

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 $\approx 14\%$ for $Z=10$ decreasing to $\approx 1\%$ 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 by⁴

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

The new quantum number here is Λ , representing the angular momentum of electrons about the internuclear axis ($\Lambda = \Sigma, \Pi, \Delta, \dots$). For $\Lambda > 0$, there are two degenerate linear combinations specified by $\epsilon, \epsilon = 0, 1$ 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 orthonormality 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 \pm 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 \mathbb{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

original integrations (some details of those are given in the Appendix of Ref. 2). We give here the generalized results.

For the amplitude itself, we find ($\Gamma \equiv j, m, \Lambda, \epsilon$; $\Gamma' \equiv j', m', \Lambda', \epsilon'$)

$$\begin{aligned} f_{\Gamma, \Gamma'}(\Omega') &= \delta_{\epsilon, \epsilon'} \delta_{\Lambda, \Lambda'} \sum a_{i\lambda\mu} Y_{i\mu}(\Omega') [(2j+1)(2j'+1)]^{1/2} \\ &\times (2J+1) \begin{pmatrix} l & j & J \\ \mu' & m & M \end{pmatrix} \begin{pmatrix} l & j & J \\ \mu & \Lambda & M' \end{pmatrix} \begin{pmatrix} j' & \lambda & J \\ m' & 0 & M \end{pmatrix} \begin{pmatrix} j' & \lambda & J \\ \Lambda & \mu & M' \end{pmatrix}. \end{aligned} \quad (2)$$

The sum in this expression goes over all indices not contained in Γ' and Γ . The $a_{i\lambda\mu}$ are fixed-nuclei scattering parameters defined as in the second paper of Ref. 6, and Ω' is the scattering angle.⁶ The parenthetical expressions are the 3- j coefficients.⁵

The differential cross section (summed over m and averaged over m') is

$$\begin{aligned} \frac{d\sigma_{\Gamma, \Gamma'}}{d\Omega'} &= \frac{k_{\Gamma'}}{k_{\Gamma}} \frac{\delta_{\epsilon, \epsilon'} \delta_{\Lambda, \Lambda'}}{4\pi} \sum a_{i_i l_j m} a_{\lambda_i \lambda_j \mu}^* (-1)^{m+\mu+J+i_j+\lambda_j} \\ &\times [(2l_i+1)(2\lambda_i+1)]^{1/2} (l_i \lambda_i 00 | L0) (l_j \lambda_j 00 | L0) \\ &\times \begin{Bmatrix} l_i \lambda_i L \\ \lambda_j l_j J \end{Bmatrix} (l_i l_j m - m | J0) (\lambda_i \lambda_j \mu - \mu | J0) \\ &\times (jJ\Lambda - \Lambda | j'0)^2 P_L(\cos\theta'). \end{aligned} \quad (3)$$

Here we have used the 6- j symbol (in braces)⁵ plus the ordinary Clebsch-Gordan coefficients to accord with the notation of Ref. 1.

The total or integrated cross section is

$$\begin{aligned} \sigma_{\Gamma, \Gamma'} &= \frac{k_{\Gamma'}}{k_{\Gamma}} \delta_{\epsilon, \epsilon'} \delta_{\Lambda, \Lambda'} \sum a_{i\lambda m} a_{\lambda \mu}^* (2\lambda+1)^{-1} (-1)^{m+\mu} \\ &\times (l\lambda m - m | J0) (l\lambda \mu - \mu | J0) (jJ\Lambda - \Lambda | j'0)^2. \end{aligned} \quad (4)$$

In Eqs. (2)–(4), the $\delta_{\Lambda, \Lambda'}$ explicitly shows that the adiabatic transitions occur within a specific electronic level. Similarly $\delta_{\epsilon, \epsilon'}$ indicates that the character under nuclear exchange cannot change. (Actually $\delta_{\Lambda, \Lambda'}$ comes about because the underlying fixed-nuclei theory was confined to elastic scattering in a fixed electronic level.⁶) As opposed to Ref. 1, the presence of the last Clebsch-Gordan coefficient for $\Lambda \neq 0$ removes the $|j-j'| = \text{even}$, selection rule.

The modified formulas for rotational excitation of a charged molecular system² (molecular ion) can be generalized trivially in the same manner as these formulas generalize the neutral results! It is understood in all these formulas that $a_{i\lambda m}$ are symbolic of scattering parameters coming from a consistently formulated fixed-nuclei theory for the appropriate non- Σ state of the target molecule.

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ERRATA

Hyperfine Structure of the 2^3S_1 State of He^{3+} , S. D. Rosner and F. M. Pipkin [Phys. Rev. A **1, 571 (1970)].** The following misprints in this article should be corrected.

(i) p. 572 " $\Delta_2 = -9.89 \pm 0.04$ ppm" should read " $\Delta_2 = -8.89 \pm 0.04$ ppm."

(ii) p. 574 Equation (43) should read " $\Delta\nu^0(\text{He}^{3+}, 2^3S_{1/2}) = \frac{16}{3} \dots$ "

(iii) p. 576 " $E(\frac{3}{2}, -\frac{3}{2}) = E_0 = \frac{1}{3}h\Delta\nu + \dots$ " should read " $E(\frac{3}{2}, -\frac{3}{2}) = E_0 = -\frac{1}{3}h\Delta\nu + \dots$ "

(iv) p. 577 "This is realized experimentally in the

hyperfine transitions with $F=1, m_f=0, \pm 1$ " . . .

should read ". . . with $\Delta F=1, \Delta m_f=0, \pm 1$."

(v) p. 577 Equation (57) has a p_{11} which should be ρ_{11} .

(vi) p. 578 " $I_0 \approx 2 \times 10^{15}$ photons/cm²sec Hz" should read ". . . $2 \times 10^5 \dots$ "

(vii) p. 580 ". . . evacuated with baking to a pressure of 10^{-3} Torr" should read ". . . 10^{-8} Torr."

(viii) p. 580 ". . . roughly 1 to 2 liters h " should read ". . . liters/ h ."

(ix) p. 581 "Harvard University J. A. Division of