameters. The effective nuclear charges ($Z_{\rm eff}$) determined by the method of O'Connell and Carroll yield numbers for the energy shifts close to the predictions of Hartree-Fock (HF) and Hartree-Fock-Slater (HFS) calculations. On the other hand, $Z_{\rm eff}$ obtained from Slater's rule gives numbers which are considerably larger than the HF and HFS values. However, the choice of screening is crucial only for low-Z elements and relativity plays an increasingly dominant role as one goes to higher atomic numbers. It is found that the relativistic effect is more pronounced for a vacancy in the L_2 subshell.

I. INTRODUCTION

The creation of a vacancy in an atomic K shell initiates primarily either of the following competing processes.

(i) An electron from an outer shell moves in and a K-x-ray photon is emitted shifting the vacancy to the higher shell.

(ii) The vacancy is filled by an electron from an outer shell X, but, rather than emitting a photon, the atom rearranges itself in such a way that the excess energy is utilized in the emission of another electron (Auger electron) from an outer shell Y into the energy continuum. In other words, a singly ionized atom with an inner-shell vacancy is converted into a doubly ionized atom with two vacancies in outer shells.

In heavy-ion collisions, simultaneously with the K vacancy, additional vacancies are produced in higher shells which have lifetimes longer than that in the K vacancy. These outer-shell vacancies affect the energies of the processes in (i) and (ii). In particular, the energies of the K x-ray and the Auger electron are shifted in opposite manners.[1] Burch *et al.*[2] have described a simple analytical model for the calculation of K-x-ray and Auger-electron energy shifts resulting from an additional vacancy in the $2p$ orbital. This model, on the one hand, gives some intuitive feelings for the magnitudes and directions of the effects and, on the other hand, allows a straight forward generalization[3] to arbitrary defect configuration.

For high-Z atoms, relativity plays a significant role in affecting the energies of the K x ray and Auger electrons.[4] It will thus be of some interest to inject the effect of relativity into the model of Burch *et al.*[2] and examine the relativistic effect, if any, on the Auger-electron and K-x-ray energy shifts in the presence of one spectator hole in the L shell. The present paper is an effort in this direction.

X-ray satellite lines arise from transitions in a level scheme associated with removal of two electrons from the inner closed shells. For example, $K\alpha$ satellites are observed when there are two vacancies in the K shell. But in our case we have one vacancy in the K shell and a spectator vacancy in the L shell. Thus the nondiagram lines considered here are different from the usual x-ray satellites.

The vacancy in the $2p$ shell gives rise to a perturbing potential for the K-shell x-ray and Auger-electron energy shifts and Burch *et al.*[2] gave an analytical model for constructing such a potential. Relativistic effects split the $2p$ level into $2p_{1/2}$ and $2p_{3/2}$ levels. In Sec. II we construct expressions for the potentials for vacancies in $2p_{1/2}$ and $2p_{3/2}$ subshells by using Dirac-Coulomb bound-state wave functions[5] and obtain their nonrelativistic limits. Using these perturbing potentials we also derive relativistic analytical expressions for the binding energy shifts of the K, L_2, and L_3, subshell electrons. In the appropriate limit, these expressions yield the nonrelativistic results of Burch *et al.*[2] In Sec. III we present numerical results for the K-shell x-ray and Auger-electron energy shifts and examine the effect of relativity on the nondiagram lines considered here. We pay special attention to the choice of screening parameters (σ) since screening is expected to play a crucial role in the hydrogenic model. In the course of our study we shall see that reliable numbers for the energy shifts can be obtained by using values of σ as given by O'Connell and Carroll[6] (CC).

