Electron scattering by N_2 at 5 and 10 eV: Rotational–vibrational close-coupling calculations and crossed beam studies of vibrational excitation*

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The ratios of differential cross sections for excitation of the first excited vibrational state to differential cross sections for elastic scattering of N_2 have been measured at scattering angles ranging from 20° to 135° at 5 and 10 eV impact energies. Using previously measured and normalized elastic differential cross sections for N_2, the ratios have been converted to inelastic cross sections. Laboratory-frame close-coupling calculations using a four-state vibrational–rotational basis set and an effective interaction potential developed previously are reported at both energies. It is shown that the four-state treatment of this potential scattering model can account for the approximate magnitude and the qualitative behavior of the cross sections, but there are some significant quantitative differences between theory and experiment.

I. INTRODUCTION

Vibrational excitation of N_2 by electrons with impact energies of 4 to 11 eV has been studied very little. This process is important in the ionosphere and thermosphere and accurate cross sections are needed at these energies for use in studies of the atmosphere.[1–14] The only experimental study of the process at these energies is that of Schulz and coworkers who measured[5] the differential cross section at 25°, 50°, and 90° at 4, 7.5, and 11 eV and later studied[6,7] a core-excited resonance (full width at half maximum about 0.7 eV) in the differential cross section near 8 eV. The only quantum mechanical calculations for vibrational excitation at these energies are those of Breig and Lin[8] and Chandra and Temkin.[9]

In the present article we report experimental differential, integral, and momentum transfer cross sections for excitation of the fundamental vibration of N_2 at eight scattering angles from 20° to 135° and at impact energies 5 and 10 eV. We also present quantum mechanical calculations of these cross sections using the truncated vibrational–rotational close-coupling approximation with a model interaction potential. These experimental and theoretical results are compared to each other and to previous experimental[5] and theoretical[8,9] results. The quantum mechanical calculations also yield cross sections for pure elastic scattering and pure rotational excitation. The elastic and total scattering cross sections are compared to previous experimental results[10–12] and the pure rotational excitation cross sections to previous quantum mechanical calculations.[9,13–15] Although the results are important for atmospheric and other applications, in this article we discuss them from the more fundamental point of view of testing quantum mechanical theories.

Vibrational excitation of N_2 by electrons with energies below 4 eV is dominated by a shape resonance which produces large cross sections for excitation of the fundamental and several overtones (the peak value of the excitation cross section for the fundamental is about 10 a_0^2). At energies from 11.5 to 30–35 eV vibrational excitation appears to be dominated by many core-excited resonances, often overlapping. These resonant processes have been well studied[5–7,16–18] (and reviewed[18,19]) and will not be considered further in this article. Nonresonant vibrational excitation of N_2 at energies 30–75 eV has also been previously studied.[20–22]

The electron scattering integral cross section for the specific process with initial vibrational and rotational quantum numbers v and j and final vibrational and rotational quantum numbers v' and j' in the ground electronic state is denoted $\sigma_{vjv'j'}$. Experimentally the rotational states have not been resolved so what has been measured is $\sigma_{vjv'j'}$ summed over j' and averaged over j. This is called $\sigma_{vv'}$. We call σ_{00} the vibrationally elastic cross section and σ_{01} the vibrational-excitation cross section. For the experimental results the distribution of j is a thermal distribution at slightly below room temperature. However in the present and previous[9] theoretical treatments the only initial value considered is $j = 0$.

II. EXPERIMENTAL DETAILS

The electron-scattering apparatus used in the present measurements has been described in detail elsewhere.[23,24] Briefly, a crossed-beam geometry is used wherein an energy-selected electron beam (having full-width at half-maximum of 0.050 eV) is focused onto the target N_2 beam which is formed by a stainless steel multichannel capillary array. Electrons scattered elastically and inelastically through the angular range 20° –

135° are then energy-analyzed and detected. The quantity measured was the ratio $R_1(E_0, \theta)$ of peak height or integrated area of the vibrational excitation ($v = 0$, $v' = 1$) feature. Correction of this ratio at small scattering angles ($\theta < 30°$) for parent beam contributions and multiplication of the corrected ratio by the absolute elastic differential cross section (as measured previously[12]) then gave the absolute differential cross section $d\sigma_{01}(E_0, \theta)/d\Omega$ for the $v = 0$ to $v' = 1$ vibrational excitation.

The parent-beam contribution was measured by pumping out the N_2 target gas to a background pressure of 8×10^{-8} torr and observing the intensity of the parent beam. This correction was 5% at 10 eV, 20° and 16% at 5 eV, 20°. Corrections were 2% or less at 30° and were negligible elsewhere.

