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Theoretical calculation of cross sections for rotational excitation in e-CO_2 scattering*

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Rotational excitation cross sections for e-CO_2 scattering in the energy range from 0.07 to 10.0 eV have been calculated using a coupled-channels procedure together with the adiabatic-nuclei (impulse) approximation. Results are presented for excitation from $j = 0$ to $j' = 0$, 2, and 4. Cross sections for $j = 0$ to $j' = 2$ in e-CO_2 scattering are compared with corresponding results for e-H_2 and e-N_2 collisions. The Born approximation for rotational excitation is examined for this problem and found to be unsatisfactory even at the lowest energies studied. Results for large initial rotational quantum number j are presented and discussed.

In the analysis of electron transport data from swarm experiments,[1] it is necessary to account for a variety of molecular excitations which can be induced by electron impact. Knowledge of cross sections for certain of these excitations obtained from various sources (e.g., theory) can reduce uncertainties in the unfolding of other cross sections via transport analysis. In the consideration of e-CO_2 scattering, the fact that the threshold for rotational excitation is quite low (typically of the order of 10^{-4} eV for small values of the final rotational state quantum number[40]) means that considerable rotational excitation is possible even for very low impact energies. To date there have been no theoretical or experimental determinations of cross sections for rotational excitation of CO_2 by electron impact. In the analyses of swarm data for this system that have been carried out so far,[2,3] the effects of rotational excitation have been ignored.[2]

Moreover, rotational excitation is an important cooling mechanism in molecular gases.[4] Since CO_2 is the dominant molecular species in the planetary atmospheres of Mars and Venus,[5] these cross sections will be needed to model correctly certain processes in these atmospheres.

In a previous paper,[6] the present authors (with L. A. Collins) reported a theoretical calculation of total integrated and differential cross sections as well as momentum-transfer cross sections for e-CO_2 collisions for incident electron energies in the range from 0.07 to 10.0 eV using a coupled-channels procedure. We shall here describe a further calculation within this theoretical framework of cross sections for rotational excitation in e-CO_2 collisions based on the adiabatic-nuclei (impulse) approximation.

Very briefly, the approach used to solve the collision problem is as follows: The fixed-nuclei approximation[7] is made, and the molecule is treated as a rigid rotor with the internuclear separation fixed at $R_{CO} = 2.194\,40 a_0$. Further, only the ground electronic state of the target is retained in the eigenfunction expansion of the scattering wave function. The coupled scattering equations are formulated in a single-center body-fixed coordinate system,[8] converted to integral equations,[9] and solved by numerical quadrature.[10] In the calculations reported, care is taken in treating the partial-wave expansion of the scattering function and the expansion of the potential energy in Legendre polynomials that enough terms are included to ensure convergence to better than 5% in the resulting cross sections.

The electron-molecule interaction potential is given by the sum of an *ab initio* static term, an approximate exchange term, and a semiempirical polarization term. (Results using this model potential are labelled SEP.) The static contribution is determined from the near-Hartree-Fock charge density of the equilibrium-configuration ground-state CO_2 molecule.[11] The exchange contribution is based on a free-electron-gas approximation[12] using the full anisotropic electron density of the target. Finally, an adiabatic polarization potential[13] is included which takes account of the spherical and nonspherical induced-polarization terms and which is truncated near the target by means of an exponential cutoff function. This function contains an adjustable parameter, the cutoff radius, which is used to position the well-known Π_u shape (potential) resonance[14] at the experimentally determined energy of about 3.8 eV. No further adjustment of the potential is made. The resultant calculated total integrated and momentum-transfer cross sections are found to be in reasonably good agreement with the measured results and exhibit the correct trends with energy, including the unusually steep rise as the scattering energy decreases below about 1.0 eV.

The parameters defining the model interaction potential used in the present study of rotational excitation as well as those describing our convergence criteria and the determination of the solution of the coupled scattering equations are described in Ref. 6(b). The same body-frame T-matrix elements were used in these calculations to determine rotational excitation cross sections [see Eq. (3) below] as were used in our earlier study of other collision processes in e-CO_2 scattering, although calculations at several additional energies were carried out in order to determine more precisely the qualitative behavior of the rotational excitation cross sections of interest.[39] The cutoff radius for the polarization potential $r_c = 2.59 a_0$, as determined[6(b)] by positioning the shape resonance as described above, was used here; no readjustment of this parameter was necessary.

