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Electron Scattering with and without Vibrational Excitation. VIII. Comment on a Theory of Small-Energy-Transfer Collisions Dominated by Long-Range Forces

Donald G. Truhlar

Chemical Dynamics Laboratory, University of Minnesota, Minneapolis, Minnesota 55455

Two methods [D. G. Truhlar and J. K. Rice, J. Chem. Phys. **52**, 4480 (1970) and B. Ritchie, Phys. Rev. A **6**, 1456 (1972)] for calculating cross sections for vibrational excitation of molecules by electron impact are compared. The former method is shown to have a greater range of applicability. Cross sections computed by the two methods differ by about a factor of 2 for excitation to the first vibrationally excited level of H_2. The neglect of the short-range potential in Ritchie's method is shown to be an important source of error in that method.

Recently, Ritchie[1] has proposed a quantum-mechanical theory for cross sections for vibrational excitation in collisions dominated by long-range central potentials. Previously, a theory applicable to such collisions had been proposed by the author and Rice.[2,3] It is of some interest to compare these theories. The latter theory is the polarized Born approximation and it includes not only the spherically symmetric part of the long-range potential but also the short-range potential and the asymmetry of the potential. The polarized Born approximation is also more general in that it does not require the assumption of small energy transfer. Ritchie's calculation evaluates the eigenphase shifts in the high-energy limit. The high-energy approximation is similar to, but not identical to, the plane-wave approximation in the polarized Born calculations; the relationship of the two approximations has been discussed elsewhere.[4,5] In the present article we consider vibrational excitation of N_2 and H_2 by electron impact.

First we consider excitation of the $v' = 1$ vibration. The data needed for the calculations by Ritchie's method are R_e (the equilibrium internuclear distance), ϵ (the vibrational excitation energy), α_{10}, and $\alpha \equiv \frac{1}{2}(\alpha_{11} - \alpha_{00})$, where

$$\alpha_{v'v} = \int \psi_{v'}^*(R) \, \alpha(R) \, \psi_0(R) \, dR \qquad (1)$$

and $\psi_{v'}(R)$ is a vibrational wave function and $\alpha(R)$ is the static dipole polarizability as a function of internuclear distance. These data were computed for H_2 by the method of Paper I and are given[6] in Table I as data set 1 (DS1). These data are essentially the same as Ritchie's data set (RDS), in which $\alpha_{vv'}$ is taken from Henry's calculations.[7]

For N_2, Ritchie used H_2 matrix elements scaled to account for the different polarizability of N_2 at R_e. This yields the data labeled RDS in Table I. A more accurate data set (ADS) was determined by the following procedure. Assume

$$\alpha(R) \cong \alpha(R_e) + \left(\frac{d\alpha}{dR}\right)\Bigg|_{R=R_e} x \,, \qquad (2)$$

where $x = R - R_e$. Define

$$x_{v'v} = \int \psi_{v'}^*(R)(R - R_e)\psi_v(R) \, dR \ . \qquad (3)$$

These matrix elements were computed by an accurate numerical method[8] using vibrational wave functions corresponding to the accurate N_2 potential function of Levine.[9] The results are $x_{00} = 7.192 \times 10^{-3}$, $x_{01} = 6.058 \times 10^{-2}$, and $x_{11} = 2.174 \times 10^{-2}$. From $d\alpha/dR \,|_{R=R_e} \cong 5.71^{10,11}$ and x_{01}, we obtain α_{01}. From

TABLE I. Matrix elements (a. u.) needed for scattering calculations by Ritchie's method.

Molecule	H_2	H_2	N_2	N_2
Data set	RDS	DS1	RDS	ADS
α	0.2355	0.2351	0.542	0.0415
α_{01}	0.739	0.7388	1.701	0.346
R_e	1.4011	1.4011	2.0741	2.0741
ϵ	0.01895	0.01895	0.01062	0.01062
σ	1.4011	1.4011	2.0741	1.3

TABLE II. Quantities important for validity of Ritchie's theory.

Molecule	H_2	N_2	N_2
Data set	DS1	RDS	ADS
α/σ^4	0.0610	0.0292	0.0145
ϵ	0.0190	0.0106	0.0106

$\alpha_{00} = 11.925$ [12] and x_{00}, we obtain $\alpha(R_e) = 11.884$ (in this model). From $\alpha(R_e)$, $d\alpha/dR \mid_{R=R_e}$, and x_{11}, we obtain $\alpha_{11} = 12.008$. The resulting data are given in Table I.

Finally the calculations involve a cutoff parameter σ. The potential causing the transition is assumed to vanish for $r < \sigma$ (where r is the distance of the incident particle from the molecular target). Ritchie assumed $\sigma = R_e$. This is reasonable enough for H_2. However, previous work[11,13,14] using similar model potentials has shown that such a value is too large for N_2 (values of 1.3,[11] 1.75,[13] and 1.19[14] were found to be close to the optimum in these various models). Hence we used $\sigma = 1.3$ for N_2.

The criterion[1] for validity of Ritchie's theory is $\alpha/r^4 >> \epsilon$ for most r, where r is the distance of the electron from the molecular target. For $r = \sigma$, these quantities are compared in Table II. For H_2 and for Ritchie's data set for N_2, the validity criterion is fairly well satisfield. But for the accurate data set for N_2, the criterion is not valid. (Note: Ritchie originally applied the criterion at $r = 1$; however, since the potential causing the transition is assumed in his method to vanish for $r < R_e$, this is inconsistent. Further, the criterion would be even farther from satisfaction by the accurate data set if we used $\sigma = R_e$.) Thus Ritchie's method is not applicable to N_2.

