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$$\sum_{ij} \Phi_i[f(\nu_i, r)\delta_{ij} - g(\nu_i, r)R_{ij}]h_j,$$

where $R_{ij} = \sum_\alpha U_{i\alpha} \tan\pi\mu_\alpha U^\dagger_{\alpha j}$ is a reaction matrix and the h_j are arbitrary coefficients. This equation reduces to (2.16) by setting $h_j = U_{j\alpha}\cos\pi\mu_\alpha$, meaning that $c_i = h_i$ and $d_i = \sum_j R_{ij}h_j$.

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PHYSICAL REVIEW A VOLUME 4, NUMBER 2 AUGUST 1971

Vibrorotational Excitations of H_2^+ by e^+ Impact. I

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(Received 17 December 1970)

Analogies between Coulomb excitations of nuclei and ionic molecules by charged projectiles are utilized to calculate vibrorotational excitations of H_2^+ molecular ions by e^+ impact by a semiclassical method developed in the nuclear case. The coupling between vibrational-rotational states of target molecules can very significantly affect the scattering cross sections for either kind of excitation on the other. In this paper we have shown that the effect of such coupling may be included very conveniently, under the present model, whenever applicable. In a subsequent paper we intend to publish results for the experimentally more accessible systems, including the $H^+ + H_2^+$ system.

I. INTRODUCTION

Recently there has been a considerable upsurge of interest in the study of rotational and vibrational energy-loss processes in diatomic molecules by electron impact. They are of much importance not only for understanding the fundamental energy exchange processes involved, but also for their applications in such allied fields as astrophysics and atmospheric physics.

In the present work we shall investigate the coupled excitation of vibrorotational states of hydrogen molecular ions H_2^+ by collision with positrons e^+. The study of such excitations with e^+ is not only important for its intrinsic significance but also for the mathematical simplicity it introduces in the formulation of the complex excitation process itself. This is due to the fact that the Pauli exchange does not enter directly into the problem.

In this work we shall adopt a semiclassical view and make use of the analogy of Coulomb excitations of nuclei, which has been studied extensively in the past.[1] The present method is semiclassical in that we shall treat the target system quantum mechanically while the motion of the projectile would be

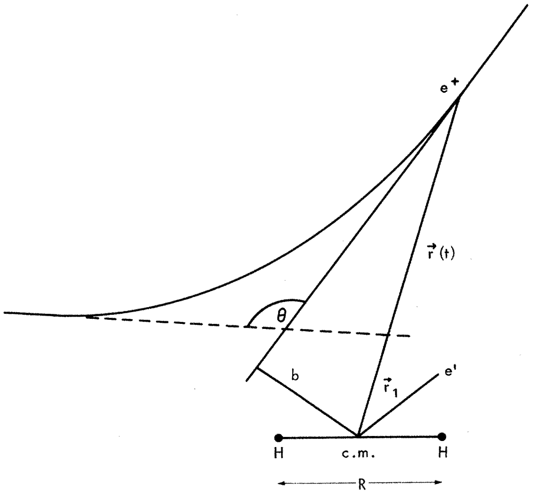

FIG. 1. Trajectory describing the collision of e^+ with H_2^+ ion. b is impact parameter, θ is angle of deviation.

assumed to be along a classical Coulomb trajectory. In the end, however, we shall attempt to modify the classical nature of the projectile motion, which does not distinguish between the initial and final states, by demanding that the principle of reciprocity be satisfied by the cross-sectional expressions and invoking the correspondence principle to be applied to such quantities as the classical velocity of the projectile.

