Dependence of electron-impact excitation cross sections on the initial vibrational quantum number in H_2 and D_2 molecules: $X\ ^1\Sigma_g^+ \to B\ ^1\Sigma_u^+$ and $X\ ^1\Sigma_g^+ \to C\ ^1\Pi_u$ transitions

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Electron-impact excitation cross sections have been calculated using the impact-parameter method for $X\ ^1\Sigma_g^+ \to B\ ^1\Sigma_u^+$ and $X\ ^1\Sigma_g^+ \to C\ ^1\Pi_u$ transitions for both H_2 and D_2 molecules as a function of incident energy and of vibrational quantum number v_i. The results show that the cross sections initially increase monotonically with increasing v_i and follow the opposite trend for higher v_i values.

I. INTRODUCTION

The knowledge of electronic excitation cross sections by electron impact, involving vibrationally excited $H_2(v_i)$ and $D_2(v_i)$ molecules, is of paramount importance in understanding the properties of H_2 and D_2 plasmas. In particular, the modeling of H^- and D^- production in multicusp magnetic plasmas requires a complete set of electronic excitation cross sections as a function of vibrational quantum number [1,2].

To our knowledge, accurate data exist only for the ground vibrational level and for the first few vibrational levels of the molecules [3]. On the other hand, complete sets of cross sections for different transitions have been obtained recently by using the modified Gryzinski method [4]. This situation prompted us to utilize a better dynamical approach for calculating the electron-impact excitation cross sections involving all vibrational levels of H_2 and D_2. In particular, in this paper we present complete sets of excitation cross sections for the $X \to B$ and $X \to C$ transitions due to their importance in the modeling of multicusp magnetic discharges.

The $X \to B$ transition for hydrogen has been studied by several authors from both experimental and theoretical points of view [5–17]. The main feature shown by the integral cross sections for $v_i = 0$ is the factor-of-2 discrepancy, not yet well understood, between experimental and theoretical results in the range of 20–60 eV. A common feature of the different *ab initio* calculations on this subject is the use of a single-configuration electronic wave function for both X and B states and the application of

the Franck-Condon approximation that neglects the vibrational motion of the molecule. In the present work, in order to study properly the dependence of the cross sections on vibrational states, we take the nuclear motion into account by use of the adiabatic-nuclei approximation without invoking the Franck-Condon approximation and, moreover, we perform configuration-interaction calculations to obtain accurate electronic wave functions. Thus the present results for $v_i = 0$ can represent a further improvement over the previous cross-section calculations for the $X \to B$ transition.

In this study, since we deal with "optically allowed" electronic transitions, we have calculated the cross sections in the framework of the impact-parameter method [11,14,18–20]. This method is particularly suitable to treat these kinds of transitions because it avoids problems arising in other quantum-mechanical theories, linked to the slow convergence in the partial-wave expansion. Section II describes briefly the so-called modified impact-parameter method, following the formulation given by Hazi [11]. In Sec. III we give some computational details, while the results are reported in Sec. IV. Finally, a summary and the conclusions are presented in Sec. V.

II. METHOD OF CALCULATION

In this section we report the basic formulas utilized in this paper. A complete treatment of the modified impact-parameter method can be found in Ref. [11].

The electronic excitation cross section in the adiabatic-nuclei approximation, for a diatomic molecule initially in the v_ith vibrational state, is given by

$$\sigma_{v_i}^{\alpha_f \alpha_i}(E) = \int d\Omega \sum_{v_f} \frac{k_{v_f}}{k_0} \left| \int_0^\infty dR\ \chi_{v_f}^{\alpha_f}(R) T_{\alpha_f \alpha_i}(k_{v_f}, k_0, \Omega; R) \chi_{v_i}^{\alpha_i}(R) \right|^2 , \tag{1}$$

where E is the incident energy, Ω is the scattering angle, k_0 and k_{v_f} are, respectively, the momenta for the incident and the scattered electron, R indicates the internuclear distance, $\chi_{v_i}^{\alpha_i}(R)$ and $\chi_{v_f}^{\alpha_f}(R)$ are the vibrational wave

functions relative to α_i and α_f electronic states, respectively, and $T_{\alpha_f \alpha_i}$ is the usual T matrix for the electronic transition $\alpha_i \to \alpha_f$ parametrically depending on R. The sum on v_f runs over the bound and continuum vibration-

al levels of the α_f electronic state.

