PHYSICAL REVIEW A VOLUME 35, NUMBER 2 JANUARY 15, 1987

Total cross sections for high-energy electron scattering by H_2 ($^1\Sigma_g^+$), N_2 ($^1\Sigma_g^+$), and O_2 ($^3\Sigma_g^-$)

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(Received 23 December 1985; revised manuscript received 20 May 1986)

Total inelastic cross sections are calculated for collisions of ground-state H_2, N_2, and O_2 with fast electrons according to the revised Bethe theory given by Inokuti *et al.* The asymptotic forms of the total elastic-scattering cross sections in the first Born approximation due to Inokuti and McDowell and including an electron exchange correction are also evaluated for these molecules. For H_2, various accurate configuration-interaction wave functions are used to compute the total inelastic and the integral elastic-scattering cross sections. Good agreement between theory and experiment is found for the total cross sections (inelastic and elastic) for high incident energies as well as incident energies near 1 keV. The cross sections are also given for N_2 and O_2. Since there are no experimental reports for the integral elastic cross section for N_2 or O_2 at very high incident energies, the comparison is made only for the experimental data at incident energies near 1 keV. It is found that the theoretical results overestimate the experimental data by about 30% for N_2. However, the Bethe total inelastic cross sections are in good agreement with experiments. Since the Born-Bethe approximation may not be valid at lower incident energies, more accurate experimental data at very high incident energies are required for valid comparison with the theoretical results reported here.

I. INTRODUCTION

The electron-atom and electron-molecule scattering processes which occur in many areas of physics, for example, astrophysics, radiation physics, etc., have been studied for many decades.[1,2] Due to the complicated interactions between atomic or molecular targets and incident electrons, there are very few accurate theoretical studies for targets containing more than two electrons.[3,4] Recently, anomalous inelastic-electron-scattering phenomena have been observed[5] when irradiating atoms with high-intensity laser beams. Currently this study is of considerable interest[6] in laser and plasma physics. The singly charged positive-ion formation from this multiphoton ionization process has been demonstrated[6] to resemble closely the stepwise ionization of atoms by electron impact. In order to understand this new phenomenon a better understanding of electron-impact ionization of atoms and molecules is a prerequisite condition. Therefore the study[3] of the total inelastic cross section has become an important topic. Due to the non-spherically-symmetric charge density in molecules, substantially different interactions between atoms and molecules with fast electrons are expected. The differences have recently[7,8] been demonstrated for collisions of fast electrons with He and H_2. The theoretical study of inelastic scattering by molecules is much less complete[3] than that of inelastic scattering by atoms. This situation is also true in the theoretical study of elastic scattering. It is difficult to obtain complete inelastic-scattering experimental data for comparison with the theoretical total inelastic cross section.[3,9,10] However, recently total-cross-section measurements for molecules at incident energies near 1 keV have been obtained with an uncertainty of a few percent.[11] Although the Born-Bethe approximation[3,12] is known to be valid for describing the *e*-atom or *e*-molecule scattering processes at high incident energies, Inokuti and McDowell[12] showed that the revised theory is quite valid for some simple atoms at incident energies near the keV region. Therefore it is quite interesting and worthwhile to present this theoretical total cross section for comparison with all the available experimental data. In general the scattering process consists of three major processes: ionization, discrete excitations (including dissociation), and elastic scattering. For H_2, in the incident energy region greater than 300 eV, van Wingerden *et al.*[13] showed that the summed cross sections from these three scattering processes are in good agreement with the total cross sections measured directly in Ramsauer-type experiments (the experimental accuracy is better than 4%). In the present work a computer program has been written for calculating the Bethe total inelastic cross sections. By combining the previous program written for elastic scattering,[8] the total cross section can be calculated for a homonuclear diatomic molecule. In order to evaluate the total inelastic cross section, the x-ray incoherent scattering factors at small momentum transfers are accurately calculated by the expansion method developed previously.[8] Atomic units are used throughout this work except where explicitly indicated otherwise.

II. THEORETICAL BACKGROUND

A. Elastic scattering

The total elastic-scattering cross section for electrons on atoms or molecules in the first Born approximation is given by[8,12,14]

$$\sigma^{\mathrm{el}}=\frac{\pi}{k_0^2}(A+B/k_0^2+C/k_0^4+\cdots), \tag{1}$$

where A for homonuclear diatomic molecules can be written as

$$A=\int_0^\infty \frac{d\sigma^{\text{el}}}{d\Omega}dQ \ , \tag{2}$$

$Q=K^2$, and B and C are defined in Ref. 12 for electron-atom scattering. Atomic values for B and C with an electron exchange correction have been calculated by Byrne;[14] the molecular values of B and C have been approximated by sums of atomic values in this work. k_0^2 is the incident electron energy in rydbergs, K is the momentum transfer, and $d\sigma^{\text{el}}/d\Omega$ is the differential elastic-scattering cross section defined in Ref. 8 for a homonuclear diatomic molecule. Note that the constant A defined in Ref. 8 should read as Eq. (2) above.