II. THEORY

According to Burch *et al.*[2] a vacancy in the $2p$ shell produces a perturbing potential (in a.u.)

$$V_{2p}(r)=\frac{1}{r}-\frac{1}{r}\int_r^\infty \rho_{2p}(r')[(r')^2-rr']dr' , \tag{1}$$

where, using hydrogenic Schrödinger wave functions,

$$\rho_{2p}(r)=\psi_{2p}^2(r)\propto r^2 e^{-Z_L r} . \qquad (2)$$

Here Z_L is the effective nuclear charge for the subshell L. Considering the vacancy to be produced in the L_i ($i=2$ and 3) subshell and using Dirac-Coulomb bound-state wave function[5] we generalize Eq. (1) as

$$V_{L_i}(r)=\frac{\alpha}{r}-\frac{\alpha}{r}I(r) \qquad (3)$$

with

$$\begin{aligned} I(r)=N_{L_i}^2 \Big\{ &(1-W_{L_i})\Big[(a_0^{L_i})^2J(0,r)+(a_1^{L_i})^2J(2,r)+2a_0^{L_i}a_1^{L_i}J(1,r)\Big] \\ &+(1+W_{L_i})\Big[(C_0^{L_i})^2J(0,r)+(C_1^{L_i})^2J(2,r)+2C_0^{L_i}C_1^{L_i}J(1,r)\Big] \\ &-r(1-W_{L_i})\Big[(a_0^{L_i})^2J(-1,r)+(a_1^{L_i})^2J(1,r)+2a_0^{L_i}a_1^{L_i}J(0,r)\Big] \\ &-r(1-W_{L_i})\Big[(C_0^{L_i})^2J(-1,r)+(C_1^{L_i})^2J(1,r)+2C_0^{L_i}C_1^{L_i}J(0,r)\Big]\Big\} . \end{aligned} \qquad (4)$$

Equations (3) and (4) are written in rational relativistic units with α, the fine-structure constant.

In deriving Eq. (4) we have used[7]

$$\begin{aligned} J(m,r)&=\int_r^\infty x^{(2\gamma_{L_i}+m)}e^{-2\lambda_{L_i}n}dx \\ &=(2\lambda)^{-(2\gamma_{L_i}+m+1)}\Gamma(2\gamma_{L_i}+m+1,2\lambda_{L_i}r) . \end{aligned} \qquad (5)$$

The quantities a, c, W, γ, λ, etc., which occur in Eqs. (4) and (5) have been given in Ref. 5 in tabular form. In the nonrelativistic limit we have

$$\begin{aligned} &\lambda_{L_2}=1,\ \ W_{L_2}=1,\ \ \lambda_{L_2}=\frac{\alpha z_{L_2}}{2} , \\ &a_0^{L_2}=2,\ \ a_1^{L_2}=-\frac{\alpha Z_{L_2}}{3} , \\ &C_0^{L_2}=0,\ \ C_1^{L_2}=-\frac{\alpha Z_{L_2}}{3},\ \ N_{L_2}=\frac{(3\alpha Z_{L_2})^{1/2}}{4} \end{aligned} \qquad (6)$$

for the L_2 subshell and

$$\begin{aligned} &\gamma_{L_3}=2,\ \ W_{L_3}=1,\ \ a_0^{L_3}=1,\ \ a_1^{L_3}=0 , \\ &C_0^{L_3}=1,\ \ C_1^{L_3}=0 , \\ &\lambda_{L_3}=\frac{\alpha Z_{L_3}}{2},\ \ N=\frac{(\alpha Z_{L_3})^{5/2}}{4\sqrt{3}} \end{aligned} \qquad (7)$$

for the L_3 subshell. The nonrelativistic result for $V_{2p}(r)$ given by Burch *et al.*[2] can now be obtained by using Eq. (6) or Eq. (7) in Eq. (3) with $Z_{L_2}=Z_{L_3}$.