To take into account the nuclear motion, we proceed in the following way. If we consider, in the usual fashion, the small spacing of the vibrational levels, for sufficiently high electron energies we can neglect the dependence of k_{v_f} and of the T matrix on v_f and use the completeness of the vibrational wave functions to obtain, from (1),

$$\sigma_{v_i}^{\alpha_f \alpha_i}(E) = \int d\Omega \frac{k}{k_0} \int_0^\infty dR \, |\chi_{v_i}^{\alpha_i}(R)|^2 |T_{\alpha_f \alpha_i}(k,k_0,\Omega;R)|^2 .$$

$$(2)$$

Setting

$$\sigma^{\alpha_f \alpha_i}(E) = \frac{k}{k_0} \int d\Omega \, |T_{\alpha_f \alpha_i}(k,k_0,\Omega;R)|^2 , \tag{3}$$

Eq. (2) becomes

$$\sigma_{v_i}^{\alpha_f \alpha_i}(E) = \int_0^\infty dR \, |\chi_{v_i}^{\alpha_i}(R)|^2 \sigma^{\alpha_f \alpha_i}(E;R) . \tag{4}$$

The quantity $\sigma^{\alpha_f \alpha_i}(E;R)$ represents the cross section for

a vertical excitation between α_i and α_f electronic states. It has been calculated in the framework of the impact-parameter approximation. In general form it can be expressed by

$$\sigma^{\alpha_f \alpha_i}(E;R) = 2\pi \int_{\rho_0}^\infty P_{\alpha_f \alpha_i}(\rho,E;\Delta E_{\alpha_f \alpha_i})\rho \, d\rho , \tag{5}$$

where $P_{\alpha_f \alpha_i}$ is the transition probability for the process $\alpha_f \to \alpha_i$, $\Delta E_{\alpha_f \alpha_i}$ is the electronic transition energy, ρ is the impact parameter, and ρ_0 is the usual cutoff replacing the lower limit of integration to avoid divergent cross sections. It depends on internuclear distance and it is determined by requiring that for high energies the impact-parameter method and Born approximation give the same cross section [11,14,18,19]. The explicit expression for $\sigma^{\alpha_f \alpha_i}(E;R)$ is given by [11]:

$$\sigma^{\alpha_f \alpha_i}(E;R) = S^{\alpha_f \alpha_i}(R) D^{\alpha_f \alpha_i}(E;R) , \tag{6}$$

where the "structural factor" $S^{\alpha_f \alpha_i}(R)$ and the "dynamical factor" $D^{\alpha_f \alpha_i}(E;R)$ are defined by

$$S^{\alpha_f \alpha_i}(R) = \frac{m^2 e^2}{3 g_i \hbar^4} \sum_{\pm \Lambda_f, \pm \Lambda_i} |M_{\Lambda_f, \Lambda_i}(R)|^2 , \tag{7}$$

$$D^{\alpha_f \alpha_i}(E;R) = \frac{2\pi \hbar^2}{m^2 u_i^2} \left\{ \gamma_i \left[K_0(\gamma_i)K_1(\gamma_i) - \frac{\pi^2}{4} S_0(\gamma_i)S_1(\gamma_i) \right] + \gamma_f \left[K_0(\gamma_f)K_1(\gamma_f) - \frac{\pi^2}{4} S_0(\gamma_f)S_1(\gamma_f) \right] \right.$$

$$+ \gamma \left[K_0(\gamma_i)K_1(\gamma_f) + K_0(\gamma_f)K_1(\gamma_i) + \frac{\pi^2}{4} S_0(\gamma_i)S_1(\gamma_f) + \frac{\pi^2}{4} S_0(\gamma_f)S_1(\gamma_i) \right]$$

$$\left. + \left[\frac{u_i^2 - u_f^2}{u_i^2 + u_f^2} \right] \left[\ln\frac{\gamma_f}{\gamma_i} + \frac{\pi^2}{2} \int_{\gamma_i}^{\gamma_f} S_0(\gamma) d\gamma \right] \right\} . \tag{8}$$