II. THEORY

Let N, n, and j denote, respectively, the electronic, vibrational, and rotational quantum numbers of the target molecule. In this paper we shall confine ourselves to the ground electronic state of the target and mostly disregard the quantum number N. One of the basic assumptions of our semiclassical approximation is that in the first approximation the incident positron moves essentially along a Rutherford trajectory around the effective positive charge of H_2^+, situated at the c.m. of the molecule. Thus, while the positron moves along its trajectory it is allowed to induce transitions in the molecular motion through the electric coupling with the various molecular charges. The transition probability b_{if} for the initial state i going to the final state f may then be given by the first-order time-dependent scattering theory of Dirac.[2] Thus we write

$$b_{if}=-i\int_{-\infty}^{\infty}e^{i\omega t}\langle f\,|\,V_{\rm int}(t)|\,i\rangle\,dt\ , \tag{1}$$

where $\omega=E_i-E_f$ is the energy difference between the states i and f and $V_{\rm int}(t)$ is the interaction potential between the incident positron and the H_2^+ target. It can easily be seen (Fig. 1) that

$$V_{\rm int}(t)=\frac{1}{|\frac{1}{2}\vec{R}-\vec{r}|}+\frac{1}{|\frac{1}{2}\vec{R}+\vec{r}|}-\frac{1}{|\vec{r}-\vec{r}_1|}-\frac{1}{r} \tag{2}$$

(the last term is subtracted to compensate for the inclusion of the leading Coulomb potential in the evaluation of the projectile trajectory), where $\vec{r}=\vec{r}(t)$ is the trajectory of the positron and $\vec{r}_1$ is the position vector of the target electron, measured from the c.m. of the molecule. The vector $\vec{R}$ stands for the separation between the two nuclei of the target.

We shall describe the target molecule in terms of simple product of normalized wave functions $\Phi_N(\vec{r}_1)$, $\chi_n(R)$, and $Y_j^{m_j}(\hat{R})$ corresponding to the electronic, vibrational, and rotational motions. Thus the total target wave function becomes

$$|\,Nnj\rangle=\Phi_N(\vec{r}_1)\ \chi_n(R)\ Y_j^m(\hat{R})\ . \tag{3}$$

In view of the fact that the incident positron repels itself from the positively charged target, we may, for sufficiently low energies, simplify the potential interaction (2) by expanding it for essentially nonpenetrating projectile orbits. Thus we find

$$V_{\rm int}(t)=-\sum_{\lambda=1,2;\ \mu=-\lambda}^{\mu=+\lambda}\frac{4\pi}{2\lambda+1}\,\frac{r_1^{\lambda}}{r^{\lambda+1}}\,Y_\lambda^{*\mu}(\hat{r}_1)\,Y_\lambda^{\mu}(\hat{r})+2\sum_{\lambda=2,4,\ldots;\ \mu=-\lambda}^{\mu=+\lambda}\frac{4\pi}{2\lambda+1}\,\frac{(\frac{1}{2}R)^{\lambda}}{r^{\lambda+1}}\,Y_\lambda^{*\mu}(\hat{R})\,Y_\lambda^{\mu}(\hat{r}),\quad r>r_1\ . \tag{4}$$

Taking the matrix elements between the initial state $|N_in_ij_i\rangle$ and the final state $|N_fn_fj_f\rangle$, we find from (3) and (4)

$$\begin{aligned}\langle f\,|\,V_{\rm int}(t)|\,i\rangle=&-\sum_{\lambda=-1,2,\ldots;\ \mu=-\lambda}^{\mu=+\lambda}\frac{4\pi}{2\lambda+1}\langle\Phi_{N_f}\,|\,r_1^{\lambda}\,Y_\lambda^{*\mu}(\hat{r}_1)|\,\Phi_{N_i}\rangle\langle\chi_{n_f}\,|\,\chi_{n_i}\rangle\langle Y_{j_f}^{m_f}(\hat{R})|\,Y_{j_i}^{m_i}(\hat{R})\rangle\frac{Y_\lambda^{\mu}(\hat{r})}{r^{\lambda+1}}\\&+2\sum_{\lambda=2,4,\ldots;\ \mu=-\lambda}^{\mu=+\lambda}\frac{4\pi}{2\lambda+1}\langle\Phi_{N_f}(\vec{r}_1)|\,\Phi_{N_i}(\vec{r}_1)\rangle\langle\chi_{n_f}\,|\,(\tfrac{1}{2}R)^{\lambda}\,|\,\chi_{n_i}\rangle\langle Y_{j_f}^{m_f}(\hat{R})|\,Y_\lambda^{\mu}(\hat{R})|\,Y_{j_i}^{m_i}(\hat{R})\rangle\frac{Y_\lambda^{\mu}(\hat{r})}{r^{\lambda+1}}\ .\end{aligned} \tag{5}$$