The binding-energy shifts of the K shell and L_2 and L_3 subshells for the potentials in (3) are given by

$$\begin{aligned} \Delta E_{K(2)}&=\langle K \mid V_{L_2} \mid K\rangle \\ &=\frac{\alpha^2 Z_K}{\gamma_K}-2\alpha N_K^2 N_{L_2}^2 \Bigg[\frac{[(a_0^{L_2})^2+(C_0^{L_2})^2]-W_{L_2}[(a_0^{L_2})^2-(C_0^{L_2})^2]}{(2\lambda_K+2\lambda_{L_2})^{(2\gamma_K+2\gamma_{L_2}+1)}} \\ &\quad\times\Gamma(2\gamma_K+2\gamma_{L_2}+1)\Bigg\{\frac{1}{2\gamma_k}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_2}+1;2\gamma_K+1;\lambda_K/(\lambda_K+\lambda_{L_2})) \\ &\quad-\frac{1}{(2\gamma_K+1)}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_2}+1;2\gamma_K+2;\lambda_K/(\lambda_K+\lambda_{L_2}))\Bigg\} \\ &\quad+\frac{[(a_1^{L_2})^2+(c_1^{L_2})^2]-W_{L_2}[(a_1^{L_2})^2-(C_1^{L_2})^2]}{(2\lambda_K+2\lambda_{L_2})^{(2\gamma_K+2\gamma_{L_2}+3)}} \end{aligned}$$

$$\times\Gamma(2\gamma_K+2\gamma_{L_2}+3)\left[\frac{1}{2\gamma_K}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_2}+3;2\gamma_K+1;\lambda_K/(\lambda_K+\lambda_{L_2}))\right.$$
$$\left.-\frac{1}{2\gamma_K+1}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_2}+3;2\gamma_K+2;\lambda_K/(\lambda_K+\lambda_{L_2}))\right]$$
$$+\frac{2[(a_0^{L_2}a_1^{L_2}-C_0^{L_2}C_1^{L_2})-W_{L_2}(a_0^{L_2}a_1^{L_2}-C_0^{L_2}C_1^{L_2})]}{(2\lambda_K+2\lambda_{L_2})^{(2\gamma_K+2\gamma_{L_2}+1)}}$$
$$\times\Gamma(2\gamma_K+2\gamma_{L_2}+2)\left[\frac{1}{2\gamma_K}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_2}+2;2\gamma_K+1;\lambda_K/(\lambda_K+\lambda_{L_2}))\right.$$
$$\left.\left.-\frac{1}{2\gamma_K+1}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_2}+2;2\gamma_K+2;\lambda_K/(\lambda_K+\lambda_{L_2}))\right]\right], \quad (8)$$

$$\Delta E_{K(3)}=\langle K\mid V_{L_3}\mid K\rangle=\frac{\alpha^2 Z_K}{\gamma_K}-2\alpha N_K^2N_{L_3}^2\left[\frac{2\Gamma(2\gamma_k+2\gamma_{L_3}+1)}{(2\lambda_K+2\lambda_{L_3})^{(2\gamma_K+2\gamma_{L_3}+1)}}\right.$$
$$\times\left[\frac{1}{2\gamma_K}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_3}+2;2\gamma_K+1;\lambda_k/(\lambda_K+\lambda_{L_3}))\right.$$
$$\left.\left.-\frac{1}{2\gamma_K+1}\,{}_2F_1(1,2\gamma_K+2\gamma_{L_3}+1;2\gamma_K+1;\lambda_K/(\lambda_K+\lambda_{L_3}))\right]\right], \quad (9)$$

