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Electron Screening in Muonic Atoms*

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Screening corrections to the muon binding energies are computed for Pb, Tl, Ba, and O. Available methods of calculation are compared. It is shown that in a broad range of atomic charges and muon states the screening of nuclear charge by the muon is almost complete, and therefore the electron density of the Z-1 element can be used in most applications. The effect of the muon on the electron cloud and the effect of the vacancies in electron shells on the screening corrections are calculated and discussed. The degree of ionization of the electron $1s_{1/2}$ orbit is determined by a cascade calculation including repopulation from the $2p$ shell.

I. INTRODUCTION

Several muonic x-ray transition energies were measured recently with accuracies of 20–50 eV.[1,2] With the new high-intensity accelerators, utilization of curved-crystal spectrometers might become feasible and accuracies of a few electron volts could be achieved for the 50–100 keV transitions. Not all measured energies agree well with the theoretical predictions; Dixit *et al.*[2] report systematic deviations exceeding substantially experimental errors. On the other hand, some of the theoretical correction terms, notably the higher-order vacuum-polarization contributions,[3,4] are in doubt. Thus both the improved experimental accuracy and the mentioned discrepancies gave an impetus for reexamination of yet another theoretical correction term in muonic atoms—electron screening.

Generally, the potential of atomic electrons is a slowly decreasing function of the radius. The constant, uninteresting part (i.e., electronic potential at the nuclear site) is approximately equal to the Thomas–Fermi expression

$$V(0)=1.8(me^3/\hbar^2)Z^{4/3}\simeq 0.049Z^{4/3}\text{ keV}.$$

The decreasing part, caused by the electronic density inside the orbit of the muon, leads to a negative contribution to the muonic x-ray energy. Its magnitude thus depends on the behavior of the electron density at distances smaller than the radius of the electron K orbit.

The effect was calculated before using various approximations, e.g., only $1s$ electrons were included,[1,2] or the calculated electron density of the atom with $(Z-1)$ protons was used.[5,6] The most sophisticated calculations were done by Fricke.[7] He used a self-consistent calculation in a system of the nucleus and atomic electrons plus muon in a given orbit. Only results for muonic lead were given. The mentioned approximations differ vastly in the complexity and in the amount of computer time involved. For the most carefully studied transition, $5g_{9/2} \rightarrow 4f_{7/2}$ in Pb^{208}, the screening corrections quoted in the literature differ by as much as 20 eV—an amount already comparable with the experimental accuracy.

II. METHOD OF CALCULATION

The screening contribution to the muon binding energy, calculated in this paper and given in Tables I–III, VIII, and IX, is obtained in the following way.

The radial Dirac equation for a muon in the given orbit is solved numerically. The potential in the equation contains a nuclear part $V_{\text{nucl}}(r)$ and a screening part $V_{\text{scr}}(r)$. The $V_{\text{nucl}}(r)$ is given by

$$V_{\text{nucl}}(r) = -\frac{4\pi e^2}{r}\int_0^r \rho_{\text{nucl}}(t)t^2\,dt - 4\pi e^2 \times \int_r^\infty \rho_{\text{nucl}}(t)t\,dt \ . \quad (1)$$

[The $\rho_{\text{nucl}}(r)$ is spherically symmetric nuclear density distribution, taken as a Fermi function here.] The results for high-n muonic states are practically independent of the details of $\rho_{\text{nucl}}(r)$, and $V_{\text{scr}}(r)$ is given by

$$V_{\text{scr}}(r) = \frac{4\pi e^2}{r}\int_0^r \rho_{\text{el}}(t)t^2\,dt + 4\pi e^2\int_r^\infty \rho_{\text{el}}(t)t\,dt \ . \quad (2)$$

Here $\rho_{\text{el}}(r)$ is the spherically averaged electron density of the atom, normalized in the usual way:

$$4\pi\int_0^\infty \rho_{\text{el}}(r)r^2\,dr = \text{number of electrons.} \quad (3)$$

Binding energies for muon in state i were calculated with screening (E^i_{scr}) and without screening (E^i_0). The screening correction is then

$$\Delta E^i = E^i_0 - E^i_{\text{scr}} > 0 \ . \quad (4)$$

The accuracy of the muonic eigenvalues (due to round-off errors in the calculation) is about 1 eV; the accuracy of ΔE^i strongly depends on $\rho_{\text{el}}(r)$. Three different methods were used for calculations of $\rho_{\text{el}}(r)$ for a given muonic atom with nuclear charge Z and nuclear mass A.