The true zero angle was determined as that angle about which the elastic scattering intensity was symmetric. The estimated error in this determination is ± 2°. The energy scale was calibrated to an estimated accuracy of ± 0.05 eV by noting the nominal positions (in energy) of the 11.48 and 11.87 eV resonances in N_2 at $\theta = 40°$ and calibrating to previously measured[16] energies of these resonances. This procedure was deemed more reliable than calibration against the 19.36 eV He resonance since a 0.1 eV difference in contact potential corrections was noted upon changing gases from He to N_2. All measurements of the ratio $R_1(E_0, \theta)$ were then carried out by leaving untouched the settings of filament current and monochromator voltage, since changes in these settings could affect the electron energy.

III. THEORY

A. Methods

The methods used for the present quantum mechanical calculations have already been presented.[22,25] Here we contrast these methods with those used by Breig and Lin[8] and Chandra and Temkin.[9]

Breig and Lin assumed that the spherical average of the polarization interaction completely dominates the quadrupole and nonspherical polarization interactions and the shorter range interactions in its contribution to the vibrational excitation cross sections. Thus they wrote the effective potential as simply

$$V(r, R) = -(\alpha(R)/2r^4)[1 - \exp(-r^n/b^n)], \quad (1)$$

where r is the distance from the electron to the center of N_2, R is the internuclear distance, and $\alpha(R)$ is the spherical average of the static electric dipole polarizability. They assumed $n = 8$ and used two different estimates of b obtained by arguments involving the size of the static charge distribution. They used plane wave scattering states.

The calculations of Chandra and Temkin involve a considerable increase in the level of sophistication. They used an accurate nonspherical static potential (including short-range and quadrupole interactions) augmented by a nonspherical polarization potential whose spherical average is of the form of Eq. (1) with $n = 6$. They set $b = 1.554\ a_0$ so that the π_g resonance energy calculated in an abbreviated version of their full method is 2.4 eV. The scattering by this potential was treated in the body frame for σ_g, σ_u, π_u, and π_g symmetries of the continuum orbital. For the first three of these they used the adiabatic-nuclei approximation[19,26,27] in which the molecular asymmetry is manifested in the coupling, for each symmetry, of waves with different values of the scattering electron's orbital angular momentum quantum number l. They converged this expansion (which required $l_{max} \cong 15$). For these symmetries, exchange was mimicked by orthogonalizing the continuum orbital to the bound orbitals, as done earlier by Burke and Chandra.[14] For the π_g symmetry they used body-frame vibrational close-coupling, neglecting exchange, and considered only l values of 2, 4, and 6. Chandra and Temkin included all four symmetries in their calculation of vibrationally elastic cross sections but since their calculations were originally applied in the resonance region where the π_g symmetry dominates the vibrational-excitation cross section they included only the π_g symmetry in the calculation of vibrational-excitation cross sections. They plan to include all four symmetries in future calculations of vibrational-excitation cross sections at these energies.[9]

The present calculations also invoke a coupled-channel treatment of an accurate nonspherical static potential augmented by a polarization potential of the form of Eq. (1) with $n = 6$. We used a similar value for the parameter b (1.592 a_0). But our calculations differ from the calculations of Chandra and Temkin in several respects. The three most important are probably the following:

(1) We neglected exchange of the scattering electron. For electron–hydrogen atom s-wave scattering in the triplet spin state, Riley and one of the authors[28] have tested the Burke–Chandra method for including exchange against the complete method involving explicit antisymmetrization of the system's wavefunction. At 5–10 eV impact energy the former included 50%–75% of the effect of exchange. Thus the use of the Burke–Chandra method to include some of the effect of exchange should improve the calculation of Chandra and Temkin. Note, however, that exchange was neglected in the π_g symmetry upon which their vibrational-excitation cross sections are based.

(2) We assumed a different R dependence of $\alpha(R)$ and the anisotropy $\alpha'(R)$ of the polarizability tensor. For $0 \rightarrow 1$ vibrational excitation, it is important that the vibrational matrix elements

$$\alpha_{10} \equiv \langle 1 | \alpha(R) | 0 \rangle \quad (2)$$

and

$$\alpha'_{10} \equiv \langle 1 | \alpha'(R) | 0 \rangle \quad (3)$$

be accurate. Our approximation to $\alpha(R)$ was a semiempirical one which, following Breig and Lin,[8] was designed to reproduce the experimental α_{10}. Our approximation to $\alpha'(R)$ was designed to give α'_{10} as accurately as possible. We have computed[25,29] these ma-

TABLE I. Vibrational matrix elements of polarizability functions of N_2.