$$\Delta E_{L_2}=\langle L_2\mid V_{L_2}\mid L_2\rangle$$
$$=N_{L_2}^2\frac{(2\gamma_{L_2}-1)!}{(2\lambda_{L_2})^{(2\gamma_{L_2}+2)}}[(2\lambda_{L_2})^2x+2\gamma_{L_2}(2\gamma_{L_2}+1)y+4\lambda_{L_2}\gamma_{L_2}T]$$
$$-N_{L_2}^4\left[\frac{x^2\Gamma(4\gamma_{L_2}+1)}{(4\lambda_{L_2})^{(4\gamma_{L_2}+1)}}\left[\frac{1}{2\gamma_{L_2}}\,{}_2F_1(1,4\gamma_{L_2}+1,2\gamma_{L_2}+1,\tfrac{1}{2})-\frac{1}{2\gamma_{L_2}+1}\,{}_2F_1(1,4\gamma_{L_2}+1;2\gamma_{L_2}+2;\tfrac{1}{2})\right]\right.$$
$$+\frac{xy\Gamma(4\gamma_{L_2}+3)}{(4\lambda_{L_2})^{(4\gamma_{L_2}+3)}}\left[\frac{1}{2\gamma_{L_2}}\,{}_2F_1(1,4\gamma_{L_2}+3,2\gamma_{L_2}+1,\tfrac{1}{2})+\frac{1}{2\gamma_{L_2}+2}\,{}_2F_1(1,4\gamma_{L_2}+3;2\gamma_{L_2}+3;\tfrac{1}{2})\right.$$
$$\left.-\frac{1}{2\gamma_{L_2}+1}\,{}_2F_1(1,4\gamma_{L_2}+3,2\gamma_{L_2}+2,\tfrac{1}{2})-\frac{1}{2\gamma_{L_2}+3}\,{}_2F_1(1,4\gamma_{L_2}+3;2\gamma_{L_2}+4;\tfrac{1}{2})\right]$$
$$+\frac{xT\Gamma(4\gamma_{L_2}+2)}{(4\lambda_{L_2})^{(4\gamma_{L_2}+2)}}\left[\frac{1}{2\gamma_{L_2}}\,{}_2F_1(1,4\gamma_{L_2}+2,2\gamma_{L_2}+1,\tfrac{1}{2})-\frac{1}{2\gamma_{L_2}+2}\,{}_2F_1(1,4\gamma_{L_2}+2;2\gamma_{L_2}+3;\tfrac{1}{2})\right]$$
$$+\frac{yT\Gamma(4\gamma_{L_2}+4)}{(4\lambda_{L_2})^{(4\gamma_{L_2}+4)}}\left[\frac{1}{2\gamma_{L_2}+1}\,{}_2F_1(1,4\gamma_{L_2}+4,2\gamma_{L_2}+2,\tfrac{1}{2})-\frac{1}{2\gamma_{L_2}+3}\,{}_2F_1(1,4\gamma_{L_2}+4;2\gamma_{L_2}+4;\tfrac{1}{2})\right]$$
$$+\frac{y^2\Gamma(4\gamma_{L_2}+5)}{(4\lambda_{L_2})^{(4\gamma_{L_2}+5)}}\left[\frac{1}{2\gamma_{L_2}+2}\,{}_2F_1(1,4\gamma_{L_2}+5,2\gamma_{L_2}+3,\tfrac{1}{2})-\frac{1}{2\gamma_{L_2}+3}\,{}_2F_1(1,4\gamma_{L_2}+5;2\gamma_{L_2}+4;\tfrac{1}{2})\right]$$
$$\left.+\frac{T^2\Gamma(4\gamma_{L_2}+3)}{(4\lambda_{L_2})^{(4\gamma_{L_2}+3)}}\left[\frac{1}{2\gamma_{L_2}+1}\,{}_2F_1(1,4\gamma_{L_2}+3,2\gamma_{L_2}+2,\tfrac{1}{2})-\frac{1}{2\gamma_{L_2}+2}\,{}_2F_1(1,4\gamma_{L_2}+3;2\gamma_{L_2}+3;\tfrac{1}{2})\right]\right], \quad (10)$$

and

$$\Delta E_{L_3}=\langle L_3\,|\,V_{L_3}\,|\,L_3\rangle=\frac{\alpha^2 Z_{L_3}}{2\gamma_{L_3}}-2\alpha N_{L_3}^4\left[\frac{2\Gamma(4\gamma_{L_3}+1)}{(4\lambda_{L_3})^{(4\gamma_{L_3}+1)}}\left\{\frac{1}{2\gamma_{L_3}}\,{}_2F_1(1,4\gamma_{L_3}+1;2\gamma_{L_3}+1;\tfrac{1}{2})-\frac{1}{2\gamma_{L_3}+1}\,{}_2F_1(1,4\gamma_{L_3}+1;2\gamma_{L_3}+2;\tfrac{1}{2})\right\}\right], \tag{11}$$