Method I. Only the two $1s_{1/2}$ electrons are used, i.e.,

$$\rho_{\text{el}}(r)4\pi r^2 = 2[g^2(r) + f^2(r)] \ , \quad (5)$$

where g, f are solutions of the Dirac equation for $1s_{1/2}$ electron in the field of point charge $(Z-1)e$.

Method II. $\rho_{\text{el}}(r)$ is the electronic density of an atom $(Z-1)$ calculated by the relativistic Hartree–Fock–Slater method. A modification of a computer program originally written by Seltzer[8] was used. First-order vacuum polarization, as well as a Fermi charge distribution for the nuclear density, was included. As usual, the nonlocal exchange potential is approximated by the local Slater free-electron exchange

$$V_{\text{ex}}(r) = -6[3\rho_{\text{el}}(r)/8\pi]^{1/3} \ . \quad (6)$$

The calculated electron eigenvalues agree with experimental binding energies within about 0.3% for the inner $K, L,$ and M shells and nuclei considered. The remaining discrepancy can probably be attributed to the nonincluded corrections for magnetic energy, self-energy, and retardation energy (see Desiderio and Johnson, Ref. 9). The error in calculation of relative quantities, like isotope shifts or shifts considered in Table V below, is, however, considerably smaller. The self-consistent iterations were terminated when relative change in $V_{\text{scr}}(r)$ was $\Delta V/V < 10^{-4}$ for r between the nuclear radius and the radius of the electron K orbit. This corresponds again to an accuracy about 1 eV in ΔE^i.

Method III. The same program as in method II is used; however, the potential due to the muon in the unperturbed orbit i is added to the nuclear Coulomb potential of a nucleus Z. The electrons partially penetrate through the muon orbit and therefore are more bound than in method II; the $V_{\text{scr}}(r)$ near the nucleus is somewhat larger. The effect is more pronounced for muon orbits with larger n or for more eccentric orbits. The perturbation of the muon eigenfunction by $V_{\text{scr}}(r)$ is so small that another iteration in this procedure is not necessary. Although the whole system of muon plus atomic electrons depends now on the state i of the muon, it is easy to see that the muonic x-ray energy is still equal to the difference of the muon eigenvalues (analog of Koopmans's theorem).

III. RESULTS AND DISCUSSION

The electron screening contributions to the muonic binding energy for a heavy nucleus $_{82}Pb^{208}$ and a medium Z nucleus $_{56}Ba^{138}$ are shown in Tables I and II. Each state is characterized by its quantum numbers and its binding energy E. The quantity E is the energy eigenvalue without screening; it does not include various quantum electrodynamic and nuclear polarization contributions necessary for comparison with experiment. Columns 3–5 of the tables contain the screening effect calculated according to methods I, II, and III. To stress the smallness of the observable part, the constant part of the screening correction was subtracted, i.e.,

$$\Delta = \Delta E^i - V_0 \ .$$

All energies are in keV. Believing that the most elaborate method (III) gives most reliable results, we see that II overestimates the effect slightly, while I underestimates it by a somewhat larger

TABLE I. Electron screening in muonic $_{82}Pb^{208}$ (parameters of ρ_{nucl}: $c=6.659$ fm, $t=2.257$ fm, all energies in keV).