	α_{10} (a.u.)	α'_{10} (a.u.)
Present[a]	0.346	0.218
Chandra and Temkin[b]	0.103	0.123
Experiment[c]	0.344	n.a.[d]

[a]Taken from Refs. 25 and 29.
[b]Computed from $\alpha(R)$ and $\alpha'(R)$ by the method of Refs. 25 and 29.
[c]Reference 30 (see also Ref. 8).
[d]Not available.

trix elements for our and their approximations to $\alpha(R)$ and $\alpha'(R)$ and they are compared to one another and to this experiment[30] in Table I. Their value for α_{10} is only 30% as large as the experimental one. The reason is that they found $\alpha(R)$ by equating a linear truncation of its Taylor series expansion in $(R - R_e)$ to the united-atom value at the origin; but this truncated series is not valid at the origin and so this procedure can lead to spurious results. Although there is no experimental result for α'_{10} we believe that their procedure is subject to the same criticism for this matrix element. It is also interesting to point out that the inner classical turning points for $v = 1$ and $v = 2$ are 1.94 a_0 and 1.90 a_0, respectively, compared to $R_e = 2.068$ a_0. Thus it is not necessary for $\alpha(R)$ to have the correct united-atom limit in order to evaluate its matrix element involving low-lying vibrational states. In summary, we believe our polarizability functions are more reliable than theirs for the present problem.

(3) We use laboratory-frame rotational–vibrational close coupling. In this treatment the molecular asymmetry is manifested in the coupling, for each total angular momentum quantum number J, of channels with different values of l and of the rotational quantum number j. We considered only $j = 0$ and 2 but converged the calculations with respect to including more l values (we used $l_{max} = 28$ at 5 eV and $l_{max} = 39$ at 10 eV, see next subsection). Since we did not converge our cross sections with respect to increasing j we have not treated the asymmetry of the potential in a complete way as Chandra and Temkin did for the σ_g, σ_u, and π_u symmetries. This is clearly a source of error and we do not know how serious it is. There are two indications from other work that it need not be too bad. First, the calculations of Burke and Chandra show that the $0 \rightarrow 2$ rotational excitation integral cross section is 2 1/2 times larger than the $0 \rightarrow 4$ one at 5 eV and that the $0 \rightarrow 4$ excitation becomes even less important relative to the $0 \rightarrow 2$ excitation at 10 eV.[14,15] This, however, is not a sufficient condition for the $j = 4$ state to be relatively unimportant in the scattering wavefunction at small r. Second, we were reasonably successful in treating elastic scattering and rotational excitation of H_2 with a two-rotational-state ($j = 1$ and 3) expansion at 10 eV.[31] However, H_2 is more nearly spherical than N_2 and the inclusion of higher rotational states is probably more important for N_2.

We will also compare the present calculations of the elastic scattering and pure rotational excitation cross sections to those obtained in two previous calculations involving the rigid-rotator assumption. The first of these, by Takayanagi and Geltman,[13] equated the potential exactly to its long-range form involving the polarization and quadrupole r^{-4} and r^{-3} interactions for $r > r_0$ and to a constant for $r \leq r_0$. The scattering was treated by distorted-wave theory with the spherical part of the potential used as a distorting potential and the parameter r_0 was adjusted to the experimental elastic scattering cross section. The second of the rigid-rotator calculations is that of Burke and Chandra.[14,15] Aside from involving the rigid-rotator assumption, this calculation is basically the same as that of Chandra and Temkin, which followed it.

B. Calculational details

The calculational procedures are described elsewhere.[22,25] The close-coupling expansion of the wavefunction is more rapidly convergent at higher J. For $J = 0$–8 we used the four-state vibrational–rotational basis with states $(v, j) = (0, 0)$, $(0, 2)$, $(1, 0)$, $(1, 2)$. For $J = 9$–12 we used only the two states $(0, 0)$ and $(0, 2)$. For $J = 13$–J_2 (where J_2 is 28 for 5 eV and 39 at 10 eV) we included only the ground state $(0, 0)$. We found $d\sigma_{00}/d\Omega$ converged within 0.4% at all angles with respect to decreasing J_2 by 2; $d\sigma_{01}/d\Omega$ converged within 1%–5% at all angles at 5 and 10 eV with respect to including only $J = 0$–10. The integral cross sections converge more rapidly. This is illustrated by Table II which gives the partial integral cross sections we calculated for the inelastic processes defined such that[32]