B. Inelastic scattering

The Bethe total inelastic cross section for atoms and molecules colliding with fast electrons given by Inokuti *et al.*[3,15] is

$$\sigma^{\text{inel}}=\frac{4\pi a_0^2}{k_0^2}[S(-1)\ln(k_0^2)+S(-1)\ln 4-2L(-1)+I_1-I_2+\gamma_{\text{tot}}/k_0^2] \tag{3}$$

with $S(-1)$ the total oscillator strength moment $(=\frac{1}{3}[\langle r^2\rangle+4\langle x_1x_2\rangle+2\langle z_1z_2\rangle])$,

$$L(-1)=\frac{d}{d\mu}S(\mu)\,|_{\mu=-1} \ , \tag{4}$$

$$I_1=\int_1^\infty S_{\text{inc}}(K)dQ/Q^2 \ , \tag{5}$$

$$I_2=\int_0^1 [S(-1)-S_{\text{inc}}(K)/Q]dQ/Q \ , \tag{6}$$

and

$$\gamma_{\text{tot}}=2Z\left[-\frac{7}{4}+\ln\left[\frac{B_e}{k_0^2}\right]\right] , \tag{7}$$

where

$$S_{\text{inc}}(K)=F_{\text{tot}}^{\text{x ray}}(K)-F_{\text{coh}}(K) \ , \tag{8}$$

$F_{\text{tot}}^{\text{x ray}}(K)$ is the total x-ray scattering factor, $F_{\text{coh}}(K)$ is the x-ray coherent scattering factor, B_e is the average binding energy of the target, and $2Z$ is the number of electrons in the target. The theory has been used for calculating total inelastic cross sections[9,10] for H_2 and H_2^+ colliding with fast charged particles. Due to the difficulty in evaluating $L(-1)$, I_1, and I_2 for molecules, there has been very little progress in applying this theory to other molecules. Since the early calculations,[16] some better computational methods[17-19] have become available to evaluate the x-ray incoherent scattering factors. Therefore the values of I_1 and I_2 can be computed accurately.

III. COMPUTATIONAL DETAILS AND RESULTS

A. Elastic scattering

In order to evaluate the integral A defined in Eq. (1), the integral is divided into two parts,

$$A=A_1+A_2$$

where

$$A_1=2\int_0^{K_{\text{max}}}\frac{d\sigma^{\text{el}}}{d\Omega}K\,dK \ ,$$

$$A_2=2\int_{K_{\text{max}}}^\infty \frac{d\sigma^{\text{el}}}{d\Omega}K\,dK \ ,$$

and K_{max} is set to be an arbitrarily large value such that the value of A_2 is less than 1% of A. The integral A_1 is numerically evaluated and the integral A_2 approximated by the independent-atom-model theory[2] as follows:

$$A_2=\int_{K_{\text{max}}}^\infty 8[Z-F(K)]^2[1+\sin(KR)/KR]\frac{dQ}{Q^2} \ , \tag{9}$$

where $F(K)$ is the x-ray scattering factor for the atom with the atomic number Z and R is the internuclear distance. Notice that a vibrational damping factor $e^{-l^2K^2/2}$ where l is the root-mean-square amplitude of vibration for diatomic molecules, should be included in the term $\sin(KR)/KR$ in Eq. (9), when the thermal vibrational averaging is considered. The value of A_2 can be further approximated by

$$A_2=4Z^2\left[\frac{1}{K^2}-\frac{4R^2}{3}\sin(KR)\left[\frac{4!}{(KR)^5}-\frac{6!}{(KR)^7}+\cdots\right]+\cos(KR)\left[\frac{3!}{(KR)^4}-\frac{5!}{(KR)^6}+\frac{7!}{(KR)^8}+\cdots\right]\right]\Bigg|_{K=K_{\text{max}}} , \tag{10}$$

where $F(K)$ in Eq. (9) is negligibly small compared to Z when $K=K_{\text{max}}$. When the thermal vibrational averaging is taken at sufficiently large K, $A_2\approx 4Z^2/K^2$. The values of A for H_2, N_2, and O_2 are given in Table I. Notice that

TABLE I. The values of the parameters defined in Eq. (1) for evaluating the elastic-scattering cross section. See Sec. III A for details of evaluation of A.