where

$$x=[(a_0^{L_2})^2+(C_0^{L_2})^2]-W_{L_2}[(a_0^{L_2})^2-(C_0^{L_2})^2]=4(1-W_{L_2})\,, \tag{12a}$$

$$y=[(a_1^{L_2})^2+(C_1^{L_2})^2]-W_{L_2}[(a_1^{L_2})^2-(C_1^{L_2})^2]=\frac{2\alpha^2 Z_{L_2}(2W_{L_2}-1)^2}{W_{L_2}^2(2\gamma_{L_2}+1)^2}\,, \tag{12b}$$

and

$$T=2[(a_0^{L_2}a_1^{L_2}+C_0^{L_2}C_1^{L_2})-W_{L_2}(a_0^{L_2}a_1^{L_2}-C_0^{L_2}C_1^{L_2})]=\frac{\alpha Z_{L_2}(1-2W_{L_2})}{(2\gamma_{L_2}+1)W_{L_2}}\,. \tag{12c}$$

The subscripts on γ, λ, W, etc., refer to subshells for which they stand. We have used the integral[8]

TABLE I. Energy shifts in a.u.

Z	Relativistic results for ΔE_K: Vacancy in L_2 subshell ($\Delta E_{K(2)}$)	Relativistic results for ΔE_K: Vacancy in L_3 subshell ($\Delta E_{K(3)}$)	Nonrelativistic results for ΔE_K ($\Delta E_{K_{NR}}$)	Relativistic results for L: ΔE_{L_2}	Relativistic results for L: ΔE_{L_3}	Nonrelativistic results for ΔE_L ($\Delta E_{L_{NR}}$)
10	0.5897	0.5944	0.5734	0.4287	0.4286	0.4295
	(1.4534)	(1.4526)	(1.4215)	(1.0634)	(1.0628)	(1.0647)
15	1.5753	1.5702	1.5309	1.1454	1.1446	1.1466
	(2.6869)	(2.6801)	(2.6365)	(1.9763)	(1.9721)	(1.9747)
20	2.5259	2.5065	2.4737	1.8354	1.8319	1.8345
	(3.9271)	(3.9053)	(3.8515)	(2.8963)	(2.8829)	(2.8847)
25	3.4468	3.4088	3.3339	2.5033	2.4947	2.4970
	(5.1824)	(5.1332)	(5.0665)	(3.8269)	(3.7962)	(3.7947)
30	4.3703	4.3030	4.2087	3.1687	3.1512	3.1522
	(6.4601)	(6.3647)	(6.2815)	(4.7717)	(4.7127)	(4.7047)
35	5.4152	5.2996	5.1831	3.9170	3.8840	3.8820
	(7.7668)	(7.6035)	(7.4965)	(5.7348)	(5.6331)	(5.6147)
40	6.5324	6.3487	6.2062	4.7127	4.6558	4.6482
	(9.1100)	(8.8506)	(8.7115)	(6.7202)	(6.5582)	(6.5247)
45	7.6619	7.3836	7.2098	5.5057	5.4155	5.3999
	(10.4974)	(10.1084)	(9.9265)	(7.7329)	(7.4889)	(7.4347)
50	8.8556	8.4544	8.2425	6.3370	6.2005	6.1734
	(11.9381)	(11.3787)	(11.1415)	(8.7780)	(8.4260)	(8.3447)
55	10.1273	9.5634	9.3044	7.2107	7.0116	6.9687
	(13.4419)	(12.6639)	(12.3565)	(9.8618)	(9.3704)	(9.2547)
60	11.4343	10.6661	10.3493	8.0926	7.8142	7.7513
	(15.0208)	(13.9668)	(13.5715)	(10.9913)	(10.3231)	(10.1647)
65	12.7889	11.7670	11.3796	8.9872	8.6105	8.5230
	(16.6888)	(15.2908)	(14.7865)	(12.1748)	(11.2849)	(11.0747)
70	14.2154	12.8790	12.4051	9.9061	9.4083	9.2911
	(18.4626)	(16.6403)	(16.0015)	(13.4222)	(12.2569)	(11.9847)
75	15.7577	14.0342	13.4524	10.8784	10.2293	10.0755
	(20.3623)	(18.0214)	(17.2165)	(14.7458)	(13.2401)	(12.8947)
80	17.4257	15.2088	14.4925	11.9070	11.0705	10.8544
	(22.4139)	(19.4426)	(18.4315)	(16.1602)	(14.2358)	(13.8047)
85	19.2541	16.4856	15.5957	12.9978	11.9310	11.6807
	(24.6491)	(20.5438)	(19.6465)	(17.6841)	(15.2450)	(14.7147)
90	21.2637	17.8010	16.6868	14.1583	12.8100	12.4979
	(27.1104)	(22.4633)	(20.8615)	(19.3418)	(16.2690)	(15.6247)
95	23.4617	19.1723	17.7608	15.3672	13.6846	13.3023
	(29.8539)	(24.1176)	(22.0765)	(21.1651)	(17.3092)	(16.5347)