$$\sigma_{vjv'j'} = \sum_l \sigma^l_{vjv'j'}. \tag{4}$$

C. Results for elastic scattering and rotational excitation

Calculated cross sections for elastic scattering and pure rotational excitation are given in Tables III and IV where they are compared to previous experimental and theoretical results. Consider first the cross sections at 10 eV. There is reasonably good agreement between all the calculations and experiments for the vibrationally elastic integral and momentum-transfer cross sections σ_{00} and σ^m_{00}. However, the present calculations seem to overestimate the rotational-excitation components of these cross sections. We have seen previously[33,34] that the two-state rotational close-coupling approximation sometimes overestimates the cross section for $j = 0$, $j' = 2$ and we suspect that the present rotational excitation cross sections may be too large due to incomplete convergence of the rotational state expansion. If so it is interesting to see what effect, if any, this has on the accuracy of $d\sigma_{00}/d\Omega$ and $d\sigma_{01}/d\Omega$. The comparison of $d\sigma_{00}/d\Omega$ to experiment and the Chandra–Temkin calculation is given in Table IV. The present calculation appears to underestimate the vibrationally elastic differential cross section from 30° to 80° and to overestimate it for $\theta \geq 90°$. This overestimation of the large-angle scattering is the reason that σ^m_{00} is overestimated (see Table III). The error in the large-angle scatter-

TABLE II. Partial integral cross sections $\sigma^l_{vjv'j'}$ and $\sigma^l_{vv'}$, and integral cross sections $\sigma_{vjv'j'}$ and $\sigma_{vv'}$ (a_0^2) for inelastic scattering.

	$E_0=5$ eV				$E_0=10$ eV			
l	σ^l_{0002}	σ^l_{0010}	σ^l_{0012}	σ^l_{01}	σ^l_{0002}	σ^l_{0010}	σ^l_{0012}	σ^l_{01}
0	1.2 (0)[a]	1.0 (−1)	4.4 (−3)	1.1 (−1)	4.5 (−1)	3.6 (−2)	2.3 (−3)	3.8 (−2)
1	2.4 (1)	1.6 (−3)	2.5 (−2)	2.6 (−2)	1.3 (1)	6.7 (−4)	3.1 (−2)	3.1 (−2)
2	1.2 (1)	3.5 (−2)	2.8 (−2)	6.4 (−2)	1.1 (1)	9.3 (−3)	9.9 (−3)	1.9 (−2)
3	2.5 (−2)	5.0 (−4)	3.5 (−4)	8.5 (−4)	4.6 (−2)	2.0 (−3)	8.4 (−4)	2.8 (−3)
4	1.2 (−2)	1.0 (−4)	2.0 (−4)	3.1 (−4)	1.4 (−2)	2.5 (−4)	1.9 (−4)	4.4 (−4)
5	6.4 (−3)	3.4 (−5)	1.0 (−4)	1.4 (−4)	5.1 (−3)	7.4 (−5)	1.1 (−4)	1.8 (−4)
6	4.1 (−3)	1.4 (−5)	5.8 (−5)	7.2 (−5)	3.5 (−3)	3.0 (−5)	6.1 (−5)	9.2 (−5)
7	2.8 (−3)	6.7 (−6)	3.7 (−5)	4.4 (−5)	2.5 (−3)	1.4 (−5)	3.8 (−5)	5.2 (−5)
8	2.0 (−3)	3.5 (−6)	2.4 (−5)	2.8 (−5)	1.8 (−3)	7.6 (−6)	2.5 (−5)	3.2 (−5)
	σ_{0002}	σ_{0010}	σ_{0012}	σ_{01}	σ_{0002}	σ_{0010}	σ_{0012}	σ_{01}
	3.75(1)	1.37(−1)	5.81(−2)	1.96(−1)	2.38(1)	4.83(−2)	4.41(−2)	9.24(−2)

[a]Numbers in parentheses are multiplicative powers of 10.

TABLE III. Integral and momentum-transfer cross sections[a] (a_0^2).

	σ_{0000}	σ_{0002}	σ_{00}	σ_{tot}	σ^m_{0000}	σ^m_{0002}	σ^m_{00}	σ^m_{tot}
$E_0=5$ eV								
Theory								
Takayanagi–Geltman[b]		0.2[c]						
Burke–Chandra[b]	36.4	9.6	49.5	59.5	22.9	10.6	37.0	37.0
Chandra–Temkin	36.3	9.7	49.8	50.0	22.6	10.6	37.1	37.3
Present	32.6	37.5	70.0	70.2	14.2	56.1	70.4	70.6
Experiment								
Brüche[d]				38				
Fisk[e]				38.7[c]				
Englehardt–Phelps–Risk							37	38
Aberth–Sunshine–Bederson[f]				45				
Golden				41				
Shyn–Stolarski–Carignan[g]			39					
Srivastava–Chutjian–Trajmar			34				28	
$E_0=10$ eV								
Theory								
Takayanagi–Geltman[b]		0.07[c]						
Burke–Chandra[b]	30.9	14.2	48.1	48.1	17.0	17.4	37.6	37.6
Chandra–Temkin	31.0	14.3	48.3	48.3	16.9	17.3	37.5	37.6
Present	20.1	23.8	43.9	44.0	10.7	35.3	46.0	46.1
Experiment								
Brüche[d]				41[c]				
Fisk[e]				37.5[c]				
Englehardt–Phelps–Risk							32	33
Aberth–Sunshine–Bederson[f]				50[c]				
Shyn–Stolarski–Carignan[g]			43					
Srivastava–Chutjian–Trajmar			43				35	