In order to calculate rotational-excitation cross sections,[15,31] we transform the body-frame T-matrix elements determined by the above procedure into a space-fixed laboratory reference frame via the appropriate unitary transformation, obtaining (for Σ target states)

$$T^{J}_{jl,j'l'} = (-1)^{l+l'} \sum_{m} C(J\,lj; -m, m) C(Jl'j'; -m, m) T^{m}_{ll'}, \tag{1}$$

where $C(j_1 j_2 j_3; m_1 m_2)$ are the usual Clebsch-Gordan coefficients.[16] This result can be used to calculate rotational-excitation cross sections for excitation from initial rotational state j to state j' via the formula[17]

$$\sigma(j \to j') = \frac{\pi}{k_j^2 (2j+1)} \sum_{J} (2J+1) \sum_{ll'} |T^{J}_{jl,j'l'}|^2, \tag{2}$$

which has been averaged over initial and summed over final m_j rotational sublevels. Since the coupled-channels procedure employs the fixed-nuclei approximation, the rotational level spacing in the target is ignored in our application of Eq. (2), and we set $k_j^2 = k^2$ for all j, where k^2 is the scattering energy in Rydbergs. The resulting formula for $\sigma(j \to j')$ is

$$\sigma(j \to j') = \frac{\pi}{k^2 (2j+1)} \sum_{J} (2J+1) \sum_{ll'} \sum_{mm'} C(Jlj; -m, m) C(Jl'j'; -m, m) \times C(Jlj; -m', m') C(Jl'j'; -m', m') [R^{m}_{ll'} R^{m'}_{ll'} + I^{m}_{ll'} I^{m'}_{ll'}], \tag{3}$$

where $R^{m}_{ll'}$ and $I^{m}_{ll'}$ are the real and imaginary parts of the body-frame T-matrix element $T^{m}_{ll'}$, respectively, and where the sum over J runs $J = 0, 1, 2, \ldots$. The total integrated cross section is invariant under this transformation of the T-operator, and we can calculate

$$\sigma_{\text{tot}} = \frac{\pi}{k^2} \sum_{ll'} \sum_{m} |T^{m}_{ll'}|^2 = \sum_{j'} \sigma(j \to j'), \tag{4}$$

which is independent of j. Equations (3) and (4) are equivalent to the adiabatic approximation applied to the rotational motion.[18,19,32] This approximation is certainly valid for e-CO_2 collisions in the energy range under consideration (0.07 to 10.0 eV), since the spacing of adjacent low-lying rotational levels[40] in the ground electronic and vibrational state of CO_2 is of the order of 10^{-4} eV. Of course, in the vicinity of the resonance, the nuclear motion should be treated beyond the adiabatic approximation.[21,33]

Our results for elastic scattering in the ground rotational state ($j = 0 \to j' = 0$) and for the low-energy excitations[22] $j = 0 \to j' = 2, 4$ are shown in Fig. 1 together with the total integrated cross section. [Although the results for σ_{tot} shown in Fig. 1 were determined by summing the rotational excitation cross sections using Eq. (4), they are identical to the results reported in Ref. 6(b).] The pronounced low-energy enhancement seen in the total and momentum-transfer cross sections[6] also appears in $\sigma(0 \to 0)$, of course, but is not seen in the inelastic cross sections. The 3.8-eV resonance appears in all cases shown in Fig. 1 as well as in the cross sections for larger $|\Delta j|$. Below the resonance, there is considerable background scattering apparent in $\sigma(0 \to 2)$. This is primarily due to the long-range quadrupole interaction and, to a lesser degree, to the anisotropic induced-polarization interaction. These contributions to the potential energy directly couple the rotational levels 0 and 2. In contrast, these long-range interactions only indirectly couple the $j = 0$ and $j' = 4$ rotational states, and the background contribution to $\sigma(0 \to 4)$ is quite small.