		Electron screening Δ		
		Only $(1s)^2$ electrons	$(Z-1)$ electrons	$(Z-1)$ electrons + muon
		I	II	III
State	E binding	$V_0=5.444$	$V_0=17.318$	$V_0=17.321$
$1s_{1/2}$	10526.607	0.000	0.000	0.000
$3d_{5/2}$	2120.378	−0.038	−0.038	−0.038
$4f_{7/2}$	1188.314	−0.084	−0.091	−0.089
$4f_{5/2}$	1197.378	−0.081	−0.091	−0.088
$5g_{9/2}$	758.972	−0.151	−0.177	−0.172
$5g_{7/2}$	761.723	−0.151	−0.176	−0.169
$6h_{11/2}$	526.481	−0.252	−0.298	−0.287
$7i_{13/2}$	386.545	−0.385	−0.457	−0.441
$7i_{11/2}$	387.020	−0.382	−0.455	−0.439
$7h_{11/2}$	387.020	−0.449	−0.535	−0.517
$7h_{9/2}$	387.686	−0.447	−0.535	−0.516
$8k_{15/2}$	295.823	−0.544	−0.650	−0.630
$8k_{13/2}$	296.060	−0.543	−0.649	−0.628
$8i_{13/2}$	296.059	−0.624	−0.746	−0.723
$8i_{11/2}$	296.377	−0.623	−0.744	−0.721
$8h_{11/2}$	296.377	−0.690	−0.825	−0.800

amount. Note also that ΔE^i depends essentially only on the orbital quantum number l, and very little on j, even for high-Z atoms.

The outer electrons contribute only to V_0; practically all variable screening comes from the electron K, L, and M shells. For example, for the muon states $4f_{7/2}$, $5g_{9/2}$, and $6h_{11/2}$ the entries in Table I are, respectively, −0.091, −0.177, and −0.295 in column 4 and −0.089, −0.170, and −0.285 in column 5, when only 28 electrons are included. The constant V_0 is, however, only 14.215 keV in such a case.

The results in column 5 of Table I agree quite well with similar numbers by Fricke.[7]

Electron screening is a major correction factor for muonic x rays going across many shells, i.e., with $\Delta n \gg 1$. Recently a number of such transitions were observed in muonic thallium (Ref. 5). In extracting the experimental screening factor, the calculated splitting and calculated intensities of unresolved fine-structure components were used.[5] The corresponding screening corrections are shown in Table III. The difference between methods II and III is still small, and general agreement with experiment is rather good. Note that screening was also calculated in Ref. 5 using a method similar to II. The results[5] are typically 30 eV larger in absolute value than in column 3 of Table III.

The screening correction is a smooth function of Z. For example, the ΔE^i in Tl(Hg) are very close to 0.98 (0.98^2) of the corresponding values in Pb. Thus interpolation or extrapolation to neighboring Z is possible.

For low-Z elements the screening is, as expected, a very small effect. The screening corrections to the Lyman series in muonic oxygen, often present in muonic experiments, are shown in Table IV.

The effect of the muon on the electron cloud, mentioned above, is exemplified in Table V. Pene-

TABLE II. Electron screening in muonic $_{56}Ba^{138}$ ($c=5.762$, $t=2.25$ fm, all energies in keV).

		Electron screening Δ		
		I	II	III
State	E	$V_0=3.242$	$V_0=9.428$	$V_0=9.428$
$3d_{3/2}$	993.265	0.000	0.000	0.000
$4f_{5/2}$	554.337	−0.017	−0.018	−0.017
$5g_{7/2}$	353.792	−0.045	−0.049	−0.047
$7i_{13/2}$	180.055	−0.143	−0.163	−0.155
$7h_{11/2}$	180.157	−0.175	−0.200	−0.190
$7g_{9/2}$	180.302	−0.200	−0.228	−0.217
$8k_{15/2}$	137.826	−0.218	−0.249	−0.237
$8i_{13/2}$	137.878	−0.258	−0.294	−0.282
$8h_{11/2}$	137.947	−0.291	−0.333	−0.320

TABLE III. Screening contribution to the muonic x-ray energy in Tl^{205} ($c=6.629$, $t=2.28$ fm). Experimental values from Ref. 5; energies in keV.