We find that in the present approximation the above equation (5) controls the entire process of transitions among the various states and the various modes of motion of the target molecule. It can easily be seen that the perturbation of the electronic motion, represented by the first sum in (5) is independent of the nuclear perturbation, represented by the second sum in (5). This is, of course, a consequence of the Born-Oppenheimer separation already assumed in the product wave function (3). We note however that the transitions among any two vibrational states $|n_i\rangle$ and $|n_f\rangle$ $(n_i \neq n_f)$, or any two rotational states $|j_i\rangle$ and $|j_f\rangle$ $(j_i \neq j_f)$, or both, lead to a vanishing of the first sum in (5). Thus the vibrational-rotational transition probabilities in the ground electronic state is found to be given by

$$b_{if} = 4\pi i \sum_{\lambda=2,4,\ldots;\ \mu=-\lambda}^{\mu=+\lambda} \frac{1}{2\lambda+1} \times 2\,\langle n_f j_f |(\tfrac{1}{2}R)^\lambda Y_\lambda^\mu(\hat{R})| n_i j_i\rangle J_{\lambda\mu},$$

$$J_{\lambda\mu} = \int_{-\infty}^{\infty} e^{i\omega t}[r(t)]^{-\lambda-1}\, Y_\lambda^\mu(\hat{r}(t))\,dt\ , \tag{6}$$

$$|nj\rangle = |\chi_n(R)\ Y_j^m(\hat{R})\rangle .$$

We note that all information regarding the trajectory of the incident positron is contained in the orbit integrals $J_{\lambda\mu}$. We shall note here that the Coulomb trajectory of e^+ can most conveniently be given by the parametric equations

$$r(t) = r_0(\epsilon\cosh\tau + 1), \qquad x(t) = r_0(\cosh\tau + \epsilon),$$

$$y(t) = r_0(\epsilon^2 - 1)^{1/2}\sinh\tau, \quad z(t) = 0, \tag{7}$$

$$t = (r_0/v_0)(\epsilon\sinh\tau + \tau)\ ,$$

where ϵ is the eccentricity, τ is the eccentric anomaly, r_0 is half the distance of closest approach, v_0 is the projectile velocity, and t is the time parameter. Substituting (7) in (6) and choosing the quantization axis along the angular momentum of the molecular rotation, it can be shown[1] that

$$J_{\lambda\mu} = r_0^{-\lambda-1}\,\omega_0^{-1}\,Y_\lambda^\mu(\tfrac{1}{2}\pi, 0)\,I_\lambda^\mu(\xi,\theta)\ , \tag{8}$$

$$I_\lambda^\mu(\xi,\theta) = \int_{-\infty}^{\infty} \exp[i\xi(\tau + (1+\epsilon^2)^{1/2}\sinh\tau)] \times \frac{[\epsilon + \cosh\tau + i(\epsilon^2-1)^{1/2}\sinh\tau]^\mu}{(1+\epsilon\cosh\tau)^{\lambda+\mu}}\,d\tau\ , \tag{9}$$

$$\xi = (E_i - E_f)/\omega_0, \quad \omega_0 = v_0/r_0, \quad r_0 = 1/2E_0\ . \tag{10}$$

The integrals (9) have been evaluated analytically for $\lambda = 1$ and numerically for $\lambda = 2$ by previous authors (see Ref. 1 as a general source). We use the data presented in Tables II.3 and II.8 of Ref. 1 for our purpose.