No attempt has been made to determine the precise locations of the resonance peaks in the calculated $\sigma(j \to j')$. The peaks are likely to be displaced slightly from 3.8 eV owing to the considerable background scattering evident, for example, in $\sigma(0 \to 2)$. Moreover, when the vibrational motion is taken into account, the resonance in the rotational excitation cross section may be broad-

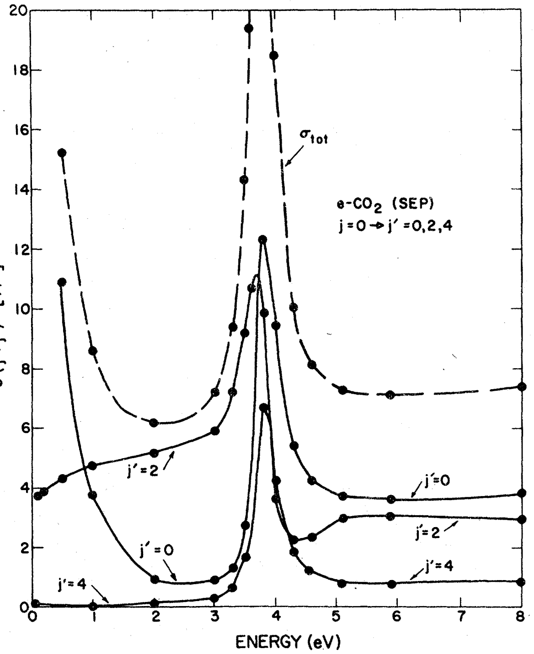

FIG. 1. Rotational excitation cross sections (in Å^2) for excitation from the ground ($j=0$) initial state to final states $j'=0, 2$, and 4 using the SEP model potential of Ref. 6. The total (integrated) cross section obtained from Eq. (4) is also shown (dashed curve). The peak value of σ_{tot} at 3.8 eV (off scale on this figure) is 19.467 Å^2. Values of σ_{tot} and $\sigma(0 \to 0)$ for energies below 0.5 eV are off scale in this figure; at 0.07 eV, $\sigma(0 \to 0) = 62.945$ Å^2 and $\sigma_{tot} = 67.270$ Å^2.

ened and may display structure[21] like that seen in the vibrational excitation cross sections.[2,3,23] Of course, some broadening of the resonance would result if our cross sections were averaged over the zero-point vibrational motion of the nuclei.

For rotational excitation of nonpolar targets,[24] it is usually the case[25] that the low-energy inelastic cross sections $\sigma(j \to j' \neq j)$ are much smaller than the corresponding elastic cross section $\sigma(j \to j)$. Figure 1 reveals that, for e-CO$_2$ collisions in the energy range from about 1.0 to 3.0 eV, $\sigma(0 \to 2)$ exceeds $\sigma(0 \to 0)$ by almost an order of magnitude. This may simply be a reflection of the complicated interference of several scattering symmetries[26] in this energy range [see Fig. 3 of Ref. 6(b)]. At very low energies (below about 0.5 eV), the scattering is almost pure Σ_g; this gives rise to the pronounced low-energy enhancement seen in σ_{tot} and $\sigma(0 \to 0)$. As the energy is increased Σ_g, Σ_u, and Π_u symmetries all contribute significantly until, near the resonance, Π_u begins to dominate. Thus from about 1.0 to 3.0 eV, no single symmetry dominates the scattering.

We have examined the contribution of various partial waves to $\sigma(j \to j')$ for $j=0$ and $j'=0, 2, 4$ by truncating the sums over l and l' in Eq. (4) at some l_{max}. We find that the elastic cross sections $\sigma(j \to j)$ for $j=0, 2, 4$ are dominated by s waves ($l=0$), especially at the lower energies. In contrast, $\sigma(0 \to 2)$ has a substantial component due to p wave ($l=l'=1$) and d wave (primarily $l=2$, $l'=0$). At the resonance energy, 3.8 eV, one must include partial waves up to f wave ($l=3$); using $l_{max}=2$ yields $\sigma(0 \to 2) = 10.722 a_0^2$ as compared to $\sigma(0 \to 2) = 35.068 a_0^2$ for $l_{max}=3$. This reflects the mixed p-f character[6] of the Π_u resonance in e-CO$_2$ scattering. At energies above a few eV, f waves make substantial contributions to $\sigma(0 \to 2)$ and to $\sigma(0 \to 4)$. For lower energies, partial waves through $l=7$ are required to converge $\sigma(0 \to 4)$ to within 1%; however, these cross sections are very