The quantity $M_{\Lambda_f, \Lambda_i}(R)$ in Eq. (7) is the usual electronic dipole transition moment defined as

$$M_{\Lambda_f, \Lambda_i}(R) = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \Psi_{\Lambda_f}^{\alpha_f *}(\mathbf{r}_1, \ldots, \mathbf{r}_N; R)$$

$$\times \left[\sum_{i=1}^N e\mathbf{r}_i \right] \Psi_{\Lambda_i}^{\alpha_i}(\mathbf{r}_1, \ldots, \mathbf{r}_N; R) , \tag{9}$$

where $\Psi_\Lambda^\alpha(\mathbf{r}_1, \ldots, \mathbf{r}_N; R)$ is the molecular electronic wave function depending on the position vectors $\mathbf{r}_1, \ldots, \mathbf{r}_N$ of the N target electrons and parametrically on the nuclear separation. Λ_i and Λ_f are, respectively, the initial and final quantum numbers of the projection of the electronic angular momentum on the molecular axis. e is the electron charge, g_i is the degeneracy of initial electronic state, and $\hbar$ is Planck's constant. K_i and S_i in Eq. (8) are the modified Bessel functions and modified Struve functions, respectively. Moreover,

$$\gamma_i = \frac{\rho_0 |\Delta E_{\alpha_f \alpha_i}|}{\hbar} \frac{1}{u_i} , \tag{10}$$

$$\gamma_f = \frac{\rho_0 |\Delta E_{\alpha_f \alpha_i}|}{\hbar} \frac{u_i}{u_f^2} , \tag{11}$$

$$\gamma = \frac{\rho_0 |\Delta E_{\alpha_f \alpha_i}|}{\hbar} \frac{2u_i}{u_i^2 + u_f^2} , \tag{12}$$

where u_i and u_f are the initial and final electron velocities. The incident energy is related to u_i by $E = mu_i^2/2$ with m the electron mass.

An improved formulation of the impact-parameter method, where the molecular motions are taken into account, has been given by Redmon et al. [14]. Generalizing Hazi's theory, they obtain, for the rotationally averaged cross section, the following expression:

$$\sigma_{v_i}^{\alpha_f \alpha_i}(E) = \sum_{v_f} S_{v_f v_i}^{\alpha_f \alpha_i} D_{v_f v_i}^{\alpha_f \alpha_i}(E) , \tag{13}$$

where

$$S_{v_f v_i}^{\alpha_f \alpha_i} = \frac{m^2 e^2}{3 g_i \hbar^4}(2-\delta_{\Lambda_f,0})(2-\delta_{\Lambda_i,0})$$

$$\times \left| \int_0^\infty dR \; \chi_{v_f}^{\alpha_f}(R) M_{\Lambda_f,\Lambda_i}(R) \chi_{v_i}^{\alpha_i}(R) \right|^2 \quad (14)$$

and $D_{v_f v_i}^{\alpha_f \alpha_i}(E)$ is given formally by Eq. (8) with $\Delta E_{\alpha_f \alpha_i}$ replaced by $\Delta E_{v_f v_i}^{\alpha_f \alpha_i}$, defined as

$$\Delta E_{v_f v_i}^{\alpha_f \alpha_i} = \varepsilon_{v_f} - \varepsilon_{v_i} \; . \quad (15)$$

ε_{v_i} and ε_{v_f} are the vibrational energy eigenvalues corresponding, respectively, to the initial and final electronic states. For energies over the dissociation threshold, ε_{v_f} is a continuum variable and in this case the sum in Eq. (13) is replaced by an integration. However, due to the small contribution to the cross section coming from dissociation, we neglect in our calculations the integration over the continuum vibrational states.

Since Eq. (13) is more general than Eq. (4), we calculated the cross section for the $X \to B$ transition using both equations to explore, by comparison of the results, the validity of our approximation.

III. COMPUTATIONAL DETAILS

The vibrational wave function in Eq. (4) is defined by

$$\left[\frac{-\hbar^2}{2\mu} \frac{d^2}{dR^2} + V_\alpha(R) - \varepsilon_v^\alpha \right] \chi_v^\alpha(R) = 0 \; , \quad (16)$$

where μ is the nuclear reduced mass of the molecule, $V_\alpha(R)$ is the electronic potential for the α state, and ε_v^α is the vibrational energy. Equation (16) was solved by expanding $\chi_v^\alpha(R)$ in harmonic-oscillator eigenfunctions. The electronic potential for every internuclear distance was obtained by linear interpolation of the data of Refs. [21,22] for X, B, and C states. We assumed the same electronic potential for both hydrogen and deuterium molecules.