Transition	Method II	Method III	Experimental
$13l_{17/2}\to 8k_{15/2}$	−1.724	−1.716	−1.67 ± 0.10
$13k_{15/2}\to 7i_{13/2}$	−1.987	−1.973	−2.36 ± 0.18
$12l_{17/2}\to 8k_{15/2}$	−1.346	−1.337	−1.37 ± 0.07
$12k_{15/2}\to 7i_{13/2}$	−1.618	−1.603	−1.71 ± 0.13
$12i_{13/2}\to 6h_{11/2}$	−1.842	−1.824	−1.80 ± 0.60
$11i_{13/2}\to 6h_{11/2}$	−1.473	−1.456	−1.24 ± 0.20

tration of the atomic electrons through a muon orbit and the corresponding increase in their binding energy is maximum for the electron $1s_{1/2}$ state. The effect depends, as expected, on the instantaneous state of the muon, decreasing as the muon cascades closer to the nucleus. Thus, atomic K x rays of, for example, muonic lead will be broader and shifted toward a higher energy when compared with standard $_{81}$Tl K x-ray lines. Observation of such an effect would yield important information about the promptness with which vacancies in the electron shells are repopulated.

IV. POPULATION OF ELECTRON 1s STATE

The small difference between methods I and II or III shows that most (80–85%) of the variable screening comes from the electron $1s$ shell. However, this state can be depleted by Auger transitions during the muonic cascade. In such a case the observable screening correction will be reduced considerably.

An attempt was made to calculate the probable population of the electron $1s$ state in various stages of the muonic cascade. A "standard" method developed by Eisenberg and Kessler[10] was used. The cascade calculation started with a statistical distribution at $n=15$ where the $1s$ electron shell is fully occupied. From energy considerations only, the L shell might have up to five vacancies then; the actual number of vacancies is certainly smaller owing to competition of other Auger processes and refilling from higher shells. The calculation was performed for two holes, i.e., four electrons in the $2p$ shell. The results are not critically dependent on that assumption as long as at least two electrons are left in the $2p$ orbit.

TABLE IV. Screening in muonic O (constant screening $V_0=510.4$ eV).

Transition	Transition energy (keV)	Screening correction (eV)
$4p_{3/2}\to 1s_{1/2}$	166.408	−2.4
$3p_{3/2}\to 1s_{1/2}$	157.714	−0.6
$2p_{3/2}\to 1s_{1/2}$	132.878	−0.1

TABLE V. Calculated difference between the electron binding energies of muonic $_{82}Pb^{208}$ and of a normal $_{81}$Tl atom. The state of the muon in Pb is shown in column 1, shifts of the electron $1s_{1/2}$, $2p_{1/2}$, and $3p_{1/2}$ states (in eV) are given columns 2, 3, and 4, respectively.

State	$\Delta 1s_{1/2}$	$\Delta 2p_{1/2}$	$\Delta 3p_{1/2}$
$1s_{1/2}$	11.4	0.1	0.01
$3d_{5/2}$	19.6	0.1	0.02
$4f_{7/2}$	39.7	0.3	0.05
$5g_{9/2}$	73.3	0.5	0.13
$6h_{11/2}$	122.2	1.0	0.25
$7i_{13/2}$	186.8	1.9	0.57
$7h_{11/2}$	218.2	2.2	0.71
$7g_{9/2}$	245.3	2.7	0.84
$8k_{15/2}$	266.1	3.0	0.92
$8i_{13/2}$	305.7	3.7	1.11
$8h_{11/2}$	338.7	4.4	1.28
$_{82}$Pb(no μ)	2491.4	503.8	139.0

Competition between Auger transitions and x-ray repopulation was first considered by de Borde.[11] The equations corresponding to the general case are given in the Appendix. Reduction of the x-ray rate P_x due to instantaneous incomplete filling of the $2p$ shell was included in the calculation. However, the possible refilling of the $2p$ shell was not included. Such a process is slower than both the K x-ray emission and most muonic transitions.