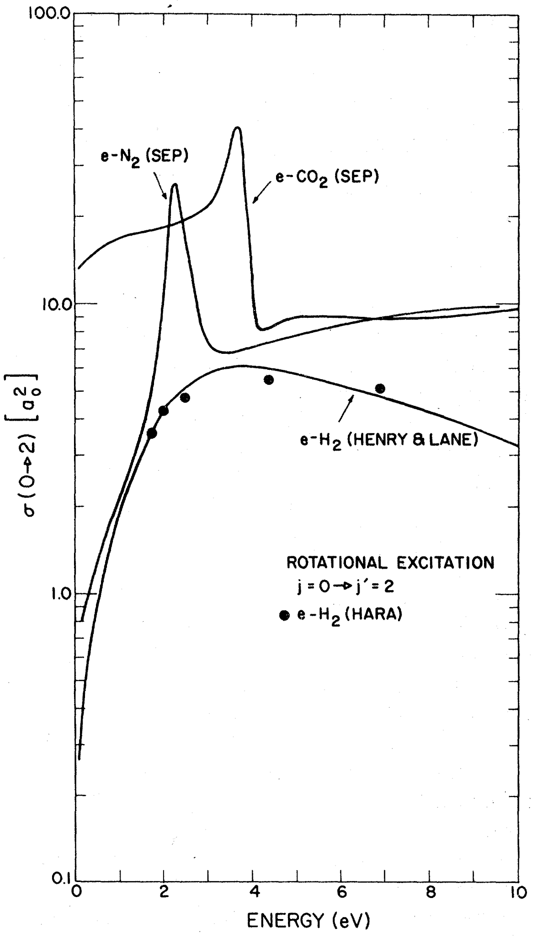

FIG. 2. Cross sections for excitation from $j=0$ to $j'=2$ for e-CO$_2$ (SEP), e-N$_2$ (SEP, Ref. 27), and e-H$_2$ (rotational close coupling, Ref. 28; and adiabatic, Ref. 19). Both of the e-H$_2$ studies include static, exchange, and (adiabatic) polarization interactions.

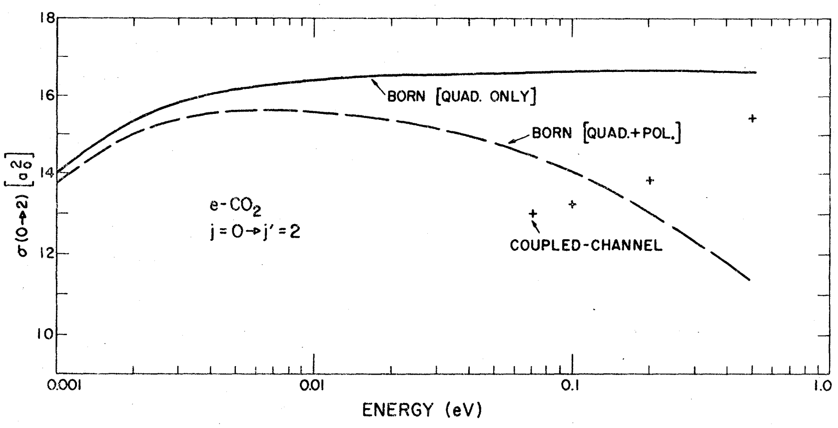

FIG. 3. Comparison of coupled-channel SEP cross sections $\sigma(0\rightarrow 2)$ for $e\rightarrow CO_2$ scattering below 0.5 eV with Born approximations to these cross sections [see Eq. (5)]. The solid curve was calculated taking account of the quadrupole interaction only (i.e., $\alpha_2 = 0$). The dashed curve was determined using quadrupole and nonspherical polarization terms.

small in this energy range.