We have defined E_0 to be the incident energy in a.u. and θ as the scattering angle. To calculate the cross sections we need the number of incident particles in a plane wave of unit flux with impact parameters between b and $b+db$. This is given by

$$2\pi b\,db = [r_0^2/4(\sin\tfrac{1}{2}\theta)^4]\,d\Omega\ ,$$

where $d\Omega$ is an elementary solid angle, and $b = r_0\cot\frac{1}{2}\theta$. The differential cross section for the λth multipole transition averaged over the initial substates m_i and summed over the final substates m_f may therefore be written as

$$\left(\frac{d\sigma}{d\Omega}\right)_\lambda = \frac{1}{2j_i+1}\sum_{m_i m_f}|b_{if}|^2 = \frac{1}{v_0^2}\,r_0^{-2\lambda+2}\,4B_\lambda(n_i j_i \rightarrow n_f j_f)\,\frac{df_\lambda(\xi,\theta)}{d\Omega}\ , \tag{11}$$

$$\frac{df_\lambda(\xi,\theta)}{d\Omega} = \frac{4\pi^2}{(2\lambda+1)^3}\sum_{\mu=-\lambda}^{\mu=+\lambda}\frac{[Y_\lambda^\mu(\frac{1}{2}\pi,0)I_{\lambda\mu}(\xi,\theta)]^2}{(\sin\frac{1}{2}\theta)^4}\ . \tag{12}$$

The total cross section is obtained by integrating (11) over all scattering angles. Thus we have

$$(\sigma)_\lambda = (1/v_0^2)\,r_0^{-2\lambda+2}\,4B_\lambda(n_i j_i \rightarrow n_f j_f) f_\lambda(\xi)\ , \tag{13}$$

with

$$f_\lambda(\xi) = \frac{16\pi^2}{(2\lambda+1)^3}\sum_{\mu=-\lambda}^{\lambda}|Y_\lambda^\mu(\tfrac{1}{2}\pi,0)|^2 \times \int_0^\pi |I_{\lambda\mu}(\xi,\theta)|^2\,\frac{\cos\frac{1}{2}\theta}{(\sin\frac{1}{2}\theta)^3}\,d\theta \tag{14}$$

and

$$Y_\lambda^\mu(\tfrac{1}{2}\pi,0) = \left(\frac{2\lambda+1}{4\pi}\right)^{1/2}\frac{[(\lambda-\mu)!\,(\lambda+\mu)!]^{1/2}}{(\lambda-\mu)!!\,(\lambda+\mu)!!}\,(-1)^{(\lambda+\mu)/2},\qquad \lambda+\mu \text{ even}$$

$$= 0, \qquad \lambda+\mu \text{ odd.}$$

In (11) and (13) the quantity B_λ is the reduced transition probability which we have defined to be

$$B_\lambda(n_i j_i \rightarrow n_f j_f) = \sum_{\mu m_f}|\langle n_f j_f|(\tfrac{1}{2}R)^\lambda Y_\lambda^\mu(\hat{R})|n_i j_i\rangle|^2 = \frac{1}{2j_i+1}|\langle n_f j_f\|(\tfrac{1}{2}R)^\lambda Y_\lambda\|n_i j_i\rangle|^2\ , \tag{15}$$

where

$$\langle n_f j_f\|(\tfrac{1}{2}R)^\lambda Y_\lambda\|n_i j_i\rangle = 2^{-\lambda}A_\lambda(n_i \rightarrow n_f)\,\langle j_f\|Y_\lambda\|j_i\rangle\ , \tag{16}$$

with the vibrational matrix elements

$$A_\lambda(n_i \rightarrow n_f) = \int_0^\infty \chi_{n_f}(R)R^\lambda\chi_{n_i}(r)\,dR \tag{17}$$

and the reduced matrix element[3]

$$\langle j_f\|Y_\lambda\|j_i\rangle = (-1)^{j_f}\left(\frac{2\lambda+1}{4\pi}(2j_i+1)(2j_f+1)\right)^{1/2} \times \begin{pmatrix} j_i & \lambda & j_f \\ 0 & 0 & 0 \end{pmatrix}. \tag{18}$$