	A			
	HF	CI	B	C
H_2	4.26[a]	4.21[b]		
N_2	125[c]	122[d]		
2N	109.10[e]		−478.06[e]	669.34[e]
O_2	131.0[f]			
2O	116.98[e]		−606.62[e]	964.20[e]

[a] Calculated using the DJ-SCF wave function (see Ref. 20).

[b] Calculated using the DJ-CI wave function (see Ref. 20).

[c] Calculated using the Cade-Wahl wave function (see Ref. 21).

[d] Calculated using the Walter Stevens wave function (see Ref. 8). (Notice that the value of A for N_2, given in Ref. 8, is 127. This was estimated as follows. K_{max} was set to 30 a.u. and A_2 was estimated by doubling the difference between A and a given in Ref. 12.)

[e] See Ref. 14, all the values are in the HF accuracy.

[f] Calculated using the Cade-Wahl wave function (see Ref. 21).

TABLE II. Comparison between direct numerical calculation and calculation using the expansion method for $F_{\text{two}}(K)$, C_1. (a) N_2, Hartree-Fock, $\int \Gamma(\mathbf{r}_1,\mathbf{r}_2,R)d\mathbf{r}_1 d\mathbf{r}_2=90.9898$, $\int \rho(\mathbf{r}_1,R) =13.999\,216\,4$. (b) H_2, minimum basis set at $R=1.4$ a.u. $\int \Gamma(\mathbf{r}_1,\mathbf{r}_2,R)d\mathbf{r}_1,d\mathbf{r}_2 =0.999\,999\,980\,38$, $\int \rho(\mathbf{r},R)d\mathbf{r}=0.999\,999\,990\,19$.

$\frac{1}{2}KR$	$F_{\text{two}}(K)$ a	$F_{\text{two}}(K)$ b	$F_{\text{two}}(K)$ c	C_1' [d]	$C_1-C_2K^2$
		(a)			
0.10	180.3421	180.3421	180.36		2.6585
0.20	175.5311	175.5313	175.55	1.6152	2.6107
0.30	167.8396	167.8402	167.86	2.3970	2.5311
0.40	157.7188	157.7171	157.74	2.4723	2.4195
		(b)			
0.10	1.965 396 97	1.965 397 00		0.8536	0.8536
0.20	1.865 723 73	1.865 721 02		0.8340	0.8330
0.30	1.712 460 09	1.712 364 76		0.8029	0.7987
0.40	1.521 969 60	1.520 962 59		0.7626	0.7507

[a] The present calculation according to Eq. (15).

[b] The present calculation according to Eq. (16).

[c] Values given in Ref. 22.

[d] Computed from Eq. (14).

the effects of the partial-wave expansion on the elastic-scattering factors are not considered for all the scattering angles.

B. Inelastic scattering

In the present work a computer program has been written to calculate the x-ray incoherent scattering factors for homonuclear diatomic molecules using a molecular wave function expanded in basis sets of Slater-type functions (STF's) or elliptical-type functions. The computational technique is given elsewhere.[17,18] To evaluate I_2, the expansion method[9] for small K is used. I_2 can be divided into two parts,

$$I_2=\int_{K=K_\epsilon}^{1}[S(-1)-S_{\text{inc}}(K)/Q)]dQ/Q + C_1K_\epsilon^2-\tfrac{1}{2}C_2K_\epsilon^4\,, \tag{11}$$

where

TABLE III. Parameters needed in Eq. (3) for evaluating the total inelastic-scattering cross section for H_2.

Wave function	$R\,(a_0)$	$-E$ (hartree)	$\left\langle \frac{1}{r_{12}} \right\rangle$	$\frac{1}{3!}\langle r_{12}^2\rangle$	$\frac{1}{4!}\langle(\mathbf{K}\cdot\mathbf{r}_{12})^4\rangle_{\Gamma,\hat{\mathbf{K}}}$	$\frac{1}{6!}\langle(\mathbf{K}\cdot\mathbf{r}_{12})^6\rangle_{\Gamma,\hat{\mathbf{K}}}$
SCF-DJ[a]	1.4009	1.333 624	0.658 42	0.858 41	0.444 36	0.179 26
SCF-Liu[b]	1.400	1.134	0.6605	0.8579	0.4434	0.1779
CI-DJ[a]	1.4009	1.173 032	0.589 82	0.928 32	0.474 37	0.175 38
CI-Liu[b]	1.400	1.174	0.5898	0.9301	0.4760	0.1755
KMS[c]	1.4009	1.174 434	0.587 39	0.938 45		
KW[d]	1.400	1.174 474	0.587 366	0.938 73		
	C_1	C_2	$S(-1)$	I_1	I_2	I_1-I_2
SCF-DJ	0.6495	0.3665	1.7168	1.5430	1.7337	0.8093
SCF-Liu	0.8807	0.3639	1.7159	1.5578	1.7392	0.8186
CI-DJ	0.7858	0.3578	1.5395	1.4683	0.6362	0.8321
CI-Liu	0.7838	0.3435	1.5389	1.4700	0.6248	0.8452
KMS				1.4505[f]	0.6380	0.8125
KW			1.5177			
			1.5487[e]			