[a]$\sigma_{vjv'j'}$ and $\sigma_{vv'}$ are defined at the end of Sec. I. σ_{tot} is the total scattering cross section, i.e., the sum of the cross sections for all processes. The corresponding momentum-transfer cross sections are $\sigma^m_{vjv'j'}$, $\sigma^m_{vv'}$, and σ^m_{tot}.

[b]Involves rigid-rotator approximation.

[c]Interpolated.

[d]E. Brüche, Ann. Phys. Leipzig **81**, 537 (1926); **82**, 912 (1927).

[e]J. B. Fisk, Phys. Rev. **51**, 25 (1937).

[f]W. Aberth, G. Sunshine, and B. Bederson, in *Atomic Collision Processes, Proceedings of the Third International Conference on the Physics of Electronics and Atomic Collisions*, edited by M. R. C. McDowell (North-Holland, Amsterdam, 1964), p. 53.

[g]T. W. Shyn, R. S. Stolarski, and G. R. Carignan, Phys. Rev. A **6**, 1002 (1972).

TABLE IV. Differential cross sections for vibrationally elastic scattering $d\sigma_{00}/d\Omega$ (a_0^2).

θ	$E_0 = 5$ eV			$E_0 = 10$ eV		
(deg)	Experiment	Chandra–Temkin	Calc[a]	Experiment	Chandra–Temkin	Calc[a]
0		7.10	19.3		12.6	20.9
10		7.30	15.5		11.6	14.2
20	5.3	7.88	12.1	8.3	10.1	9.15
30	5.6	8.26	9.36	7.5	8.94	5.93
40	5.1	7.90	7.05	6.3	7.68	3.77
50	4.1	6.82	5.16	5.0	6.08	2.30
60	3.1	5.38	3.77	3.9	4.29	1.42
70	2.4	4.04	2.95	2.7	2.77	1.05
80	1.89	3.08	2.69	1.79	1.81	1.10
90	1.54	2.53	2.92	1.29	1.47	1.49
100	1.43	2.30	3.52	1.43	1.61	2.12
110		2.27	4.38		2.01	2.88
115	1.57		4.88	2.0		3.29
120		2.33	5.40		2.52	3.70
130		2.44	6.54		3.05	4.57
135	2.3		7.13	3.4		5.02
140		2.58	7.71		3.57	5.48
150		2.75	8.84		4.06	6.39
160		2.90	9.79		4.46	7.20
170		3.00	10.4		4.70	7.76
180		3.03	10.7		4.79	7.96

[a]Present calculation.

ing might be caused by the nonconvergence of the rotational-state expansion since this nonconvergence reflects an incomplete treatment of the short-range l coupling caused by the strong short-range forces responsible for large-angle scattering.

The present calculations appear to be less accurate at 5 eV (see Table III). One expects that exchange is much more important at 5 than 10 eV and that its neglect is responsible for the vibrationally elastic cross section being too large at 5 eV. But our lack of explicit exchange is compensated to some extent by the fact that the parameter in our polarization potential was adjusted by Burke and Chandra[14] to the π_g resonance at 2.4 eV and exchange was neglected during this adjustment. Since the exchange effect is larger at 2.4 than at 5–10 eV this might even overestimate exchange. However the d-wave resonant scattering at 2.4 eV might not be sensitive to the shorter range part of the exchange effect.

Table III shows that the calculation of rotational-excitation cross sections by Takayanagi and Geltman[13] is quite inaccurate.

IV. RESULTS FOR VIBRATIONAL EXCITATION

The present measurements and calculations of the ratios $R_1(E_0, \theta)$ are shown in Figs. 1 and 2 at 5 and 10 eV, respectively. The errors given for $R_1(E_0, \theta)$ represent one standard deviation as determined by 2–5 measurements at each E_0 and θ. The absolute differential cross sections are given in Figs. 3 and 4 and Table V at the two energies. The errors here represent the root mean square of the error in $R_1(E_0, \theta)$ and of the estimated error (± 15%) in the absolute elastic differential cross sections of Ref. 12.