III. SYMMETRIZATION OF CLASSICAL CROSS SECTIONS

In the present approach, the projectile orbit has been described classically and consequently the cross-sectional expressions (11) and (13) do not distinguish between the initial and final states of the trajectories. One of the most successful ways of introducing the initial and final parameters for the orbits is to impose the principle of reciprocity on the cross-sectional expressions and replace various classical parameters by their corresponding quantal analogs via the correspondence principle. To satisfy the reciprocity relation between the cross section σ_{if} for the direct process and σ_{fi} for its inverse, we must have

$$\omega_i v_i^2 \sigma_{if} = \omega_f v_f^2 \sigma_{fi} \ , \tag{19}$$

where ω_i, v_i and ω_f, v_f are, respectively, the statistical weights and velocities (in a.u.) for the initial and final states of the system. For the present problem we have

$$\omega_i = (2j_i+1), \quad \omega_f = (2j_f+1) \ . \tag{20}$$

From (19) and (20) we conclude that σ_{if} must have the form

$$\sigma_{if} = \frac{v_f}{v_i}\left(\frac{2j_f+1}{2j_i+1}\right)^{1/2} \times (\text{cross-sectional expression symmetric in } i \text{ and } f) \ . \tag{21}$$

Extending Kramers-type prescriptions for the principal quantum number $n \rightarrow n+1$ to the positive energy continuum where n is replaced by $i\eta$, Biedenharn and Brussaard[4] obtain the correspondence

$$\eta \rightarrow (\eta^2+1)^{1/2} \tag{22}$$

for the so-called Sommerfeld number η, where

$$\eta^2 = r_0 \left| z_1 z_2 e^2 m \right| = (z_1 z_2 e^2)^2/\hbar^2 v_0^2 \tag{23}$$

is given in terms of half the distance of closest approach r_0, or the incident velocity v_0. In (23) m_0 and z_1 are the mass and charge of the projectile and z_2 stands for the effective charge of the target. In our case $z_1 = z_2 = +1$. From the fundamental correspondence between the quantum-mechanical matrix elements and the classical Fourier components and from the relation (22), it can be shown (for a concise derivation and an elegant discussion see Ref. 4) that the classical η yields the final correspondence

$$\eta \rightleftarrows \left(\frac{2(\eta_i^2+1)(\eta_f^2+1)}{(\eta_i^2+1)^{1/2}+(\eta_f^2+1)^{1/2}}\right)^{1/3} \ . \tag{24}$$

We note that in terms of the initial and final parameter η_i and η_f, the quantity ξ defined in (10) reduces to

$$\xi = \eta_f - \eta_i \ . \tag{25}$$

For the cross-sectional expression to be inserted in Eq. (21) we shall adopt the classical expression (13) and symmetrize it through the use of Eqs. (22)–(24) as follows:

$$\eta^2 = \left(\frac{z_1 z_2 e^2}{\hbar v_0}\right)^2 = \frac{1}{v_0^2} \Rightarrow [(\eta_i^2+1)(\eta_f^2+1)]^{1/2} \ , \tag{26}$$

$$r_0^{-2\lambda+2} \Rightarrow \left(\frac{2(\eta_i^2+1)(\eta_f^2+1)}{(\eta_i^2+1)^{1/2}+(\eta_f^2+1)^{1/2}}\right)^{(4-4\lambda)/3} (z_1 z_2 m_0)^{2\lambda-2} \ . \tag{27}$$

Finally, substituting (26) and (27) in (13) and combining the result with (21) we obtain

$$\sigma_{if} = \frac{\eta_i}{\eta_f}[(\eta_i^2+1)(\eta_f^2+1)]^{1/2}\left(\frac{2(\eta_i^2+1)(\eta_f^2+1)}{(\eta_i^2+1)^{1/2}+(\eta_f^2+1)^{1/2}}\right)^{(4-4\lambda)/3} \times 4B_\lambda(n_i j_i \rightarrow n_f j_f) f_\lambda(\xi = \eta_i - \eta_f) \ . \tag{28}$$

An expression similar to (28) is obtained for the differential cross section with $f_\lambda(\xi)$ replaced by $df_\lambda(\xi, \theta)/d\Omega$.