[a] See Ref. 20.

[b] Bowen Liu (private communication).

[c] The values quoted in B. S. Sharma and A. J. Thakkar, J. Phys. B **17**, 3405 (1984) (see Table I) are taken; also see Ref. 19.

[d] See footnote c and W. A. Kolos and L. Wolnewicz, J. Chem. Phys. **43**, 2429 (1965).

[e] The value quoted in Ref. 9, for details see L. Wolniewicz, J. Chem. Phys. **45**, 515 (1966).

[f] The values of I_2 for integrating from $K=0$—0.2 a.u. is approximated to 0.0310 a.u. obtained from CI-Liu wave function and the rest of the integral, I_2 is calculated using the value $S(-1)=1.5177$ a.u. (see footnote d) and the x-ray incoherent scattering factors given in Ref. 19.

$$C_1=\tfrac{1}{3}\langle(\mathbf{K}\cdot\mathbf{r}_1)^2(\mathbf{K}\cdot\mathbf{r}_2)^2\rangle_{\Gamma,\hat{\mathbf{K}}}-\tfrac{1}{4}\langle(\mathbf{K}\cdot\mathbf{r}_1)^3(\mathbf{K}\cdot\mathbf{r}_2)\rangle_{\Gamma,\hat{\mathbf{K}}}$$
$$+\tfrac{1}{12}\langle(\mathbf{K}\cdot\mathbf{r})^4\rangle_{\hat{\mathbf{K}}}-\tfrac{1}{4}\langle(\mathbf{K}\cdot\mathbf{r})^2\rangle^2_{\hat{\mathbf{K}}}\,, \tag{12}$$

$$C_2=\tfrac{1}{360}\langle(\mathbf{K}\cdot\mathbf{r})^6\rangle_{\hat{\mathbf{K}}}+\tfrac{1}{60}\langle(\mathbf{K}\cdot\mathbf{r}_1)^5(\mathbf{K}\cdot\mathbf{r}_2)\rangle_{\Gamma,\hat{\mathbf{K}}}$$
$$-\tfrac{1}{24}\langle(\mathbf{K}\cdot\mathbf{r}_1)^4(\mathbf{K}\cdot\mathbf{r}_2)^2\rangle_{\Gamma,\hat{\mathbf{K}}}$$
$$+\tfrac{1}{36}\langle(\mathbf{K}\cdot\mathbf{r}_1)^3(\mathbf{K}\cdot\mathbf{r}_2)^3\rangle_{\Gamma,\hat{\mathbf{K}}}$$
$$+\tfrac{1}{24}\langle(\mathbf{K}\cdot\mathbf{r})^2\rangle_{\hat{\mathbf{K}}}\langle(\mathbf{K}\cdot\mathbf{r})^4\rangle_{\hat{\mathbf{K}}}\,. \tag{13}$$

K_ϵ is set to be an arbitrary small value, e.g., 0.2 a.u., such that I_2 can be accurately evaluated, $\langle\ \rangle_{\hat{\mathbf{K}}}$ and $\langle\ \rangle_{\Gamma,\hat{\mathbf{K}}}$ denote

$$(1/4\pi)\int\int d\hat{\mathbf{K}}\,d\mathbf{r}\,\rho(\mathbf{r},R)$$

and

$$(1/4\pi)\int\int\int d\hat{\mathbf{K}}\,d\mathbf{r}_1 d\mathbf{r}_2\Gamma(\mathbf{r}_1\mathbf{r}_2,R)\,,$$

respectively, and $\rho(\mathbf{r},R)$ and $\Gamma(\mathbf{r}_1,\mathbf{r}_2,R)$ are the one-electron and two-electron densities, respectively. C_1 and C_2 can be expressed in terms of the electronic moments (see Appendix A). Notice that when K is sufficiently small, $K\approx K_\epsilon$, and the two-electron density is properly normalized, C_1 expressed in terms of moments in Eq. (12) is approximately equal to the value of C_1', where