The electronic transition dipole moment and the transition energies were obtained by carrying out configuration-interaction calculations. We used a basis set of Cartesian Gaussian functions, consisting of $6s\,6p$, centered on the nuclei and $4s\,4p$ at midpoint [23]. The values of the dipole moment and of the transition energies for X, B, and C states were checked by comparison with the "exact" values of Kolos and Wolniewicz [21,22,24]. Table I reports some results. The integration in Eq. (4) has been carried out using 100-point Gauss-
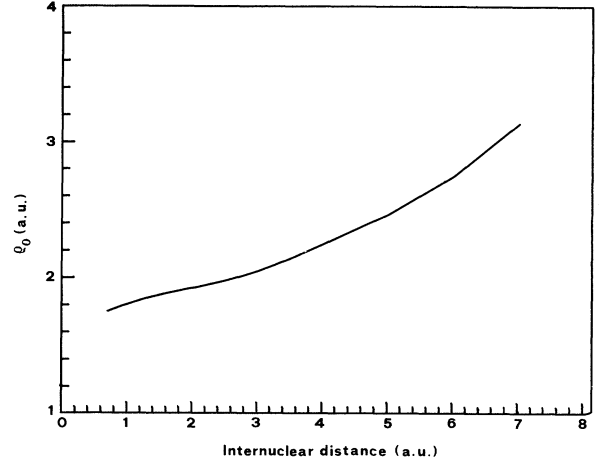

FIG. 1. Cutoff parameter ρ_0 as a function of internuclear distance for the $X\ ^1\Sigma_g^+ \to B\ ^1\Sigma_u^+$ electronic transition of H_2 molecule.

Legendre quadrature. The dipole moment, the transition energy, and impact parameter were calculated at 20 points in the range $0 < R < 7$ (atomic units) and all other values required in the integration were linearly interpolated. Finally, the cutoff ρ_0 was calculated by requiring that both the impact-parameter method and Born approximation cross sections were the same at 500 eV. Figure 1 shows the dependence of ρ_0 on internuclear distance for the $X \to B$ transition.

The same computational methods have been applied to Eq. (13). The cutoff parameter ρ_0 in this case has been computed following Refs. [14,18]. By using the Franck-Condon approximation and considering the vibrational states to be degenerate, Eq. (13) becomes

$$\sigma_{v_i}^{\alpha_f \alpha_i}(E) \cong \frac{m^2 e^2}{3 g_i \hbar^4} |M_{\Lambda_f,\Lambda_i}(\bar{R})|^2 (2-\delta_{\Lambda_f,0})$$

$$\times (2-\delta_{\Lambda_i,0}) D^{\alpha_f \alpha_i}(E) \; , \quad (17)$$

where $\bar{R}$ is a particular fixed internuclear distance. For sufficiently high incident energies the above expression becomes [18,19]

$$\sigma_{v_i}^{\alpha_f \alpha_i}(E) \cong -\frac{2\pi e^4}{E|\Delta E_{\alpha_f \alpha_i}|} f_{\alpha_f \alpha_i} \ln \left[\frac{\rho_0 |\Delta E_{\alpha_f \alpha_i}|}{\hbar (2E/m)^{1/2}} \right] , \quad (18)$$

where $f_{\alpha_f \alpha_i}$ is the generalized oscillator strength given by

TABLE I. Transition energies and dipole moments in atomic units as a function of internuclear distance for $X\ ^1\Sigma_g^+ \to B\ ^1\Sigma_u^+$ and $X\ ^1\Sigma_g^+ \to C\ ^1\Pi_u$ electronic transitions of H_2.

Transition	Internuclear distance	Transition energy[a]	Transition energy[b]	Dipole moment[a]	Dipole moment[c]
$X \to B$	1.4	0.4670	0.4687	0.9821	0.9799
$X \to C$	2.0	0.4198	0.4199	0.8460	0.8629

[a]Present work.
[b]References [21] and [22].
[c]References [24].

$$f_{\alpha_f \alpha_i} = \frac{2m}{3g_i \hbar^2 e^2} |\Delta E_{\alpha_f \alpha_i}|(2 - \delta_{\Lambda_f, 0})$$

$$\times (2 - \delta_{\Lambda_i, 0}) |M_{\Lambda_f, \Lambda_i}(\bar{R})|^2 . \tag{19}$$

By evaluating $\sigma_{v_i}^{\alpha_f \alpha_i}(E)$ in the Born approximation we can calculate ρ_0 from Eq. (18). In the case of the $X \to B$ transition, setting $\bar{R}$ equal to the equilibrium internuclear distance of 1.4 a.u. we obtained, for the cutoff parameter ρ_0, the value of 1.86 a.u. The computer program utilized to calculate the cross section in Eq. (13) was tested by reproducing the results of Redmon et al. (see Table III and Fig. 5 of Ref. [14]).