We shall emphasize the fact that the symmetrization procedure adopted here for the classical cross sections is by no means unique in character. Nevertheless it has been found that an essentially similar procedure adopted by Biedenharn and Brussaard[4] in nuclear excitation problems produced excellent agreement with the corresponding quantal calculations. We note, however, that our symmetrization procedure has the advantage over that of the previous authors in that it yields the correct threshold law[5]: $\sigma_{if} \simeq e^{-2\pi\eta_f}$ for the repulsive Coulomb scattering while the other expression yields $\sigma_{if} \sim (1/\eta_f^{1/3}) \times e^{-2\pi\eta_f}$ near the excitation threshold. In a complete quantum calculation one requires the Wigner threshold law for Coulomb scattering to emerge naturally. The unsymmetrized result is incapable of yielding this behavior, and at the same time it numerically overestimates the cross sections by large factors. The present calculation is, however, not completely classical in nature as we treat the target states quantum mechanically and symmetrize the result to satisfy the detailed-balance theorem. The present symmetrization is found to lead to the correct quantum limit at the threshold. In comparing our symmetrization with that of Ref. 4 we find that for the present problem they differ very little numerically. Thus, for example, we calculate for a typical $\Delta E_{if} = 0.02$ a.u. the ratio between the two cross sections to be 1.03, 1.01, and 1.00 for (typical) incident energies E_i(a.u.) = 0.03, 0.10, and 0.25, respectively.

IV. NUMERICAL CALCULATIONS

In the present calculation we have retained the quadrupole term $\lambda = 2$ only; the dipole term $\lambda = 1$ and the next-higher-order term $\lambda = 3$ vanish identically for homonuclear diatomic target H_2^+. The vibrational matrix elements are calculated using Morse functions[6]:

$$\chi_n(R) = N_n e^{-z/2} z^{(k-2n-1)/2} \sum_{i=0}^{n} (-1)^i \binom{n}{i} z^i \Big/ (k-2n)(k-2n+1)\cdots(k-2n+i-1) \ ,$$

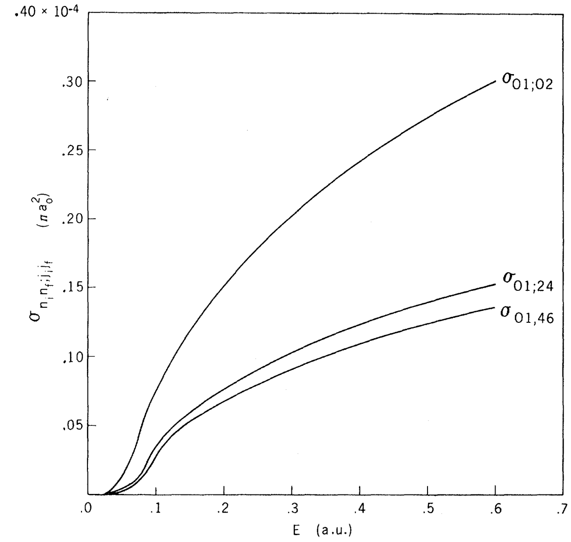

FIG. 2. Total cross sections for 0 → 2, 2 → 4, and 4 → 6 rotational excitations accompanied by 0 → 1 vibrational excitation.

where

$$z = k e^{-\beta(R-R_0)} ,$$

$$k = (2/\beta)(2M_0D)^{1/2} \equiv 1/\chi_e , \quad R_0 = R(\text{at equilibrium})$$

$$N_n^2 = \frac{(k-n-1)(k-n-2)\cdots(k-2n)}{n!\,\Gamma(k-2n-1)}\beta ,$$

and where M_0 is the reduced mass of the target and D is the dissociation energy. For H_2^+ molecular ions we chose $D = 0.10265$ a.u., $\beta = 0.6678\,(\text{a.u.})^{-1}$, $M_0 = 918.334$ a.u., and $R_0 = 2.00$ a.u.