$$\int_0^\infty x^{\mu-1}e^{-\beta x}\Gamma(\gamma,ax)dx = \frac{a^\gamma \Gamma(\mu+\gamma)}{\mu(a+\beta)^{\mu+\gamma}}\,{}_2F_1(1,\mu+\gamma,\mu+1,1-a/(a+\beta))\,, \quad (13)$$

$\mathrm{Re}(a+\beta)>0,\ \ \mathrm{Re}\beta>0,\ \ \mathrm{Re}(\mu+\gamma)>0\ .$

Note that an incorrect result for the value of this integral has been quoted by Gradshteyn and Ryzhik,[7] p. 663. A useful check on the fairly complicated expressions (8)–(11) is that in the nonrelativistic limit they yield the appropriate results of Burch *et al.*[2]

III. RESULTS AND DISCUSSION

Based on Eqs. (8)–(11) we have calculated energy shifts for the K shell and L_2 and L_3 subshells for a single vacancy in the L_2 or L_3 subshell. In order to examine the role of effective nuclear charges ($Z_{\rm eff}=Z_K$, Z_{L_2}, or Z_{L_3} as the case may be) we have chosen to work with two different types of screening parameters. For our first choice we followed O'Connell and Carroll who fitted screening constants for the electronic wave functions[3,6] to measured binding energies. Second, we determined $Z_{\rm eff}$ by the use of Slater's rule. Note that in the method of O'Connell and Carroll effective nuclear charges are different for different subshells. This is, however, not true for Slater's rule. For example, in Slater's rule $Z_{\rm Li}=Z-4.15$ for all subshells with $i=1$, 2, and 3. In Table I we present our results for $Z=10$–95 in steps of 5. The numbers without parentheses represented calculated values of the energy shifts for the first choice of $Z_{\rm eff}$, while those inside the parentheses are for our second choice.

Looking closely into our numbers we see that the effects of screening is more prominant for low-Z atoms. For $Z=10$ the Slater screening parameters yield number for $\Delta E_{K(i)}$ ($i=2,3$), $\Delta E_{K_{\rm NR}}$, ΔE_{L_2}, ΔE_{L_3}, and $\Delta E_{L_{\rm NR}}$ which are larger than the corresponding results obtained

TABLE II. Transition energy shifts for x rays and Auger electrons in a.u.