The shaded rectangles in Figs. 1 and 2 were obtained

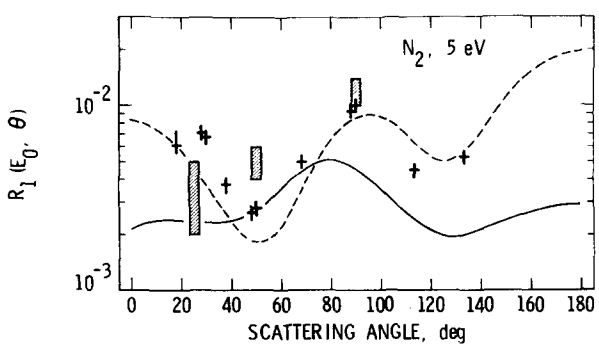

FIG. 1. The ratio $R_1(E_0, \theta)$ as a function of scattering angle θ for vibrational excitation at 5 eV. The solid line is the result of the present calculations and the dashed line represents the calculations of Ref. 9. Present experimental results and error estimates are shown by crosses, while shaded rectangles are interpolated estimates from Fig. 2 of Ref. 5.

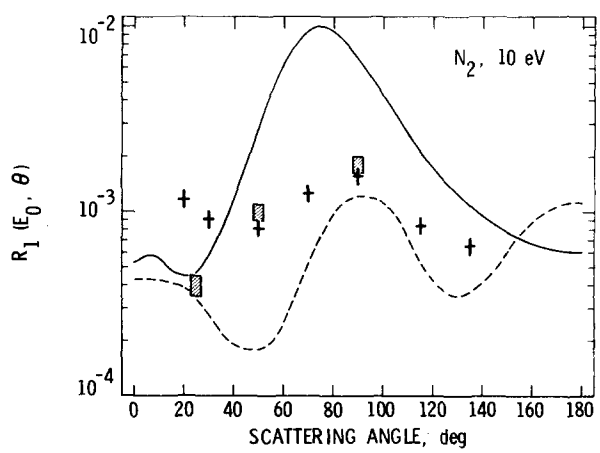

FIG. 2. Same as Fig. 1 but at 10 eV incident energy.

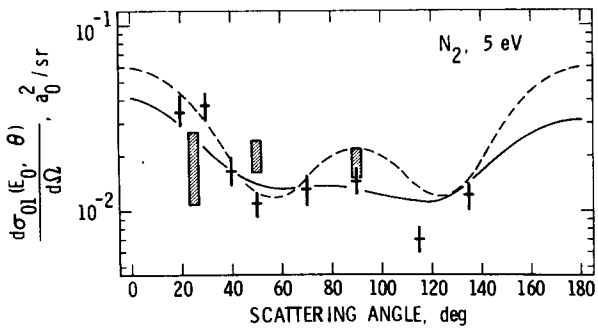

FIG. 3. Absolute differential cross section $d\sigma_{01}(E_0,\theta)/d\Omega$ for e^-–N_2 vibration excitation ($v=0$ to $v'=1$) at 5 eV. Notations are same as in Fig. 1. The present ratio estimates and those of Ref. 5 were placed on the absolute scale by use of the absolute elastic differential cross sections of Ref. 12.

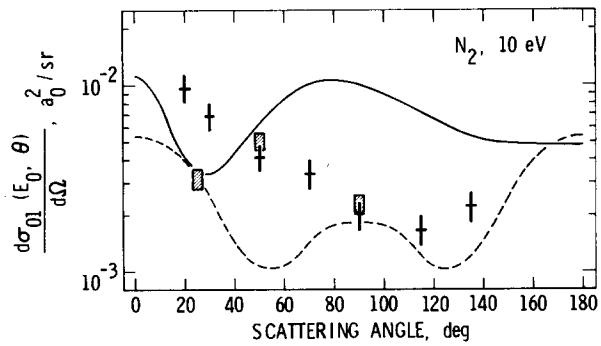

FIG. 4. Same as Fig. 3 but at 10 eV incident energy.

from Ref. 5, Fig. 2 by interpolation. Their sizes indicate our estimates of the errors due to interpolation. The agreement between the interpolated values and the present results is good to satisfactory to 90° and 50°, but poor at 20°–25°. This disagreement at low angles is difficult to reconcile. There are two important sources of systematic error that could be present. First, parent beam contributions would lower the ratio $R_1(E_0,\theta)$ over its true value. In the present experiments this contribution has been measured and a correction has been made. Second, possible nonlinearities in detector–amplifier–multichannel scalar counting efficiencies could lead to erroneous ratios $R_1(E_0,\theta)$ in the range 10^{-2}–10^{-3}. This effect was investigated at 10 eV, 20° and it was found that R_1 was independent of count rate for elastic scattering count rates of 0.25–11.8 kHz, a range which included rates encountered in the present data.