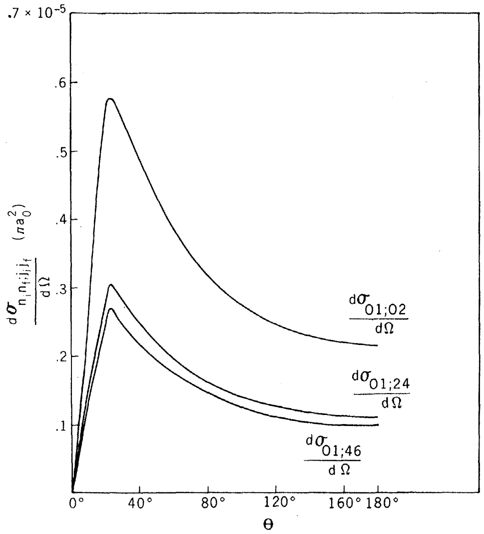

FIG. 3. Differential cross sections for 0 → 2, 2 → 4, and 4 → 6 rotational excitations accompanied by 0 → 1 vibrational excitation.

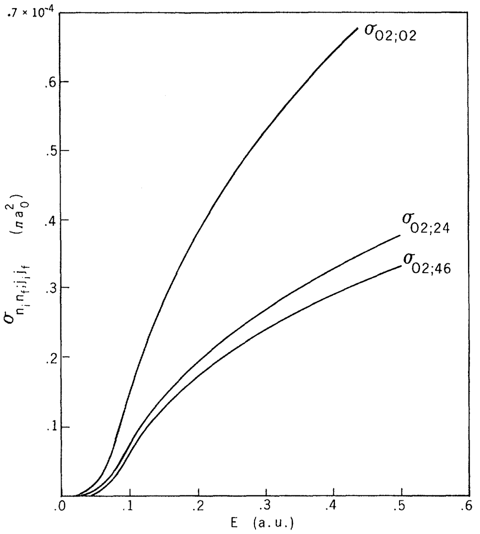

FIG. 4. Total cross section for 0 → 2, 2 → 4, and 4 → 6 rotational excitations accompanied by 0 → 2 vibrational excitation.

Following Heaps and Herzberg[6] the vibrational matrix elements are found to be

$$\int \chi_{n_f}(R)\,R^2\,\chi_{n_i}(R)\,dR = \frac{(-1)^{n_i+n_f+1}}{\beta^2 n_f!}\,\frac{2C_{n_f n_i}H_{n_f n_i}}{1-(n_f+1)\chi_e} ,$$

where

$$C_{n_f n_i} = \left(\frac{[1-(2n_i+1)\chi_e][1-(2n_f+1)\chi_e]\chi_e^{n_f-n_i}n_f!}{[1-(n_i+1)\chi_e][1-(n_i+2)\chi_e]\cdots(1-n_f\chi_e)n_i!}\right)^{1/2}$$

and $H_{n_f n_i}$ is a polynomial the first few of which are

$$H_{n_f 0} = (n_f-1)!\,\ln[1-(n_f+\tfrac{3}{2})\chi_e] + a_{n_f} ,$$

with

$$a_1 = 0, \quad a_2 = 1, \quad a_3 = 3, \quad a_4 = 11, \quad a_5 = 50, \ldots .$$

V. RESULTS AND DISCUSSIONS

We present here both the differential as well as the total cross sections for vibrorotational transitions between the ground state and the first few excited vibrational-rotational states. In Figs. 2 and 3 we compare the difference between different rotational excitations and a fixed vibrational transition $n_i = 0 \rightarrow n_f = 1$. We find that the cross sections for $j_i = 0 \rightarrow j_f = 2$ are by far the largest compared to the rest and those between $j_i = 2, 4, 6 \rightarrow j_f = 4, 6, 8$, respectively, are comparable with each other. In Figs. 4 and 5 we have similar results between the same set of rotational states but with a different vibrational transition: $n_i = 0 \rightarrow n_f = 2$. Comparing Figs. 4 and 5 with Figs. 2 and 3 we find that the magnitude of all the 0 → 2 cross sections are an order of magnitude or more larger than those for

