

POSITRON-RUBIDIUM SCATTERING

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ABSTRACT

A 5-state close-coupling calculation (5s-5p-4d-6s-6p) has been carried out for e^+ -Rb scattering in the energy range 3.7–28.0 eV. In contrast to the results of similar close-coupling calculations for e^+ -Na and e^+ -K scattering the (effective) total integrated cross section has an energy dependence which is contrary to recent experimental measurements.

INTRODUCTION

During the past several years there have been a number of elaborate close-coupling calculations for e^+ -Na¹⁻⁴ and e^+ -K²⁻⁵ scattering in the energy region from 0.5 to 100 eV. In addition, there have been other calculations for these two systems based upon the core-corrected modified Glauber approximation^{6,7}. So far the total cross sections, as determined by both of these theoretical approaches, have been in satisfactory agreement with the corresponding experimental data for Na⁸ and K^{9,10} both with respect to the shape and magnitude of the cross sections.

In comparing theory with experiment it is necessary, particularly at the very low energies, to compensate for the fact that experimentally it is not possible to discriminate against positrons scattered *elastically* through small angles about the forward direction. Thus, in making their comparison with experiment, Ward *et al.*²⁻⁵ determined the elastic differential cross section and from this computed an effective elastic cross section and hence an effective total cross section.

We report here the first close-coupling calculation for e^+ -Rb scattering and compare our results with the recent experimental measurements of Stein *et al.*¹¹

THEORY

The close-coupling calculations for the alkalis have so far been based upon a one-electron model for the atom where the valence orbital, either in the ground or an excited state, moves in the central potential of a fixed (frozen) ion core.

This model can be most easily accommodated within the standard frozen-core Hartree-Fock approximation.¹² Here, the core orbitals of the closed-shell alkali ion are first computed via the standard fully-varied Hartree-Fock procedure and then, with these core orbitals held fixed, a single Hartree-Fock equation is solved in turn for each of valence orbitals (including the ground state) of the alkali atom. Although this simple model for the alkali atoms and alkali-like ions has met with some success in the determination of ionization energies and oscillator

strengths for these systems¹³⁻¹⁶ the overall accuracy of this model deteriorates with increasing size of the ion core.

However, this model can be significantly improved, and at the same time retain its one-electron character, if core polarization of the valence electron is incorporated into the model. Two different approaches to the inclusion of core polarization have so far proved quite successful. One method involves the use of a model potential which includes both the dipole and quadrupole polarizabilities of the alkali core.¹⁷ The other method first determines a core polarization potential for the closed shell Hartree-Fock alkali ions via an adiabatic polarized-orbital procedure¹⁸ and then solves variationally a single Hartree-Fock equation, which includes this core polarization potential, for the ground and excited valence states of the atom.^{19,20}

In the close-coupling calculations of Ward *et al.*²⁻⁵ for positron scattering from Li, Na and K the model potentials of Peach¹⁷ were primarily used to determine the atomic wavefunctions. In the present calculations for e^+ -Rb scattering we have chosen to use polarized Hartree-Fock orbitals. Table 1 contains the ionization energies of the first few s-, p- and d-levels of Rb as obtained via the regular frozen-core Hartree-Fock procedure (FC-HF) and the polarized frozen-core Hartree-Fock method (PFC-HF). Also included are the corresponding experimental values for these ionization energies.²¹

TABLE 1. Ionization energies of Rb in atomic units.

| Level | FC-HF | PFC-HF | Experiment |
|-------|----------|----------|------------|
| 5s | 0.137202 | 0.153621 | 0.153508 |
| 6s | 0.058140 | 0.061719 | 0.061772 |
| 7s | 0.032209 | 0.033591 | 0.033624 |
| 5p | 0.090135 | 0.096921 | 0.095472 |
| 6p | 0.043652 | 0.045643 | 0.045218 |
| 7p | 0.025887 | 0.026760 | 0.026575 |
| 4d | 0.060066 | 0.072899 | 0.065319 |
| 5d | 0.033972 | 0.039773 | 0.036399 |
| 6d | 0.021570 | 0.024397 | 0.022793 |

In the determination of the core polarization potential for Rb⁺ only the 3d, 4s and 4p core Hartree-Fock orbitals were polarized. As can be seen from the table, the ionization energies for the s- and p-levels which were determined within the PFC-HF framework are in far better agreement with experiment than those obtained without core polarization. On the other hand neither model does

particularly well for the d-levels. This is most probably an indication that the 'one-electron' model is beginning to break down for an alkali the size of Rb.