In order to obtain "experimental" values of σ_{01} and σ_{01}^m we had to extrapolate $d\sigma_{01}/d\Omega$ to 0° and 180° and integrate. The extrapolations were done assuming the experimental (exp) differential cross sections had the theoretical (th) *shapes* in those regions, e.g.,

$$\frac{d\sigma_{01}^{\text{exptl}}(E_0,\theta)}{d\Omega} = \frac{d\sigma_{01}^{\text{theor}}(E_0,\theta)}{d\Omega} \times \frac{d\sigma_{01}^{\text{exptl}}(E_0,20°)}{d\Omega}\left[\frac{d\sigma_{01}^{\text{theor}}(E_0,20°)}{d\Omega}\right]^{-1}.$$

Thus we obtain two different sets of experimental in-

TABLE V. Experimental and quantum mechanical values of $R_1(E_0,\theta)$ and $d\sigma_{01}(E_0,\theta)/d\Omega$ for pure vibrational excitation of N_2 at 5 and 10 eV.

	$R_1(E_0,\theta)$ (10^{-3})						$\frac{d\sigma_{01}(E_0,\theta)}{d\Omega}$ (10^{-3} a_0^2/sr)					
θ(deg)	Experiment		Theory						Theory			
			Present		Chandra–Temkin		Experiment		Present		Chandra–Temkin	
	5 eV[a]	10 eV[a]	5 eV	10 eV	5 eV	10 eV	5 eV[b]	10 eV[b]	5 eV	10 eV	5 eV	10 eV
0	···	···	2.16	0.537	8.30	0.43	···	···	41.7	11.2	58.9	5.36
10	···	···	2.39	0.564	7.48	0.43	···	···	37.1	8.00	54.6	5.00
20	6.50	1.16	2.37	0.452	5.58	0.39	34.4	9.61	28.7	4.13	43.9	3.93
30	6.68	0.919	2.34	0.571	3.68	0.28	37.4	6.89	21.9	3.39	30.4	2.50
40	3.25	···	2.39	1.15	2.35	0.19	16.7	···	16.9	4.32	18.6	1.43
50	2.69	0.815	2.70	2.76	1.83	0.18	11.0	4.11	13.9	6.35	12.5	1.07
60	···	···	3.48	5.99	2.25	0.25	···	···	13.1	8.49	12.1	1.07
70	5.39	1.26	4.55	9.56	3.89	0.52	13.1	3.37	13.4	10.0	15.7	1.43
80	···	···	5.11	9.58	6.50	0.99	···	···	13.7	10.6	20.0	1.79
90	9.56	1.57	4.56	6.75	8.61	1.21	14.7	2.02	13.3	10.1	21.8	1.79
100	···	···	3.51	4.26	8.68	1.11	···	···	12.4	9.03	20.0	1.79
110	···	···	2.60	2.72	6.92	0.71	···	···	11.4	7.83	15.7	1.43
115	4.47	0.841	2.29	2.19	···	···	7.02	1.68	11.2	7.21	···	···
120	···	···	2.08	1.79	5.21	0.42	···	···	11.3	6.64	12.1	1.07
130	···	···	1.96	1.26	5.13	0.35	···	···	12.8	5.76	12.5	1.07
135	5.35	0.657	2.01	1.08	···	···	12.2	2.23	14.3	5.44	···	···
140	···	···	2.11	0.947	7.20	0.40	···	···	16.3	5.19	18.6	1.43
150	···	···	2.40	0.766	11.0	0.62	···	···	21.2	4.90	30.4	2.50
160	···	···	2.67	0.671	15.2	0.88	···	···	26.2	4.83	43.9	3.93
170	···	···	2.88	0.622	18.2	1.06	···	···	30.0	4.83	54.6	5.00
180	···	···	2.96	0.606	19.4	1.12	···	···	31.5	4.82	58.9	5.36

[a]Errors (one standard deviation) at 5 and 10 eV are 9% ($^{+20}_{-9}$% at 20°) and ±11%, respectively.
[b]Errors at 5 and 10 eV are ±17% ($^{+25}_{-17}$% at 20°) and ±19%, respectively.

TABLE VI. Integral and momentum-transfer cross sections (a_0^2) for vibrational excitation.