The cross sections for $\Delta j = 2$ are especially interesting because they are strongly affected by nonspherical long-range forces as well as the short-range expansion coefficients in the potential energy. In Fig. 2, we compare $\sigma(0\rightarrow 2)$ for the present e-CO_2 study with the corresponding cross sections from a separate treatment of e-N_2 scattering using the same theory[27] and a rotational close-coupling treatment of e-H_2 collisions by Henry and Lane.[28] (Also shown are the results obtained by Hara[19] for e-H_2 scattering in the adiabatic approximation.) The peak in the e-N_2 cross section at about 2.3 eV is due to a Π_g shape resonance.[29] The behavior of the e-H_2 cross sections with energy has been interpreted[30] as a broad $p\sigma$ shape resonance.[33] Below the resonance energies, $\sigma_{CO_2}(0\rightarrow 2)$ exceeds $\sigma_{N_2}(0\rightarrow 2)$ and $\sigma_{H_2}(0\rightarrow 2)$ by more than an order of magnitude. This result partly reflects the fact that the quadrupole moment[6] of CO_2 ($q_{CO_2} = -3.86ea_0^2$) is considerably larger in magnitude than that[27] of N_2 ($q_{N_2} = -0.94ea_0^2$) or of[28] H_2 ($q_{H_2} = +0.49ea_0^2$). However, even at the lowest energy studied, 0.07 eV, the collision cannot be described strictly in terms of the long-range interactions (see Fig. 3); the short-range static and exchange effects must be taken into account. For energies greater than about 6.0 eV, well above the N_2 and CO_2 resonances, $\sigma_{H_2}(0\rightarrow 2)$ dies off more rapidly than either $\sigma_{N_2}(0\rightarrow 2)$ or $\sigma_{CO_2}(0\rightarrow 2)$ because the electron-molecule interaction potential for e-H_2 collisions is far more nearly spherical than are the potentials for the other two systems.

The first Born approximation (BA) has frequently been used to calculate rotational-excitation cross sections for low-energy electron collisions.[31,32] It is certainly true that for *very* low-energy electrons this is a valid procedure, since essentially all of the scattering arises from the long-range region, where the ratio of the interaction energy to the kinetic energy of the electron is quite small.[34,35] For simple molecules (e.g., N_2) the Born approximation is valid[25] for scattering energies below a few tenths of an eV. The BA has been applied to electron-homonuclear diatomic molecule scattering by Gerjuoy and Stein[35] (quadrupole only) and by Dalgarno and Moffett[36] (quadrupole and polarization). In general, the BA cross section for a $|\Delta j| = 2$ transition, taking into account the long-range quadrupole and nonspherical induced-polarization interactions, can be written as

$$\sigma(j\rightarrow j\pm 2) = \frac{k_{j'}}{15k_j}\left(8\pi q^2 + \frac{\pi^2}{2}\,\frac{q\alpha_2}{k_j}(3k_j^2 + k_{j'}^2) + \frac{9\pi^3\alpha_2^2}{128}(k_j^2 + k_{j'}^2)\right)F_\pm(j)\,, \tag{5}$$

where α_2 and q are the nonspherical polarizability and quadrupole moment, respectively. The function $F_\pm(j)$ is given by

$$F_\pm(j) = \begin{cases} \dfrac{(j+2)(j+1)}{(2j+1)(2j+3)} & \text{for } j\rightarrow j+2 \\[2ex] \dfrac{j(j-1)}{(2j-1)(2j+1)} & \text{for } j\rightarrow j-2\,, \end{cases} \tag{6}$$

and k_j^2 and $k_{j'}^2$ are defined by

$$2\epsilon_j + k_j^2 = 2\epsilon_{j'} + k_{j'}^2\,. \tag{7}$$

In Eq. (7), ϵ_j is the energy (in atomic units) of the jth rotational state, which we take to be

$$\epsilon_j(\text{hartree}) = (4.5563\times 10^{-6})B_{\text{rot}}(\text{cm}^{-1})\,j(j+1)\,. \tag{8}$$

For CO_2, the rotational constant[20] is $B_{\text{rot}} = 0.3937$ cm^{-1}. We also use[37] $\alpha_2 = 9.19a_0^3$ and our value[6] of $q = -3.8598ea_0^2$ for the nonspherical polarizability and the quadrupole moment, respectively. The resulting cross sections for $\sigma(0\rightarrow 2)$ in the BA with quadrupole only, and with quadrupole and polarization, are compared with the coupled-channel results including static, exchange, and induced-