The FC-HF model yields a dipole polarizability of $510 a_0^3$; the PFC-HF procedure gives $353 a_0^3$ which is

approximately 10% higher than the experimental value of $319 \pm 6 a_0^3$.²²

The close-coupling equations can be written, in differential equation form, as

$$\left[\frac{d^2}{dr^2} - \frac{l_2(l_2+1)}{r^2} - 2V_c(r) + k_\nu^2 \right] F_{\nu LS}(r) = -2 \sum_{\nu'} V(\nu, \nu')_L F_{\nu' LS}(r) \quad (1)$$

where $\nu = n_1 l_1 l_2$

$$V_c(r) = \frac{Z}{r} - \sum_{nl} 2(2l+1) y_0(nl, nl; r) \quad (2)$$

$$V(\nu, \nu')_L = \sum_{\lambda} f_{\lambda}(l_1 l_2, l'_1 l'_2; L) y_{\lambda}(n_1 l_1, n'_1 l'_1; r) \quad (3)$$

and

$$y_{\lambda}(n_1 l_1, n'_1 l'_1; r) = r^{-\lambda-1} \int_0^r P_{n_1 l_1}(x) P_{n'_1 l'_1}(x) x^{\lambda} dx + r^{\lambda} \int_r^{\infty} P_{n_1 l_1}(x) P_{n'_1 l'_1}(x) x^{-\lambda-1} dx \quad (4)$$

The functions $F_{\Gamma}(r)$ describe the radial motion of the incident positron and the P 's are the radial atomic orbitals. The summation in equation (2) is over the core orbitals and the coefficients f_{λ} as well as the subscript Γ are defined in Percival and Seaton.²³

In this work we have solved the equivalent integral equation formulation of the close-coupling equations by a technique which is similar to that used by McEachran and Fraser.²⁴ From the asymptotic form of the solutions to these equations one can obtain, with the help of asymptotic correction procedures,²⁵ the elements, $R_{\nu\nu'}^{LS}$, of the R matrix and hence the corresponding elements of the S and T matrices.

The total cross section for the excitation of an alkali atom from the state $n'_1 l'_1$ to $n_1 l_1$ is given (in units of πa_0^2) by

$$\sigma(n'_1 l'_1 \rightarrow n_1 l_1) = \sum_{LS} \sum_{l_2 l'_2} \frac{(2L+1)(2S+1)}{4k_\nu^2 (2l'_1+1)} |T_{\nu\nu'}^{LS}|^2 \quad (5)$$

Experimentally it is impossible to discriminate against positrons scattered elastically through small angles about the forward direction. Thus a knowledge of the elastic differential cross section enables one to estimate how

much flux has been lost by means of this effect. We have therefore calculated an effective elastic cross section defined as

$$\sigma_{el}^{eff} = 2\pi \int_{\theta_0}^{\pi} \sin \theta \frac{d\sigma_{el}}{d\Omega} d\theta \quad (a_0^2) \quad (6)$$

where θ_0 is the lower limit of the experimental angular discrimination. An estimate of this quantity has been made in the experimental measurements of Stein *et al*¹¹ for each energy of the incident positron. This effective elastic cross section is then added to the various excitation cross sections to yield an effective total cross section which can, more meaningfully, be compared with the experimental data.

RESULTS

In table 2 we present our 5-state close-coupling results for the elastic, the various excitation cross sections and the total cross section for e^+ -Rb scattering for energies between 3.7 and 28.0 eV. Also included in the table are results for the effective total cross section. The energies

TABLE 2. The elastic, excitation and total integrated cross sections (πa_0^2) for e^+ -Rb scattering in the energy range 3.7-28.0 eV.

| Energy (eV) | 5s-5s | 5s-5p | 5s-4d | 5s-6s | 5s-6p | σ_{tot} | σ_{tot}^{eff} |
|-------------|--------|-------|-------|-------|-------|----------------|----------------------|
| 3.7 | 124.23 | 92.20 | 67.65 | 4.67 | 0.91 | 289.66 | 209.28 |
| 5.8 | 62.76 | 76.18 | 75.12 | 2.50 | 2.51 | 219.07 | 170.83 |
| 7.8 | 42.16 | 77.68 | 61.02 | 1.58 | 3.14 | 185.58 | 151.47 |
| 17.8 | 17.64 | 73.12 | 20.52 | 0.98 | 2.72 | 114.98 | 102.69 |
| 28.0 | 12.79 | 60.27 | 10.23 | 0.88 | 1.95 | 86.12 | 80.31 |

chosen are such that they coincide with those given in the experimental data of Stein *et al.*¹¹

We note that the elastic as well as the 5s-5p and 5s-4d excitation cross sections are the dominate contributors to the total cross section. By comparing the total cross section with the corresponding effective one it can be seen that at 3.7 eV almost 2/3 of the elastic scattering flux will not be detected experimentally; this fraction increases to nearly 4/5 at 7.8 eV. Nonetheless, our effective total cross section increases monotonically as the incident energy of the positron decreases. This behaviour

of the effective total cross section, as predicted by our 5-state close coupling approximation, is in contrast to the experimental data of Stein *et al.*¹¹ which has a maximum in the low energy region. Unfortunately we can not offer any explanation for this discrepancy as yet.

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