Z	Relativistic results for $\Delta E_{K\alpha}$: $\Delta E_{K\alpha_1}$	$\Delta E_{K\alpha_2}$	Nonrelativistic results for $\Delta E_{K\alpha}$	Relativistic results for ΔE_{KLL}: $\Delta E_{KL_2L_2}$	$\Delta E_{KL_3L_3}$	Nonrelativistic results for ΔE_{KLL}
10	0.1658	0.1610	0.1439	−0.2677	−0.2628	−0.2856
	(0.3898)	(0.3900)	(0.3568)	(−0.6722)	(−0.6730)	(−0.7079)
15	0.4256	0.4299	0.3843	−0.7155	−0.7190	−0.7623
	(0.7080)	(0.7106)	(0.6618)	(−1.2573)	(−1.2641)	(−1.3129)
20	0.6746	0.6905	0.6393	−1.1449	−1.1573	−1.1953
	(1.0224)	(1.0308)	(0.9668)	(−1.8387)	(−1.8605)	(−1.9179)
25	0.9141	0.9435	0.8369	−1.5598	−1.5806	−1.6601
	(1.3406)	(1.3555)	(1.2718)	(−2.4100)	(−2.4592)	(−2.5229)
30	1.1518	1.2016	1.0565	−1.9671	−1.9994	−2.0957
	(1.6520)	(1.6884)	(1.5768)	(2.9653)	(−3.0607)	(−3.1279)
35	1.4156	1.4982	1.3011	−2.4188	−2.4686	−2.5809
	(1.9704)	(2.0320)	(1.8818)	(−3.7028)	(−3.6627)	(−3.7329)
40	1.6929	1.8197	1.5580	−2.8930	−2.9629	−3.0902
	(2.2924)	(2.3898)	(2.1868)	(−4.3304)	(−4.2658)	(−4.3379)
45	1.9681	2.1562	1.8099	−3.3495	−3.4474	−3.5900
	(2.6195)	(2.7645)	(2.4918)	(−4.9684)	(−4.8694)	(−4.9429)
50	2.2529	2.5186	2.0691	−3.8184	−3.9466	−4.1043
	(2.9527)	(3.1601)	(2.7968)	(−5.6179)	(−5.4733)	(−5.5479)
55	2.5518	2.9166	2.3357	−4.2941	−4.4598	−4.6330
	(3.2935)	(3.5801)	(3.1018)	(−6.2817)	(−6.0769)	(−6.1529)
60	2.8519	3.3417	2.5980	−4.7509	−4.9623	−5.1533
	(3.6437)	(4.0295)	(3.4068)	(−6.9618)	(−6.6794)	(−6.7579)
65	3.1565	3.8017	2.8566	−5.1855	−5.4540	−5.6664
	(4.0059)	(4.5140)	(3.7118)	(−7.6608)	(−7.2790)	(−7.3629)
70	3.4707	4.3093	3.1140	−5.5968	−5.9376	−6.1771
	(4.3834)	(5.0404)	(4.0168)	(−8.3818)	(−7.8704)	(−7.9679)
75	3.8049	4.8793	3.3769	−5.9991	−6.4244	−6.6985
	(4.7813)	(5.6169)	(4.3218)	(−9.1293)	(−8.4588)	(−8.5729)
80	4.1383	5.5187	3.6381	−6.3883	−6.9322	−7.2163
	(5.2068)	(6.2537)	(4.6268)	(−9.9065)	(−9.0290)	(−9.1779)
85	4.5546	6.2563	3.9150	−6.7415	−7.3764	−7.7657
	(5.2988)	(6.9650)	(4.9318)	(−10.7191)	(−9.9462)	(−9.7829)
90	4.9910	7.1090	4.1889	−7.0529	−7.8190	−8.3090
	(6.1943)	(7.7686)	(5.2368)	(−11.5732)	(−10.0747)	(−10.3879)
95	5.4877	8.0945	4.4585	−7.2727	−8.1969	−8.8438
	(6.8084)	(8.6888)	(5.5418)	(−12.4763)	(−10.5008)	(−10.9924)

by the use of CC screening parameters by a factor of about 2.5. For this atom, as expected, relativity plays an insignificant role in affecting the energy shifts. This is true for both choices of the screening parameters. In general, as we go to heavier atoms relativistic corrections tend to dominate over the effects of screening.