$$C_1'=[S(-1)-S_{\text{inc}}(K)/Q]/Q\mid_{K=K_\epsilon}\,. \tag{14}$$

The two-electron scattering factor $F_{\text{two}}(K)$ can be defined and written as

$$F_{two}(K)=F_{\text{tot}}^{\text{x ray}}(K)-2Z$$
$$=\frac{1}{4\pi}\int\int\int\Gamma(\mathbf{r}_1,\mathbf{r}_2,R)e^{i\mathbf{K}\cdot\mathbf{r}_{12}}d\mathbf{r}_1 d\mathbf{r}_2 d\hat{\mathbf{K}}\,. \tag{15}$$

The values at small K can be rewritten as

$$F_{\text{two}}(K)=2Z(2Z-1)-\frac{1}{2!}\langle(\mathbf{K}\cdot\mathbf{r}_{12})^2\rangle_{\Gamma,\hat{\mathbf{K}}}$$
$$+\frac{1}{4!}\langle(\mathbf{K}\cdot\mathbf{r}_{12})^4\rangle_{\Gamma,\hat{\mathbf{K}}}$$
$$-\frac{1}{6!}\langle(\mathbf{K}\cdot\mathbf{r}_{12})^6\rangle_{\Gamma,\hat{\mathbf{K}}}+\cdots\,. \tag{16}$$

Equation (16) can be used to check the accuracy of the calculation according to Eq. (15). In Table II the values $F_{\text{two}}(K)$ at very small K are shown for a few systems. The values for $S(-1)$, I_1, I_2, C_1, and C_2, are given in Tables III and IV.

IV. COMPARISON WITH EXPERIMENTS

A. H_2

Ever since the early calculation[9] of the Bethe total inelastic cross section for H_2, efforts have been made to extend the theoretical result to low-incident-energy collisions.[24] It was suggested[24] that the values of (I_1-I_2) reported[9] earlier may be too large. In the present work the values of (I_1-I_2) are given for various wave functions of H_2. In Table III, it is shown that the effect of electron correlations on I_1-I_2 is not very important. The value computed using the accurate configuration-interaction (CI) wave function is not very different from the values calculated using the self-consistent-field (SCF) wave function. The improvement over the value previously computed from the two-term CI wave function[25] is not significant but the present value does differ from the value computed from the five-term CI wave function.[26] Neglecting the correction due to thermal vibration and using the accurate value[19] of I_1-I_2 given in Table III, the Bethe total inelastic cross section can be written as

$$\sigma^{\text{inel}}=\frac{4\pi a_0^2}{k_0^2}[1.5487\ln(k_0^2)+2.4036+\gamma_{\text{tot}}/k_0^2]\,. \tag{17}$$

Neither the value 2.4036 given in the present work, nor 2.2212 quoted in Ref. 9 is in agreement with the value 1.53 given in Ref. 24.

The differential elastic-scattering cross section for H_2 computed earlier[18] by using the Davidson and Jones (DJ) CI wave function[20] is almost identical to the most accurate value reported by Kolos *et al.* (KMS).[19] Therefore the former is sufficiently accurate to evaluate the constant A. The total elastic-scattering cross section can be written as

$$\sigma^{\text{el}}=\frac{\pi}{k_0^2}(4.2106-2/k_0^2)\,. \tag{18}$$

The integral elastic cross section $\sigma^{\text{el}}=0.00789\pm0.000\,10$ a.u.^{2} at 25 keV reported by Ulsh, Wellenstein, and Bonham[27] is in good agreement with the present theoretical value of Eq. (18). Their reported incoherent

TABLE IV. Parameters needed in Eq. (3) for evaluating the total inelastic-scattering cross section for N, O, N_2, and O_2.

	Wave function	$R\,(a_0)$	C_1	C_2	$S(-1)$	$L(-1)$	I_1	I_2	I_1-I_2
N_2	HF[a]	2.068	2.6745	1.7035	6.0895		6.7370	2.2676	4.4694
2N	CI				5.134[c]	2.7732[b]	6.414[c]	2.036[c]	4.378[c]
N_2					4.747[b]	3.091[b]			
O_2	HF[a]	2.282	2.0171	1.2968	5.9758		7.0429	2.9245	4.1184
2O	CI				4.648[c]	2.6512[b]	6.512[c]	1.504[c]	5.008[c]
O_2					4.652[b]	2.7853[b]			

[a] The present calculation in the Hartree-Fock approximation.