IV. RESULTS

In Fig. 2 we compare the e-H_2 cross sections calculated using Eq. (4), with the final vibrational levels treated as degenerate, and Eq. (13) with the sum on v_f carried out explicitly. The comparison is made for some representative values of initial vibrational quantum number. The agreement between the two sets of results is very satisfactory for low v_i values over the entire range of energies considered, while for $v_i = 12$ we find some discrepancy particularly evident at low energies, probably due to the fact that in Eq. (13) the sum on v_f is performed explicitly. On the other hand, this difference can be attributed also to the particular value used in Eq. (13) for the cutoff parameter ρ_0 in the range of high vibrational quantum numbers. Actually, to calculate ρ_0 by Eqs. (17)–(19) we used, for the internuclear distance $\bar{R}$, the same value for all vibrational states, suppressing in this way the dependence of ρ_0 on the vibrational quantum number v_i. The value of 1.4 a.u. used for $\bar{R}$ is a "good value" for $v_i = 0$ and for low v_i values, as is shown in Fig. 2, while for high v_i a more suitable choice could produce better results [25]. However, considering also that the discrepancy observed in Fig. 2 is not too large (about 15% at 25 eV), we can
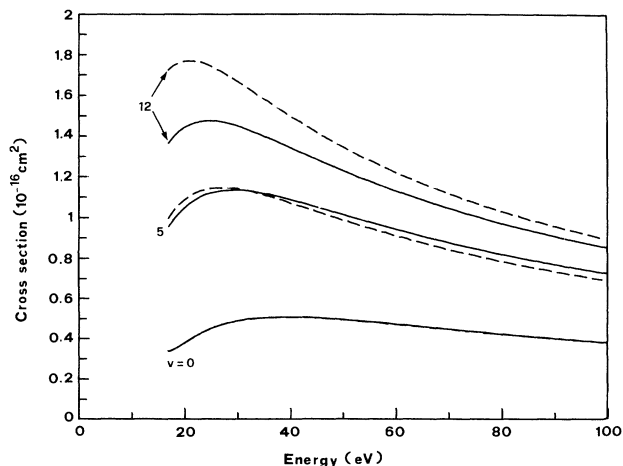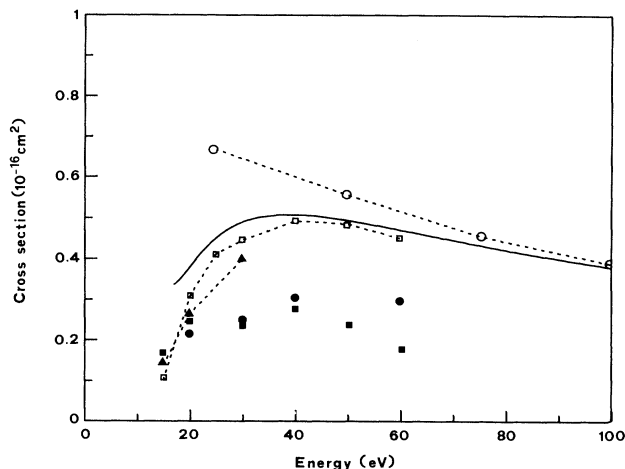

FIG. 3. Cross sections as a function of incident energy for the $X\ ^1\Sigma_g^+ \to B\ ^1\Sigma_u^+$ transition of H_2: O, Born approximation [7]; ——— impact-parameter method (present results); □, distorted-wave approximation [9]; ▲, Schwinger multichannel method [16]; ■, experiment [6(b)]; ●, experiment [15].

confidently use Eq. (4) over the range of initial vibrational quantum number.

In Figs. 3 and 4 the present cross sections for the colliding system e-$H_2(v_i = 0)$ are compared with other theoretical and experimental results for both electronic excitations $X \to B$ and $X \to C$, respectively [6(b),7,9,15,16]. The present cross sections are in good agreement with the other theoretical calculations. For the $X \to B$ transition, our values are slightly smaller than those obtained in Ref. [11], where the Franck-Condon approximation was used.

