PHYSICAL REVIEW
LETTERS

VOLUME 22 | 19 MAY 1969 | NUMBER 20

FINE-STRUCTURE TRANSITIONS AND SHAPE RESONANCES*

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(Received 11 April 1969)

A partial-wave description is employed to calculate the cross sections for fine-structure transitions in the ^2P state of sodium in collisions with helium. The cross sections show an oscillatory behavior with energy that is related to the occurrence of shape resonances in the elastic-scattering channels.

Considerable attention has been given to measurements of the cross sections for excitation transfer between the $^2P_{1/2}$ and $^2P_{3/2}$ levels in alkali atoms induced by collisions with inert-gas atoms.[1] The quantitative theoretical analyses[2] have been based upon semiclassical descriptions of the process which are not valid near the reaction threshold and which suppress certain quantum oscillatory phenomena.

If, as is usually assumed, the process can be attributed to an effective orientation-dependent interaction, the calculation of the cross section for changing the total internal angular momentum of a particle A by collision with a particle X in a ^1S state throughout the collision becomes precisely the problem formulated by Arthurs and Dalgarno,[3] provided the rigid-rotator wave function in their analysis is replaced by the appropriate internal wave function of system A. Following Callaway and Bauer[2] we adopt the effective interaction at large separations R:

$$V(\vec{R}) = -R^{-6}\alpha_X \langle r^2\rangle_A \{P_0(\vec{r},\vec{R}) + P_2(\vec{r},\vec{R})\},$$

where $\vec{r}$ is the position vector of the electron in A and $\vec{R}$ is the vector from A to X, where $\langle r^2\rangle_A$ is the expectation value of r^2 for atom A, and where α_X is the dipole polarizability of X. If we write more generally

$$V(\vec{R}) = \sum_\mu v_\mu(R) P_\mu(\vec{r},\vec{R}),$$

the coupling matrix elements for the channel wave functions formed in a state of total angular momentum J from the states $|(LS)j\rangle$ of A and the orbital momenta l of relative motion are given in a standard notation[4] by

$$\langle (LS)j'l'J|V|(LS)j''l''J\rangle = \sum_\mu v_\mu(R)(-1)^{J-S-\mu}(2L+1)\{2l'+1)(2l''+1)(2j'+1)(2j''+1)\}^{\frac{1}{2}}$$

$$\times \bar{V}\begin{pmatrix} L & L & \mu \\ 0 & 0 & 0 \end{pmatrix} \bar{V}\begin{pmatrix} l' & l'' & \mu \\ 0 & 0 & 0 \end{pmatrix} \bar{W}\begin{pmatrix} j' & j'' & \mu \\ l'' & l' & J \end{pmatrix} \bar{W}\begin{pmatrix} j' & j'' & \mu \\ L & L & S \end{pmatrix}.$$

For ^2P states of A, $L=1$ and the only nonzero matrix elements are those with $\mu=0$ or $\mu=2$. The resulting coupled equations describing the scattering divide into two sets, one with even and the other with odd values of l.

In calculating the cross sections we include in v_0 and v_2 a short-range repulsion containing variable parameters. Figure 1 shows the cross sections for

$$\mathrm{Na}(3p^2P_{1/2}) + \mathrm{He} \rightarrow \mathrm{Na}(3p^2P_{3/2}) + \mathrm{He}$$

with $\alpha_{\mathrm{He}} = 1.384a_0^3$, $\langle r^2\rangle_{\mathrm{Na}} = 40.1a_0^2$,[4] and short-range repulsions in v_0 and v_2 of CR^{-12} with C chosen to yield a well depth for v_0 of 0.01 eV.

The shape is qualitatively similar to the semiempirical universal curve constructed by Gallagher[5] from a study of excitation transfer of Ru and Cs in collisions with various inert gases. However, for barycentric energies less than 0.01 eV the calculated curve contains considerable structure which is associated with the shape resonances that occur in the elastic channels. Their location and appearance is much modified by the coupling between the different channels. For the other alkali atoms, the energy defect is sufficiently large that the resonances may appear at laboratory temperatures. Their observation would yield detailed information on the interaction potentials.

At a temperature of about 390°K the predicted cross section for the $^2P_{1/2}$-$^2P_{3/2}$ transition is 2.2×10^{-15} cm^2 compared with the experimental value[6] of 8.6×10^{-15} cm^2. It is unlikely that any acceptable modification of the interactions will give a cross section much in excess of 5×10^{-15} cm^2 and the discrepancy, though small, suggests that some nonadiabatic mechanism is operative. Measurements at other temperatures would be instructive.

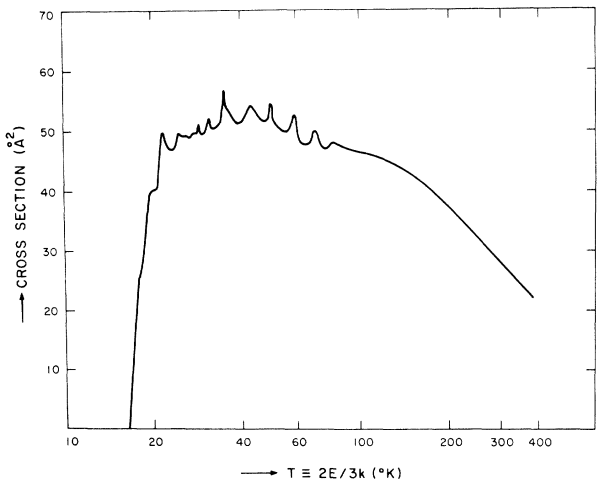

FIG. 1. Computed cross section for $\mathrm{Na}(3p^2P_{1/2}) + \mathrm{He} \rightarrow \mathrm{Na}(3p^2P_{3/2}) + \mathrm{He}$.

*Work partly supported by the National Aeronautics and Space Administration under Grant No. NGR 22-007-136.

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