[b] Zeiss *et al.* (see Ref. 23).

[c] Inokuti and co-workers (see Ref. 3).

TABLE V. Total inelastic σ^{inel}, integral elastic σ^{el}, and total σ^{tot} cross sections for H_2 (units of 10^{-16} cm^2).

k_0^2 (eV)	σ^{el}	$\sigma^{\text{el}^{\text{a}}}$	σ^{inel}	σ^{tot}	$\sigma^{\text{tot}^{\text{b}}}$	$\sigma^{\text{tot}^{\text{c}}}$
100.0	0.471	0.89	2.401	2.872	2.56±0.3	2.52
150.0	0.321	0.52	1.852	2.173	1.98±0.1	2.00
200.0	0.244	0.36	1.514	1.758	1.69±0.03	1.61
300.0	0.164	0.23	1.122	1.287	1.27±0.03	1.22
400.0	0.124	0.15	0.900	1.024	1.04±0.03	0.97
500.0	0.099	0.12	0.755	0.855	0.87±0.02	0.83
600.0	0.083		0.653	0.736		0.71
700.0	0.071	0.073	0.577	0.648		0.64
750.0	0.067		0.546	0.612		0.60
800.0	0.062		0.518	0.580		
1000.0	0.050	0.050	0.431	0.481		
2000.0	0.025	0.027	0.242	0.267		

[a] Reference 28.
[b] Reference 29.
[c] Reference 13.

scattering factors for H_2 are also in good agreement with the accurate theoretical values reported here and elsewhere.[7,9,17–19] In order to see if the Born-Bethe approximation[3,12] is valid for describing the total collision processes at lower incident electron energies, in Table V the total cross sections (integral elastic and total inelastic) are shown for comparison with experiments. Notice that the integral elastic-scattering cross sections reported by van Wingerden *et al.*[28] have a 10% uncertainty. Therefore, the integral elastic-scattering cross sections[28] and the total cross sections[13,29] agree very well with the present theoretical calculation for incident energies near 1 keV.

B. N_2

Due to the fact that accurate wave functions of N_2 are not available even for the ground state (e.g., a target wave function with at least 75% correlation energy), accurate values for the parameters in Eq. (3) for evaluating the total inelastic cross section are not easily obtained. Zeiss *et al.*[23] made an extensive study using the Thomas-Reiche-Kuhn sum rule to obtain accurate values of $S(-1)$, $L(-1)$ for a few diatomic molecules. Their values are more accurate than those of Kosman and Wallace (KW) (Ref. 30) who studied N_2 using multiple scattering theory, and the Hartree-Fock (HF) level values calculated here because the latter calculations omit the effect of electron correlations. According to the calculation for H_2 and for some other atoms,[3] the effect of electron correlations on I_1-I_2 is not very important compared with the effect on the other parameters in Eq. (3). We assume this to be true for the other diatomic molecules studied here. By using the values of $S(-1)$ and $L(-1)$ given by Zeiss *et al.*, the total inelastic cross section is written as

$$\sigma^{\text{inel}}=\frac{4\pi a_0^2}{k_0^2}[4.742\ln(k_0^2)+4.8612+\gamma_{\text{tot}}/k_0^2]\ . \qquad (19)$$

There is no experimental integral elastic cross section for N_2 at very high incident energies; some experimental data[31,32] for the differential cross sections at small scattering angles exist but this is not sufficient to estimate the integral elastic cross sections. However, there are experimental data[33,34] available at incident energies near 1 keV. In Fig. 1(a) the theoretical results in the HF approximation are shown to be too large by 30% as compared to the experimental data[33,34] and other theoretical results.[35] The disagreement is probably due to the failure of the Born theory for collisions at low incident energy. In order to know the accuracy of the calculated Bethe total inelastic cross section, comparisons with high-energy data will be necessary. The total cross sections made up of the calcu-