Figure 5 shows the cross sections for the $X \to B$ transition, for the system e-$H_2(v_i)$, with v_i covering the range 0–14. The cross sections increase monotonically from
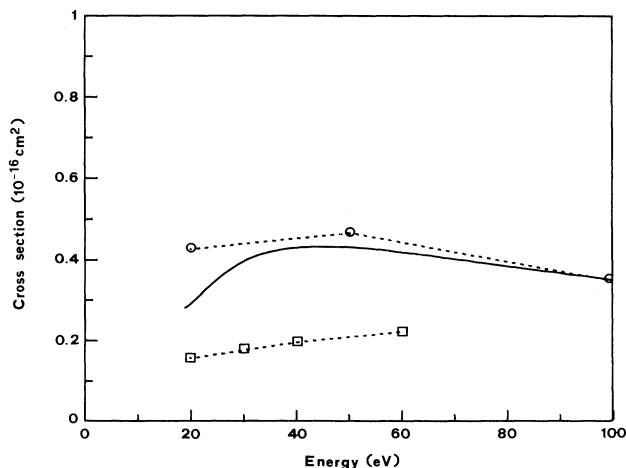

FIG. 2. Comparison of cross sections calculated by Eq. (4) ——— and Eq. (13) – – – (see text), for the process $H_2(X\ ^1\Sigma_g^+,\ v_i = 0, 5, 12) + e \to H_2(B\ ^1\Sigma_u^+) + e$. For $v_i = 0$ the curves overlap.

FIG. 4. Cross sections as a function of incident energy for the $X\ ^1\Sigma_g^+ \to C\ ^1\Pi$ transition of H_2: O, Born approximation [10]; ———, impact-parameter method (present results); □, experiment [15].

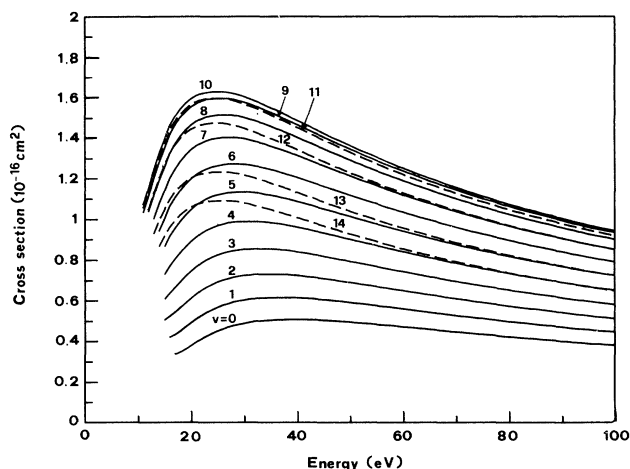FIG. 5. Cross sections as a function of incident energy for the process $H_2(X\ ^1\Sigma_g^+,\ v_i=0-14)+e\rightarrow H_2(B\ ^1\Sigma_u^+)+e$.

FIG. 7. Same as Fig. 5 but for the process $H_2(X\ ^1\Sigma_g^+,\ v_i=0-14)+e\rightarrow H_2(C\ ^1\Pi_u)+e$.

$v_i=0$ through $v_i=10$, with an increment in the maximum up to a factor of 4, and follow the opposite trend for $v_i>10$. To understand this unexpected behavior, we plotted in Fig. 6 the quantity $\sigma^{\alpha_f\alpha_i}(E;R)$ [see Eq. (4)] as a function of the internuclear separation R for a fixed incident energy $E=25$ eV. In the same figure we report also the cross section for the $X\rightarrow C$ transition for $E=40$ eV. The shape of these curves is determined by the trend of the transition dipole moment with internuclear distance. A comparison with the results of Wolniewicz [24], who calculated the electronic transition moment for the same electronic excitation of the H_2 molecule and for several internuclear distances, shows in fact that the cross section $\sigma^{\alpha_f\alpha_i}(E;R)$ is strongly influenced by the behavior of the transition moment.