The results are shown in Tables VI and VII, where the average number of the atomic electrons present on the $1s$ orbit at the moment when the muon has reached the corresponding state is shown This number is obtained by averaging the quantity $2a_{f2}+a_{f1}$ from Eqs. (A6) and (A7) through all possible ways of the muonic state population. Refilling of the electron $1s$ state competes with the muonic transition in the next step of the cascade. Thus the actual number of the $1s$ electrons $\bar{n}_{i\to f}$ [(A9)], which determines the screening effect, is somewhat increased. For the most strongly affected $7i\to 6h$ transitions, $\bar{n}_{i\to f}$ is 1.94 (1.69) in Pb(Ba), compared to the initial $1s$-electron orbit population (given in Tables VI and VII) of 1.75 (1.42).

The electron $2p$ shell is strongly depleted by combination of the Auger and x-ray processes; there are about 2.5 $2p$ electrons left in Pb and only one left in Ba for lower ($n\leq 6$) stages of the cascade. The $2s$ state is not affected by the x-ray emission; there are about 66% (50%) of $2s$ electrons left in Pb (Ba).

TABLE VI. Muonic cascade in Pb. The muonic states are characterized by the n, l quantum numbers in the first column and row, respectively. For each state the upper entry gives probability of population (in %). The lower entry gives the average number of atomic 1s electrons present when the muon has reached the corresponding n, l state.

n \ l	2	3	4	5	6	7	8	9	10
11	0.1 2.0	0.3 2.0	0.4 2.0	1.7 2.0	3.4 2.0	5.9 2.0	9.4 2.0	13.6 2.0	18.4 2.0
10	0.1 1.82	0.4 1.85	1.0 1.88	2.3 1.91	4.7 1.94	8.6 1.97	14.1 1.98	21.0 1.99	
9	0.2 1.90	0.5 1.91	1.4 1.91	3.5 1.93	7.4 1.94	14.2 1.92	25.4 1.96		
8	0.2 1.94	0.8 1.93	2.4 1.93	6.4 1.93	15.0 1.94	32.7 1.96			
7	0.4 1.92	1.5 1.88	5.2 1.84	15.7 1.80	41.5 1.75				
6	0.7 1.96	3.2 1.93	13.7 1.90	51.0 1.86					
5	1.6 1.98	10.5 1.96	62.0 1.92						
4	6.5 1.98	75.1 1.95							
3	86.2 1.96								

The effect of vacancies in electron $1s_{1/2}$, $2s_{1/2}$, or $3s_{1/2}$ states on the screening correction is shown in Tables VIII and IX. The simpler method (II) was used; columns denoted a were calculated with "frozen" $\rho_{el}(r)$ of a neutral $Z-1$ atom from which the corresponding electron was removed. In column b the relaxation of $\rho_{el}(r)$ was included. There is almost no difference in observable screening be-

TABLE VII. Muonic cascade in Ba. Same as Table VI.

n \ l	2	3	4	5	6	7	8	9	10
11	0.1 2.0	0.6 2.0	1.3 2.0	2.3 2.0	3.8 2.0	5.9 2.0	8.8 2.0	12.2 2.0	14.7 2.0
10	0.4 1.51	0.9 1.55	1.8 1.60	3.0 1.65	4.6 1.72	6.8 1.80	10.1 1.90	16.8 1.96	
9	0.4 1.60	1.1 1.58	2.5 1.58	4.7 1.58	7.7 1.60	12.4 1.66	23.5 1.81		
8	0.4 1.75	1.3 1.74	3.2 1.73	6.5 1.75	12.4 1.78	29.6 1.86			
7	0.7 1.70	2.5 1.63	6.8 1.56	15.4 1.49	37.3 1.42				
6	1.1 1.83	4.6 1.74	14.3 1.63	43.6 1.45					
5	2.4 1.90	11.9 1.80	53.6 1.57						
4	8.3 1.89	67.0 1.65							
3	80.0 1.70								

TABLE VIII. Influence of one-electron vacancies in the electron shells in muonic Pb on the screening correction. Energies in keV. Columns a were calculated with the electron density ρ_{el} of a neutral $Z-1$ atom, with corresponding electron removed. In columns b the relaxation of ρ_{el} was included.