	Extrap.[a]	σ_{01}	σ_{01}^m
$E_0 = 5$ eV			
Theory			
Chandra–Temkin		0.259	0.259
Present		0.195	0.190
Experiment			
Present	Chandra–Temkin	0.205	0.197
Present	Present	0.189	0.167
Present	Average	0.197	0.182
$E_0 = 10$ eV			
Theory			
Chandra–Temkin		0.0196	0.0196
Present		0.0924	0.0909
Experiment			
Present	Chandra–Temkin	0.0449	0.0382
Present	Present	0.0412	0.0282
Present	Average	0.0430	0.0332

[a]Extrapolation column tells which theoretical cross sections were used to extrapolate experimental ones to 0° and 180°.

tegral and momentum-transfer cross sections, depending upon whether the Chandra–Temkin or the present theoretical calculations are used to extrapolate. The two sets are presented and compared to theory in Table VI. For discussion purposes we will consider the experimental result to be the average of these two extrapolations; this is also given in Table VI.

V. DISCUSSION OF VIBRATIONAL-EXCITATION CROSS SECTIONS

Comparison of the two theoretical calculations to each other and to experiment provides some surprises. Both calculations of $d\sigma_{01}/d\Omega$ agree reasonably well with each other and with the available experiments at 5 eV. This is surprising because of the important differences in the calculations and in the results for elastic scattering and rotational excitation. Apparently $d\sigma_{01}/d\Omega$ is less sensitive to these differences than is $d\sigma_{00}/d\Omega$ or σ_{0002}. At 10 eV, however, the results are quite different. The present value of σ_{01} is 4.7 times larger than Chandra and Temkin's value at 10 eV. The present result might have been expected to be larger than theirs because of the larger value of α_{10} (in fact, if the long-range spherically averaged polarization potential dominated the interaction, as assumed by Breig and Lin, the cross section in first-order perturbation theory would be proportional to α_{10}^2 and the present value of σ_{01} would be expected to be 11.3 times larger than Chandra and Temkin's) but this factor is apparently not too important or is cancelled by another factor since at 5 eV the present σ_{01} is only 0.75 times that obtained by Chandra and Temkin. Thus the cross section calculated by Chandra and Temkin at 10 eV is apparently too low because only the π_g symmetry is included. The present comparison of their result to experiment is not really a test of their complete method, rather it is a test of how well one can do including only the symmetry which is resonant at lower energy. The present theoretical result at 10 eV is 2.15 times greater than experiment, which in turn is 2.19 times larger than the result of the Chandra–Temkin calculation. Thus both integral cross sections are in reasonably good agreement with experiment. The differential cross sections for vibrational excitation are quite different and neither agrees very well with experiment. We expect the Chandra–Temkin calculation will agree better with experiment when the other symmetries are included.

We have pointed out in other articles that the experimental differential cross sections are subject to larger errors than the ratios of differential cross sections. The same is true of the present results. Thus the figures showing $R_1(E_0, \theta)$ are particularly interesting. At 5 eV the Chandra–Temkin calculation of $R_1(E_0, \theta)$ seems to agree better with experiment than does the present calculation; neither calculation agrees as well with the experimental $R_1(10\text{ eV}, \theta)$. The ratios $\sigma_{01}(10\text{ eV})/\sigma_{01}(5\text{ eV})$ and $\sigma_{01}^m(10\text{ eV})/\sigma_{01}^m(5\text{ eV})$ are also interesting: the experimental values are 0.22 and 0.18, respectively. Chandra and Temkin calculated 0.08 and 0.08, respectively, and the present calculations yield 0.47 and 0.48, respectively. Thus the predicted energy dependences of the integral cross sections are quite different and neither agrees with experiment within a factor of 2.

Convergence of the laboratory-frame close-coupling expansion of the wavefunction may actually be quite slow. Thus the results of the four-state laboratory-frame close-coupling expansion (used here) may differ appreciably from a converged close-coupling calculation. In this case it may be useful to consider the present approximation not as a truncated close-coupling approximation but rather as a unitarized distorted-wave-type calculation which includes the nonspherical distortion in the initial and final states and treats the coupling and back coupling between these states, including degeneracies, to infinite order. Since the distorted wave approximation is a basic one in all fields of scattering, it deserves wide testing of its detailed limits of applicability. In our opinion, the few-state close-coupling approximation represents a logical and consistent next higher order of approximation and it too deserves testing. The present results at 5 and 10 eV and our previous results[22,25] at 30–75 eV show that while the four-state close-coupling approximation can account for many of the qualitative features of the scattering, it is not accurate enough for many quantitative purposes, at least for the present choice of polarization potential and neglecting exchange.

Note added in proof: Chandra and Temkin have now calculated $d\sigma_{01}/d\Omega$ by their hybrid theory including the contributions of nonresonant symmetries. Their results will be published soon in this journal.

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