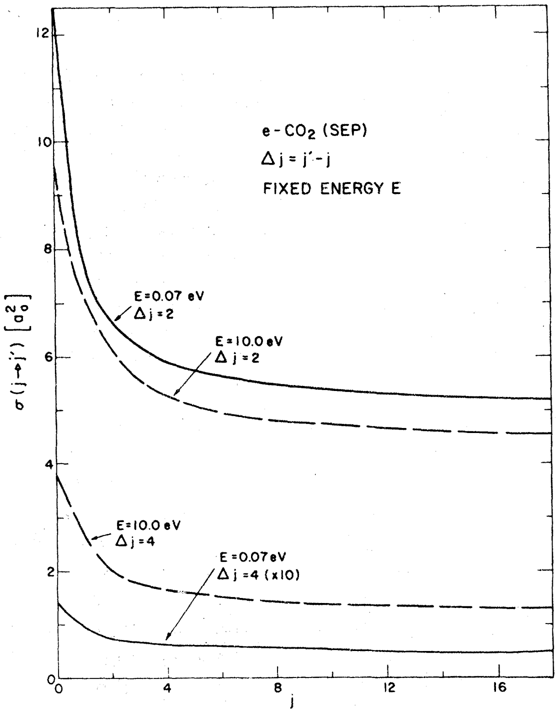

FIG. 4. Behavior of $\sigma(j \rightarrow j')$ for e-CO_2 scattering with increasing initial rotational quantum number j for two scattering energies, 0.07 eV (solid curves) and 10.0 eV (dashed curves). Two transitions $\Delta j = 2$ and 4 are shown for each case. The results at 0.07 eV for $\Delta j = 4$ have been multiplied by 10 for purposes of clarity.

polarization interactions (SEP) in Fig. 3. When polarization is included in the BA for e-CO_2 scattering, the cross section decreases with increasing energy due to cancellation of the quadrupole and nonspherical polarization interactions. This behavior is also seen in e-N_2 scattering.[36] (The threshold for the excitation $j = 0 \rightarrow j' = 2$ in N_2 is 0.0003 eV.) Although the energy range over which the quadrupole interaction is important is fairly large for e-CO_2 collisions, it is clear that the Born approximation will certainly be unreliable for the lowest energies studied here and probably for energies above about 0.03 eV. It seems unlikely that a straightforward application of the distorted-wave method[17,38] to low-energy e-CO_2 scattering would be successful. The nonspherical interaction potential in this problem is so strong compared to the spherical potential [see Fig. 1 of Ref. 6(b)] that we would expect this essentially "perturbation-theory" approach to fail.

In considerations of cooling rates and electron energy distribution functions for CO_2, one must keep in mind that as the gas temperature T_g increases, the peak in the Maxwell-Boltzmann distribution function, which governs the distribution of target molecules among initial rotational states, moves to higher values of j. Thus in CO_2, at $T_g = 100$, 300, and 500 °K the peak occurs at $j = 8$, 16, and 20, respectively. The behavior of $\sigma(j \rightarrow j')$ for e-CO_2 collisions as j increases is illustrated in Fig. 4 for $\Delta j = 2$ and 4 transitions at the two extremes of energy studied, 0.07 and 10.0 eV. The results shown here are typical of the entire energy range studied, and exhibit smooth behavior with increasing j. The nearly constant nature of the results at large j reflects the fact that the ratio of statistical weights of the initial and final states approaches unity as $j \rightarrow \infty$.

In this paper we have presented and discussed theoretical cross sections for rotational excitation of CO_2 by low-energy electrons. Preliminary studies of the electron energy distribution functions which obtain when these rotational-excitation cross sections are incorporated into the transport analysis suggests that they do not significantly alter the results obtained when rotational excitation is ignored. Cooling rates due to rotational excitation in CO_2 gases are presently being calculated and will be reported elsewhere.

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[39] The additional results for the total integrated cross sections for e-CO_2 scattering are (in units of a_0^2): $\sigma_{tot}(0.2\text{ eV})=119.112$, $\sigma_{tot}(3.3\text{ eV})=33.625$, $\sigma_{tot}(3.6\text{ eV})=69.525$, $\sigma_{tot}(4.3\text{ eV})=35.909$, and $\sigma_{tot}(4.6\text{ eV})=29.071$. These supplement the results given in Table IV of Ref. 6(b).

[40] The rotational constant of CO_2 in the ground electronic and vibrational state (see Ref. 20) is 0.3937 cm^{-1}, so the energy of state j' relative to the ground rotational state ($j=0$) in eV is $4.888\times10^{-5} j'(j'+1)$.