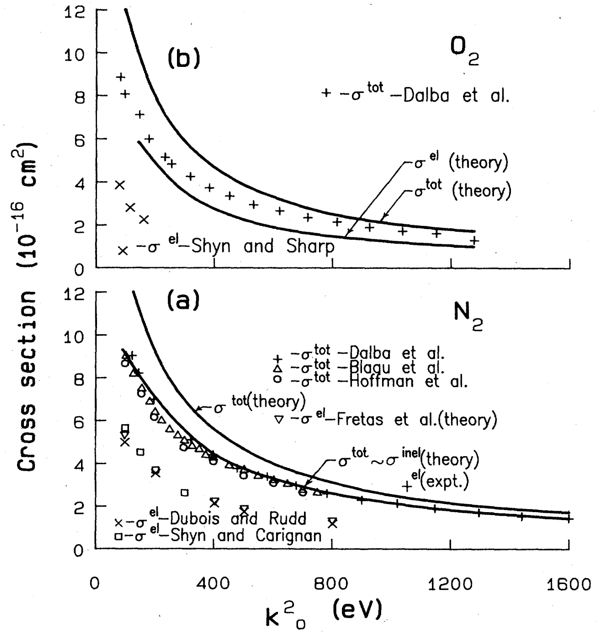

FIG. 1. Total cross section and integral elastic-scattering cross section for N_2 and O_2.

lated Bethe inelastic total cross sections and the experimental integral elastic cross sections are given for comparison with various experimental total cross sections[29,36–38] at incident energies near 1 keV. The experimental values reported by Sueoka and Mori[38] are in good agreement with other experiments[29,36,37] and they are not included in Fig. 1(a) which presents a comparison between theory and experiment. Good agreement is found at incident energies near 1 keV. This implies that the Born-Bethe theory may be adequate to describe the total collision processes at such low incident energies, but as pointed out already, not the separate cross sections.

C. O_2

Here the situation is less clear. O_2 is an open-shell diatomic molecule for which accurate wave functions are not available in the literature. In Table IV the value of $S(-1)$ calculated from the HF molecular wave function of O_2 is slightly smaller than the values reported for N_2. By using the values of $S(-1)$ and $L(-1)$ given by Zeiss *et al.* the values of (I_1-I_2) in the HF approximation, the Bethe total inelastic cross section is written as

$$\sigma^{\text{inel}}=\frac{4\pi a_0^2}{k_0^2}[4.652\ln(k_0^2)+4.9969+\gamma_{\text{tot}}/k_0^2] \; . \tag{20}$$

The total elastic-scattering cross sections for O_2 according to Eq. (1) can be calculated by using the constants A, B, and C given in Table I. There are no experimental data available for either total or integral elastic cross sections for O_2 at very high incident energies. Furthermore there is only one experimental measurement reported for the total cross section[37] and the integral elastic cross section[39] at incident energies near 1 keV. Figure 1(b) shows that the disagreement between theory and experiment at incident energies in the 100-eV range is very similar to the case of N_2. Neither the total cross sections nor the integral elastic cross sections are in agreement with the experimental data.[37,39] This shows again the failure of the Born approximation for O_2.

V. DISCUSSION AND CONCLUSIONS

The Born-Bethe approximation according to Inokuti and co-workers[3,12] is shown to be valid for studying the total cross sections for H_2 from very high incident electron energies to near 1 keV. In applying the theory to N_2 and O_2, the situation is not clear because accurate experimental integral elastic cross section at incident energies above 30 keV are not available. Since the accuracy of $S(-1)$ for N_2 as reported by Zeiss *et al.* and $S_{\text{inc}}(K)$, have been assured by a recent experimental study (private communication[40] from Professor R. A. Bonham), and the error for (I_1-I_2) for N_2 due to the HF approximation will not be more than 4% for incident energies near 30 keV, we believe that the total inelastic cross sections reported here for N_2 are quite accurate. (This assumes that the effect of electron correlation on the form factor is not more than 20%—see also the last papers in Ref. 3 for the assessment of the correlation effect due to the N atoms.) The disagreement between theory and experiment for the total cross section at low incident energies is most probably due to the failure of the first Born approximation for the elastic scattering. Therefore, accurate experimental data for both total cross sections and integral elastic cross sections for N_2 and O_2 at very high incident energies are urgently needed in order to compare with the theoretical values reported here.

ACKNOWLEDGMENTS

The author wishes to thank Professor R. A. Bonham and Professor M. Fink for a copy of Ref. 31 and their continued interest and encouragement during the course of this work, and Professor V. H. Smith, Jr. for unpublished results (Ref. 14). Thanks are also due to Dr. G. C. Lie and Professor A. J. Thakkar for their helpful discussions, and to the Chemistry Department, Indiana University for the use of their computing facilities. Finally, constructive comments from Professor R. A. Bonham are gratefully acknowledged.