Muon in state	One electron missing in shell: K a	K b	L_I a	L_I b	M_I a	M_I b	No vacancy
$3d_{5/2}$	14.584	14.779	16.610	16.749	17.033	17.126	17.280
$4f_{7/2}$	14.552	14.747	16.558	16.697	16.979	17.072	17.227
$5g_{9/2}$	14.503	14.700	16.481	16.621	16.897	16.990	17.141
$6h_{11/2}$	14.433	14.626	13.367	16.506	17.777	16.871	17.021
$7i_{13/2}$	14.340	14.532	16.218	16.356	16.621	16.715	16.861
$7h_{11/2}$	14.295	14.487	16.145	16.285	16.544	16.638	16.783
$7g_{9/2}$	14.257	14.449	16.085	16.223	16.481	16.575	16.719
$8k_{15/2}$	14.228	14.419	16.037	16.176	16.431	16.525	16.668
$8i_{13/2}$	14.171	14.362	15.948	16.086	16.337	16.431	16.572
$8h_{11/2}$	14.125	14.315	15.873	16.011	16.259	16.352	16.493

tween cases a and b. It is seen that approximately 82% of the observable screening effect comes from the $1s_{1/2}$ electrons, 12% from the $2s_{1/2}$ electrons, and 3% from $3s_{1/2}$ electrons.

The incomplete filling of the electron shells will cause broadening and asymmetrical shapes of the muonic lines. The positions of the maximum of the lines can be derived from the numbers given in Tables VI–IX.

V. CONCLUSIONS

The calculations have shown that the relatively simple method II can replace the more complicated but more consistent method III for most applications. The largest uncertainty in the screening correction is connected with incomplete filling of the electron shells in the latter phases of muonic cascade.

Observation of energy shifts of atomic x rays accompanying the muonic cascade or high-precision (5% or better) measurement of the screening effect in a broad range of Z would help to resolve this problem and give therefore unique information about the early history of a muonic atom.

TABLE IX. Influence of one-electron vacancies in the electron shells in muonic Ba on the screening correction. Energies in keV. Columns a were calculated with the electron density ρ_{el} of a neutral $Z-1$ atom, with a corresponding electron removed. In columns b the relaxation of ρ_{el} was included.

Muon in state	One electron missing in shell: K a	K b	L_I a	L_I b	M_I a	M_I b	No vacancy
$3d_{3/2}$	7.821	7.960	9.048	9.145	9.290	9.344	9.428
$4f_{5/2}$	7.802	7.950	9.031	9.128	9.273	9.327	9.410
$5g_{7/2}$	7.785	7.932	9.001	9.098	9.242	9.296	9.379
$7i_{13/2}$	7.720	7.867	8.894	8.990	9.129	9.183	9.265
$8k_{15/2}$	7.671	7.817	8.812	8.909	9.045	9.098	9.169

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APPENDIX: COMPETITION BETWEEN RADIATION, AUGER ELECTRON EMISSION, AND REPOPULATION OF ELECTRON 1s STATE

At time $t=0$ the muon is in a given initial state i. We want to consider the muonic transition $i\to f$ with radiative rate P_R. P_K is the rate for Auger $1s$ electron emission from a fully occupied $1s$ state. Equations for P_R and P_K can be found in Ref. 10. The partially filled $1s$ shell contains originally 2 (1, 0) electrons with probabilities a_{i2} (a_{i1}, a_{i0}). The rate of the $2p\to 1s$ x-ray transition (for one vacancy in $1s$) was calculated by Scofield[12]; it is denoted P_x here.