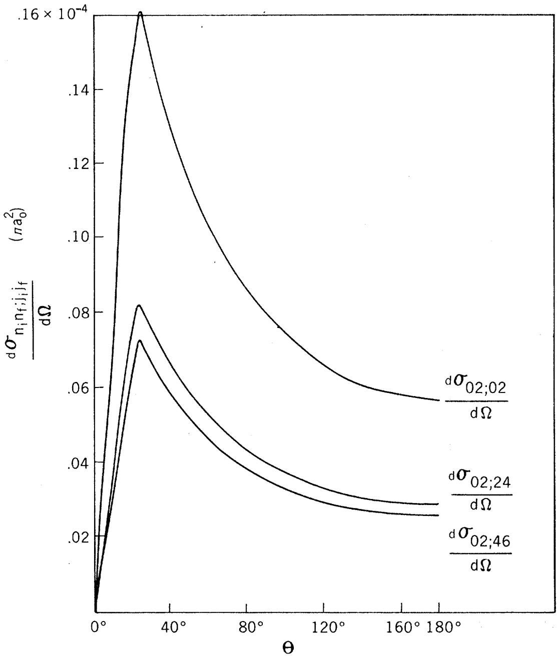

FIG. 5. Differential cross sections for 0 → 2, 2 → 4, and 4 → 6 rotational excitations accompanied by 0 → 2 vibrational excitation.

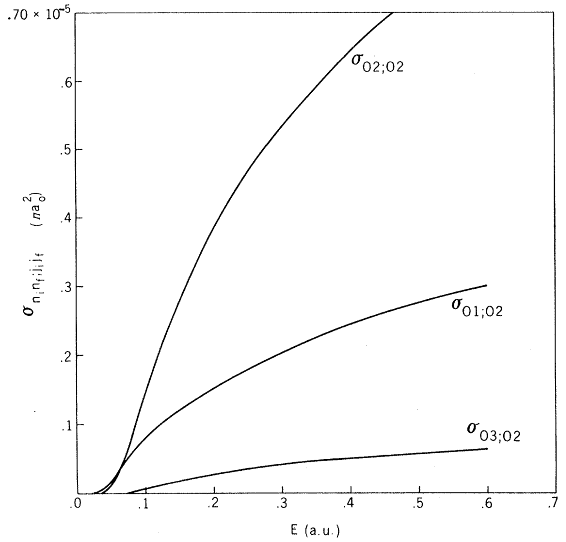

FIG. 6. Total cross sections for 0 → 1, 0 → 2, and 0 → 3 vibrational excitations accompanied by 0 → 2 rotational excitation.

the 0 → 1 transitions. Finally, in Fig. 6 we compare the total cross sections for a fixed rotational excitation $j_i = 0 \rightarrow j_f = 2$, with various vibrational excitations: $n_i = 0 \rightarrow n_f = 1$, $n_i = 0 \rightarrow n_f = 2$, and $n_i = 0 \rightarrow n_f = 3$.

This result again shows that the $n_i = 0 \rightarrow n_f = 2$ vibrational transition is much larger than those for $n_i = 0 \rightarrow n_f = 1$ and $n_i = 0 \rightarrow n_f = 3$; while the last two cross sections are comparable in magnitude. Although we have not plotted the cross sections for $n_i = 0 \rightarrow n_f = 4$, we noted that it was somewhat smaller than that for $n_i = 0 \rightarrow n_f = 3$ in the energy range under consideration.

We believe that the present method is particularly suitable for the energy range $E_i = 0.0$ to $E_i \leq 0.5$ Ry for the following reasons:

(i) In this energy range the distance of closest approach is $\geq 2a_0$ and is expected to be large enough to allow essentially nonpenetrating orbits for the projectiles.

(ii) Since the threshold for positronium formation is at 0.705 Ry, we may neglect such channels for positron energies below 0.705 Ry.

We conclude by noting that the calculated absolute transition probabilities are all very small so that the application of a first-order theory is generally satisfactory.

ACKNOWLEDGMENTS

I would like to thank Dr. A. Temkin for his helpful comments and Dr. A. B. Ritchie and Dr. D. Morgan for their interest in this work.

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