APPENDIX: EVALUATION OF THE INTEGRALS C_1 and C_2

$$C_1=(\tfrac{1}{6}a_4+\tfrac{1}{2}\langle r^2\rangle^2-\tfrac{2}{3}\langle x^2\rangle^2$$

$$-\tfrac{4}{3}\langle x^2\rangle\langle z^2\rangle-\tfrac{1}{2}a_{22}+\tfrac{2}{3}a_{31})/5 \; ,$$

$$a_4=2\langle x^4\rangle+\langle z^4\rangle+2\langle x^2y^2\rangle+4\langle x^2z^2\rangle \; ,$$

where

$$a_{22}=\tfrac{4}{3}(2\langle x_1z_1x_2z_2\rangle+\langle x_1y_1x_2y_2\rangle)+2\langle x_1^2x_2^2\rangle+\langle z_1^2z_2^2\rangle+\tfrac{2}{3}(\langle x_1^2y_2^2\rangle+2\langle x_1^2z_2^2\rangle) \; ,$$

$$a_{31}=2(\langle x_1^3x_2\rangle+\langle x_1^2y_1y_2\rangle+\langle x_1^2z_1z_2\rangle+\langle z_1^3z_2\rangle) \; ,$$

$$C_2=(\tfrac{1}{30}b_6+\tfrac{1}{5}b_{15}+\tfrac{1}{3}b_{33}-\tfrac{1}{2}b_{42}+\tfrac{1}{2}b_{24})/42 \; ,$$

$$b_6=\langle z^6\rangle+2\langle x^6\rangle+6(\langle x^2z^4\rangle+\langle x^4z^2\rangle+\langle x^2y^4\rangle+\langle x^2y^2z^2\rangle) \; ,$$

$$b_{24}=\tfrac{1}{5}(\langle r^2\rangle a_4+4\langle z^2\rangle\langle z^4\rangle+8\langle x^2\rangle\langle x^4\rangle-4\langle z^2\rangle\langle x^2y^2\rangle-8\langle x^2z^2\rangle\langle x^2\rangle) \; ,$$

$$b_{15}=\langle z_1^5z_2\rangle+2(\langle x_1^5x_2\rangle+\langle x_1^4z_1z_2\rangle+\langle x_1z_1^4x_2\rangle+\langle x_1^4y_1y_2\rangle+\langle x_1^2y_1^2z_1z_2\rangle)$$

$$+4(\langle x_1^2z_1^3z_2\rangle+\langle x_1^3z_1^2x_2\rangle+\langle x_1^2y_1z_1^2y_2\rangle+\langle x_1^3y_1^2x_2\rangle) \; ,$$

$$
\begin{aligned}
b_{33}=&\langle z_1^3 z_2^3\rangle+2\langle x_1^3 x_2^3\rangle+\tfrac{6}{5}(\langle x_1^2 z_1 z_2^3\rangle+3\langle x_1 z_1^2 x_2 z_2^2\rangle+\langle x_1^3 x_2 z_2^2\rangle+2\langle x_1^2 y_1 y_2 z_2^2\rangle+\langle z_1^3 x_2^2 z_2\rangle\\
&+\langle x_1^2 z_1 y_2^2 z_2\rangle+3\langle x_1^2 z_1 x_2^2 z_2\rangle+\langle x_1 z_1^2 x_2^3\rangle+\langle x_1 z_1^2 x_2 y_2^2\rangle+3\langle x_1^2 y_1 x_2^2 y_2\rangle\\
&+\langle x_1^3 x_2 y_2^2\rangle+\langle x_1^2 y_1 y_2^3\rangle+2\langle x_1 y_1 z_1 x_2 y_2 z_2\rangle)\ ,\\
b_{42}=&\langle z_1^4 z_2^2\rangle+2\langle x_1^4 x_2^2\rangle+\tfrac{12}{5}(\langle x_1^2 z_1^2 z_2^2\rangle+\langle x_1^2 z_2^2 x_2^2\rangle+\langle x_1^2 y_1^2 x_2^2\rangle)\\
&+\tfrac{2}{5}(\langle x_1^4 z_2^2\rangle+\langle z_1^4 x_2^2\rangle+\langle x_1^4 y_2^2\rangle+\langle x_1^2 y_1^2 z_2^2\rangle+\langle x_1^2 z_1^2 y_2^2\rangle+\langle y_1 z_1^3 x_2^2\rangle)\\
&+\tfrac{16}{5}(\langle x_1 z_1^3 x_2 z_2\rangle+\langle x_1^3 z_1 x_2 z_2\rangle+\langle x_1 y_1^2 z_1 x_2 z_2\rangle+\langle x_1 y_1^3 x_2 y_2\rangle)+\tfrac{8}{5}\langle x_1 y_1 z_1^2 x_2 y_2\rangle\ ..PM
\end{aligned}
$$

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