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Z Dependence of the *K-LL* Auger Rates*

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A comparison between the nonrelativistic total *K-LL* Auger rates of McGuire and our calculations is presented. The effects of the exchange approximations on the Auger rates are also presented.

In recent papers,[1,2] McGuire has reported on the nonrelativistic *K-LL* Auger transition rates for $Z \leq 54$. It is the purpose of this paper to report that the *K-LL* Auger calculations of McGuire are often erroneous by as much as 25%, and exhibit a strange local structure versus atomic number.

We have also investigated the effects of two exchange approximations in the Hartree-Fock-Slater (HFS) model by considering Slater[3] exchange and Kohn and Sham,[4] and Gaspar[5] (KSG) exchange. The results for the *K-LL* Auger transition rates are presented here.

METHOD OF CALCULATIONS

In our work[6] and that of McGuire, a nonrelativistic HFS program[7] has been utilized to obtain bound-state wave functions. In this procedure, the free-electron exchange potential (in the notation of Ref. 7) is

$$V^{\text{exch}} = -6C[(3/8\pi)|\rho|]^{1/3} . \qquad (1)$$

The Slater exchange approximation ($C = 1$) was used.

We differ from McGuire in the calculations of the continuum wave functions. McGuire approximates the screening function associated with the HFS model by a series of straight lines and then obtains analytic continuum solutions in terms of Whittaker functions.[8] The relevant continuum wave functions were numerically calculated for the HFS potential in the present work. The calculated Auger electron energies used in our computations are in agreement ($\leq 0.5\%$) with the experimentally measured energies.

All our computations correspond to an initial state in which a *K*-shell electron is missing, and we have calculated the *K*-shell Auger rates for every *Z* between 10 and 54.

The *K-LL* Auger rates were also calculated with the Kohn-Sham-Gaspar (KSG)[4,5] exchange approximation [$C = \frac{2}{3}$ in Eq. (1)] using the same Auger energies as those for Slater exchange.

RESULTS AND DISCUSSION

Figure 1 contains a comparison of theoretical *K-LL* Auger transition rates of McGuire and this work for $C = 1$. We note that the results of McGuire are consistently lower for $Z < 22$ and higher for $Z > 26$ as compared to the present work. The discrepancy is $\approx 25\%$ in a large number of cases. The relativistic HFS calculations of Bhalla and Ramsdale[9] are in agreement (within a few percent) with our work for $35 < Z < 55$.

A local structure in the *K–LL* Auger rates of McGuire is found in Fig. 1. Our calculations show a smooth dependence of the *K-LL* Auger rates versus atomic number. Similarly, the theoretical results of Callan[10] (using the hydrogenic wave functions with the effective *Z* approximation for the atomic screening) show no local structure in the *K-LL* Auger rates. We believe that the reason for the local structure in McGuire's theoretical results lies in the calculational procedure for the continuum-state wave functions. McGuire approximates the screened potential and then obtains an analytical solution in terms of the Whittaker functions. We calculate the continuum-state wave functions by the numerical integration of the Schrödinger equation with the appropriate screened potential.

The effects of the KSG exchange approximation on the *K-LL* Auger rates were also investigated. The rates using $C = \frac{2}{3}$ are smaller as compared to those

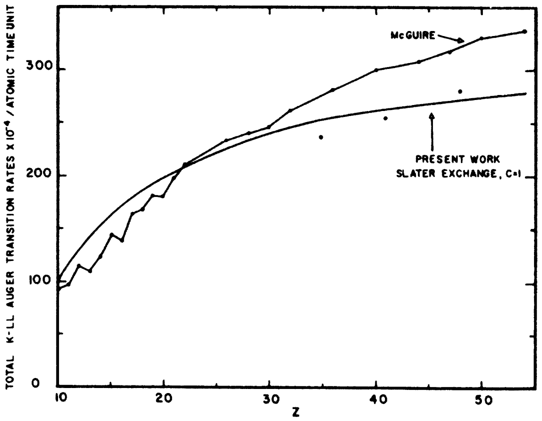

FIG. 1. Calculated total *K-LL* Auger transition rates versus atomic number. The present work is with the nonrelativistic Hartree-Fock-Slater model. The theoretical rates of McGuire are joined by lines to emphasize the local structure. The unconnected circles represent the relativistic Hartree-Fock-Slater calculations of Bhalla and Ramsdale.

with the Slater approximation. The difference in the two theoretical rates (with $C = 1$ and $C = \frac{2}{3}$) decreases smoothly with atomic number starting with a value of ≈ 14% for Z=10 decreasing to ≈ 1% for Z=54.

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Adiabatic Theory of Rotational Excitation of Non-Σ States

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The formulas for the rotational excitation of diatomic molecules in the adiabatic theory are generalized to include rotational excitation within molecular states of arbitrary Λ symmetry. For Λ not equal to zero (non-Σ states), the rotational quantum number can change by any integer, and not only an even integer as is the case for Σ states.

In two recent papers[1,2] we developed explicit formulas for the rotational excitation of diatomic molecules by electron impact in the framework of the adiabatic theory.[3] In those papers we (inadvertently) took the rotational wave functions to be ordinary spherical harmonics $Y_{jm}(\Omega_0)$. That, however, is only correct for Σ electronic states, and the results of Refs. 1 and 2 are implicitly restricted to rotational excitation of Σ states.

More generally, the relevant part of the electronic-rotational wave functions is given by[4]

$$\psi_{\text{rot}}(\vec{\beta}_0) = [(2j+1)/16\pi^2]^{1/2} [\mathfrak{D}^{(j)}_{\Lambda,m}(\vec{\beta}_0) + (-1)^{J-\Lambda+\epsilon} \mathfrak{D}^{(j)}_{-\Lambda,m}(\vec{\beta}_0)] \chi_\epsilon . \tag{1}$$

The new quantum number here is Λ, representing the angular momentum of electrons about the internuclear axis ($\Lambda = \Sigma, \Pi, \Delta \ldots$). For $\Lambda > 0$, there are two degenerate linear combinations specified by ϵ, $\epsilon = 0, 1$ defining the spatial symmetry of the wave function under exchange of the nuclei.[4] χ_ϵ is the complementary nuclear spin function with the usual orthornormality properties

$$\langle \chi_{\epsilon'}, \chi_\epsilon \rangle = \delta_{\epsilon'\epsilon} .$$

For nuclei which are composite bosons, only the space symmetric solutions $\epsilon = 0$ exist. [Correspondingly, for such homonuclear molecules the splitting (Λ doubling) that does occur for composite fermion nuclei diatomics by virtue of the finite mass of nuclei, does not occur.] The situation is fundamentally different for $\Lambda > 0$ as opposed to $\Lambda = 0$. In the latter case, there is a unique correlation between the ± character of the Σ state, and its nuclear exchange character (cf. Table 14.1 of Ref. 4). Therefore, one does not have to refer explicitly to the nuclear-exchange character ϵ in that case.

To complete the definitions of quantities in Eq. (3), the $\mathfrak{D}$ functions are the rotational harmonics, which is our name for the well-known irreducible-representation coefficients of the rotation group.[5] The angles $\vec{\beta}_0 \equiv (\alpha_0, \beta_0, \gamma_0)$ can be taken to be the three Euler angles needed to rotate a coordinate system attached to the body-fixed internuclear axis into a space-fixed system most conveniently defined by the incident direction of the impinging electron beam.[6] The integrations needed for the rotational function [Eq. (1)] are simple generalizations of the