Using data set 1 the calculation for excitation of the fundamental vibration of H_2 by Ritchie's method proceeds as follows:

$$Q_{01} = (\tfrac{1}{32}\pi p_c G\sigma^2)(1 - \tfrac{1}{120}G + \tfrac{1}{23040}G^2) , \qquad (4)$$

where

$$p_c = 4\chi_c^2/(1 + \chi_c^2)^2 ,$$

$$\chi_c = (S - \alpha)/\alpha_{10} ,$$

$$S = (\alpha^2 + \alpha_{10}^2)^{1/2} ,$$

$$G = (\pi S/k\sigma^3)^2 ,$$

and $Q_{0v'}$ is the integral cross section for excitation of v' quanta of vibration. Equation (4) is an expansion in powers of G. For H_2, $G = 0.7842/k^2$. Since the vibrational excitation cross section is dominated by a resonance at low energies,[15,16] the direct excitation mechanism is not applicable there (e.g.,

even at 10 eV, the resonance accounts for at least $\tfrac{1}{4}$ of the excitation cross section; see Paper III[16]). Thus we will restrict attention to energies $E \geq 10$ eV. At high energies there is a different difficulty because at high energies the polarization-potential model used here to obtain the dominant long-range potential breaks down.[17-20]

Calculations for excitation of the $v' = 1$ state of H_2 by electron impact using Ritchie's method and using the polarized Born method of Papers I and III with data set 1[2,16] (the latter calculations are labeled simply B/P since they are our most complete polarized Born calculations) are compared in Table III. The comparison shows that for energies of 45 eV and higher, Ritchie's method yields results lower than the B/P calculation by about a factor of 2. This can be explained by considering two calculations of integral cross sections which, like Ritchie's method, consider only the central potential. One, labeled "P_0^{D5}" by the convention of Paper I and called "B/P with modified potential" here, includes only the spherically symmetric part of the polarization potential of the complete B/P calculation. The other, labeled "$S_0 P_0^{D5}$" in Paper I and called "B/P with spherically symmetric potential" here, includes the spherically symmetric part of the whole potential (short-range static potential

TABLE III. Integral cross sections (in a_0^2) for vibrational excitation of the fundamental vibration of H_2 as functions of impact energy E.

E(eV)	Complete B/P[a]	Ritchie's method	B/P using Ritchie's potential[b]	B/P using modified potential[c]
10	0.290[d]	0.185[e]	0.275	0.106[f]
13.6	0.178[d]	0.136	0.203	0.0782[f]
20	0.139[d]	0.0930	0.141	0.0536[f]
45	0.0801[d]	0.0414	0.0658	0.0239[f]
60	0.0627[d]	0.0311	0.0495	0.0179[f]
81.6	0.0473[d]	0.0229	0.0367	0.0132[f]
100	0.0390[d,f]	0.0187	0.0301	0.0107[f]
200	0.0202[f]	0.00934	0.0152	0.00537
412	0.0100[f]	0.00453	0.00739	0.00261

[a]Using data set 1 of Ref. 2.
[b]P_0^C with $a_p = 1.4011a_0$ in the notation of Ref. 2.
[c]P_0^{D5} with $a_p = 2.1a_0$ in the notation of Ref. 2.
[d]Paper III.
[e]Reference 1.
[f]Paper I.

plus polarization potential) of the complete B/P calculation. Figure 10 of Paper I shows that the former cross sections are only about half or less than half of the latter ones for $v'=1$. Figures 15 and 17 of Paper I show the ratio is even less for higher v'. Thus, it is a poor approximation to neglect the short-range static potential and it becomes worse for higher v'. For example, Table XI of Paper I A shows the B/P with modified potential model predicts $Q_{02}/Q_{01} = 0.0092-0.0093$, for $E = 10-100$ eV. But the B/P with spherically symmetric potential calculation predicts $0.0169-0.0239$ for the same quantity (the complete B/P calculation predicts $0.0141-0.0264$ for this quantity and including exchange by the BOR/P method changes this to $0.0148-0.0268$).[2] Similar considerations indicate that the B/P with modified potential method underestimates Q_{03}/Q_{02} in the 10-100-eV energy range by a factor of about $\frac{5}{2}$.

Finally we carried out plane-wave calculations for exactly the same central potential used in Ritchie's method. These calculations would be labeled P_0^C by the convention of Paper I since the polarization potential is of the C type.[2,9] These calculations, shown in Table III, also yield results higher than those obtained by Ritchie's method. This shows that part of the difference between columns 2 and 3 of Table III is in the treatment of the dynamics for a given potential. Since the short-range potential cannot be treated realistically by Ritchie's method, and since we have shown in the previous paragraph that the short-range potential is expected to be very important, the values computed by the B/P method are preferable to the values computed by Ritchie's method. However, the empirical accuracy of either method cannot be finally assessed until they can be compared with experiment in a greater number of cases in which the experiment is independently normalized.[21]

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Electronic Stopping Cross Sections*

A. E. S. Green and R. K. Hill

Department of Physics, University of Florida, Gainesville, Florida 32601

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We examine a three-parameter formula for the electronic stopping cross section at nonrelativistic velocities of Brice based upon the Firsov formalism. We show that it is substantially a special case of a simple formula applied earlier by Green and Peterson, and that the work of Brice provides an approximate rule relating two of their four parameters.

I. INTRODUCTION

Recently Brice[1] has proposed a three-parameter semitheoretical formula for the electronic stopping cross section of heavy particles,

$$S(\epsilon) = (Z_1 + Z_2)(4\hbar^2/5m)f_e(\epsilon)f(u),\tag{1}$$

where