Denote by $\chi_0(t)$ the probability that the muon is still in the state i, $\chi_R(t)$ the probability of a radiative process, and by $\chi_A(t)$ the probability of an Auger transition. We have then

$$\dot{\chi}_R = P_R\chi_0\ , \tag{A1}$$

$$\dot{\chi}_A = [a_{i2} + a_{i1}\tfrac{1}{2}(2-e^{-P_xt}) + a_{i0}(2-e^{-P_xt})\tfrac{1}{2}(1-e^{-P_xt})]P_A\chi_0\ , \tag{A2}$$

$$\dot{\chi}_A + \dot{\chi}_R = -\dot{\chi}_0\ . \tag{A3}$$

Denote further

$$\varphi_1(t) = \exp\left[(P_A/2P_x)(1 - e^{-P_x t})\right],$$

$$\varphi_0(t) = \exp\left[(3P_A/2P_x)(1 - e^{-P_x t})\right] \times \exp\left[(P_A/4P_x)(1 - e^{-2P_x t})\right].$$

Then

$$\chi_0(t) = \left[a_{i2} + a_{i1}\varphi_1(t) + a_{i0}\varphi_0(t)\right] e^{-(P_A+P_R)t}. \qquad \text{(A4)}$$

The total Auger transition rate P_A^1 (corrected for partial population of the 1s state) can be determined from the equation

$$\chi_R(\infty) \equiv \frac{P_R}{(P_A^1 + P_R)} = P_R \int_0^\infty \chi_0(t)\, dt\ . \qquad \text{(A5)}$$

The population of the electron 1s state when the muon reaches the state f is given by

$$a_{f2} = P_R \int_0^\infty \left[a_{i2} + a_{i1}(1 - e^{-P_x t})\varphi_1(t) + a_{i0}(1 - e^{-P_x t})^2 \varphi_0(t)\right] e^{-(P_A+P_R)t}\, dt\ , \qquad \text{(A6)}$$

$$a_{f1} = \int_0^\infty \{P_A a_{i2} + a_{i1}\varphi_1(t)[(P_R - P_A)e^{-P_x t} + P_A] + a_{i0}\varphi_0(t) \times [P_R(1 - e^{-P_x t})e^{-P_x t} + P_A(1 - e^{-P_x t})^2\} e^{-(P_A+P_R)t}\, dt, \qquad \text{(A7)}$$

$$a_{f0} = \int_0^\infty \{a_{i1}\varphi_1(t)\tfrac{1}{2}P_A e^{-P_x t} + a_{i0}\varphi_0(t) e^{-P_x t} \times [P_R + \tfrac{1}{2}P_A(1 - e^{-P_x t})]\} e^{-(P_A+P_R)t}\, dt\ . \qquad \text{(A8)}$$

The average number of 1s electrons actually present during the muonic radiative $i \to f$ transition is

$$\bar{n}_{i\to f} = 2a_{f2} + a_{f1} + [P_A^1/(P_A^1 + P_R)]\ . \qquad \text{(A9)}$$

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Excited Electronic States of O_2^-

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Excited electronic states of the O_2^- molecule have been calculated with configuration-interaction (CI) variational trial functions that assure formally correct asymptotic behavior as well as the single-configuration self-consistent-field (SCF) approximation. CI results were obtained by both multiconfiguration self-consistent-field (MC-SCF) and pseudonatural orbital (PNO) techniques. The MC-SCF results are most accurate and are used to analyze the energy curves and wave functions of these states for internuclear separations larger than 3 a.u. All the excited states are found to have equilibrium-internuclear separations at least 1 a.u. larger than the ground state. The two lowest energy states, the $^4\Sigma_u^-$ and $^2\Pi_u$, are characterized, respectively, as shape and valence Feshbach resonances. They are sufficiently bound to make it likely they play a role in low-energy-electron scattering by oxygen.

I. INTRODUCTION

The experimental and theoretical understanding of the excited states of O_2^- is very limited. Simple adiabatic correlation rules determine that 24 energy curves arise from the interaction of ground state $O(^3P)$ and $O^-(^2P)$. Of all these energy curves only the ground state $X^2\Pi_g$ of the ion has been studied extensively. In particular, there has been a considerable experimental effort toward the determination of the electron affinity of O_2.[1] A recent calculation has also shown that an accurate electron