Further, we find that the relativistic effect is more pronounced when we have a vacancy in the L_2 subshell. For example, for $Z=95$, the relativistic correction to ΔE_K for a vacancy in the L_2 subshell is about 80% (56%) but a similar correction is only 23% (22%) for the vacancy in the L_3 subshell. The percentages inside the parentheses refer to numbers for the Slater screening parameters. As for ΔE_{L_2} $(=\langle L_2 \mid V_{L_2} \mid L_2 \rangle)$ and ΔE_{L_3} $(=\langle L_3 \mid V_{L_3} \mid L_3 \rangle)$ we see that the numbers for ΔE_{L_2} exhibit more deviation from the nonrelativistic values than shown by the numbers for ΔE_{L_3}. The reason for this may be understood as follows.

In the case of inner-shell electrons of heavy atoms, the large component of the relativistic wave function is pulled in considerably when compared to the nonrelativistic one. This pulling in of the relativistic wave function which results from the mass velocity effect[9] is dominant for the L_2 electrons and is not that significant[5] for the L_3 electrons.

Results for $\Delta E_{K\alpha}$ $(=\Delta E_K - \Delta E_L)$ and ΔE_{KLL} $(=\Delta E_K - 2\Delta E_L)$ are presented in Table II for a vacancy in the $2p$ subshell. In the relativistic theory the spin-orbit coupling splits the $\Delta E_{K\alpha}$ to $\Delta E_{K\alpha_1}$ and $\Delta E_{K\alpha_2}$ while ΔE_{KLL} splits to $\Delta E_{KL_2L_2}$ and $\Delta E_{KL_3L_3}$. For $\Delta E_{K\alpha_1}$ and $\Delta E_{K\alpha_2}$ we have the spectator vacancy in L_3 and L_2 subshells, respectively. More specifically, we write $\Delta E_{K\alpha_1} = \langle K \mid V_{L_3} \mid K \rangle - \langle L_3 \mid V_{L_3} \mid L_3 \rangle$ and $\Delta E_{K\alpha_2} = \langle K \mid V_{L_2} \mid K \rangle - \langle L_2 \mid V_{L_2} \mid L_2 \rangle$. Also

$$\Delta E_{KL_2L_2} = \langle K \mid V_{L_2} \mid K \rangle - 2\langle L_2 \mid V_{L_2} \mid L_2 \rangle$$

and

$$\Delta E_{KL_3L_3} = \langle K \mid V_{L_3} \mid K \rangle - 2\langle L_3 \mid V_{L_3} \mid L_3 \rangle .$$

For Ne our results for $\Delta E_{K\alpha}$ based on CC choice of screening parameters compare quite well with the Hartree-Fock (HF) result (0.1911 a.u.) of Bhalla and Hein.[10] The experimental result[1] for $\Delta E_{K\alpha}$ is 0.2573 a.u. The Slater screening parameters yield a result which deviates considerably from the quoted HF value. Extensive Hartree-Fock or Hartree-Fock-Slater (HFS) calculations are not available for comparison with other results presented in this table. Parente *et al.*[11] have tabulated theoretical energies for the L x-ray satellite that arise from transitions in the presence of one spectator hole in the M and N shells. The computations are relativistic. Therefore, extension of our work for the L shell will be interesting. This is, however, quite a program and we propose to deal with this in a future publication.

Some HFS calculations[2] indicate that the magnitude of ΔE_{KLL} approaches that of $\Delta E_{K\alpha}$. We find that for both choices of our screening parameters this is not true for the nonrelativistic model. But from our relativistic calculations we see that $|\Delta E_{K\alpha_2}| \rightarrow |\Delta E_{KL_2L_2}|$ for $Z \geq 70$, particularly for the CC choice of screening parameters. Unfortunately, this type of correlation is a little inaccurate for $|\Delta E_{K\alpha_1}|$ and $|\Delta E_{KL_3L_3}|$.

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