The peaked shape of $\sigma^{\alpha_f\alpha_i}(E;R)$ for the $X\rightarrow B$ transition determines the dependence of the total cross section

on the initial vibrational quantum number observed in Fig. 5. For low v_i values, due to the rapid falloff of the vibrational wave functions as $R\rightarrow\infty$, the most important contribution to the integral in Eq. (4) comes from the rising part of the $X\rightarrow B$ curve of Fig. 6, while for higher v_i values $(v_i>10)$ the main contribution to the integration comes from the range of larger internuclear distances corresponding to the decreasing part of the $X\rightarrow B$ curve. This effect is strongly reduced in the v_i dependence of the total cross sections reported in Fig. 7 for the $X\rightarrow C$ transition. In fact, the almost constant value of $\sigma^{\alpha_f\alpha_i}(E;R)$ for $R\gtrsim4$ a.u. seen in Fig. 6 determines the weak dependence of the total cross sections on the vibrational quantum number $(v_i=12,13,14)$. The same behavior, as expected, is observed in Figs. 8 and 9 where we report the electron-impact total cross sections for the $D_2(v_i)$ molecule, for the $X\rightarrow B$ and $X\rightarrow C$ transitions and for v_i in the range 0–20.
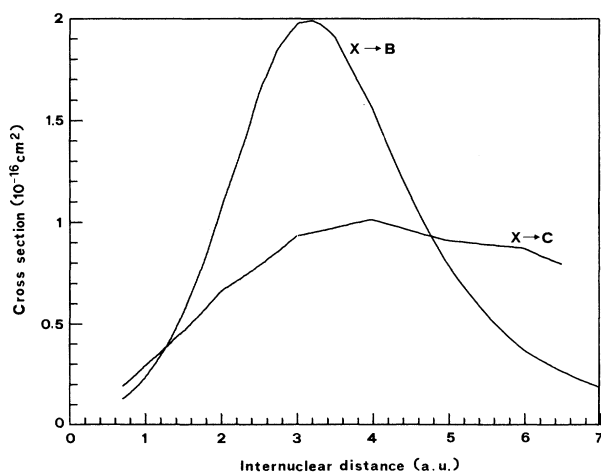

FIG. 6. $\sigma^{\alpha_f\alpha_i}(E;R)$ as a function of internuclear distance for the $X\ ^1\Sigma_g^+\rightarrow B\ ^1\Sigma_u^+$ and $X\ ^1\Sigma_g^+\rightarrow C\ ^1\Pi_u$ transition of H_2 with $E=25$ and 40 eV, respectively.
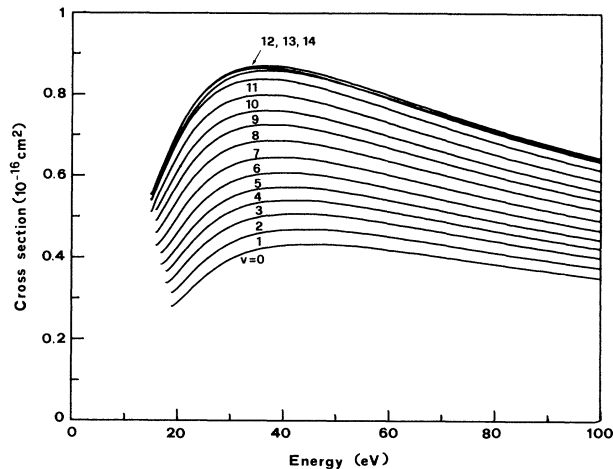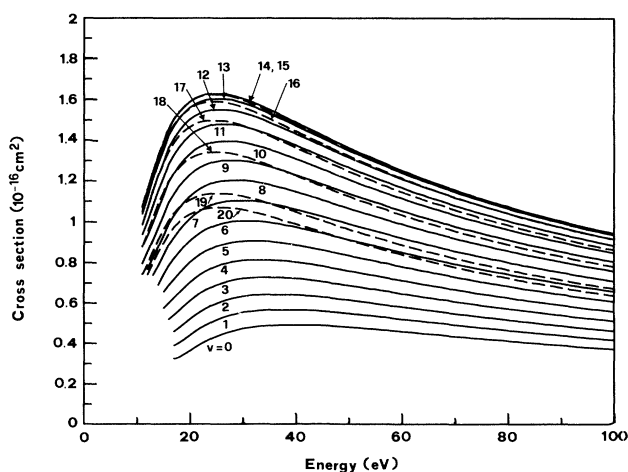

FIG. 8. Same as Fig. 5 but for the process $D_2(X\ ^1\Sigma_g^+,\ v_i=0-20)+e\rightarrow D_2(B\ ^1\Sigma_u^+)+e$.
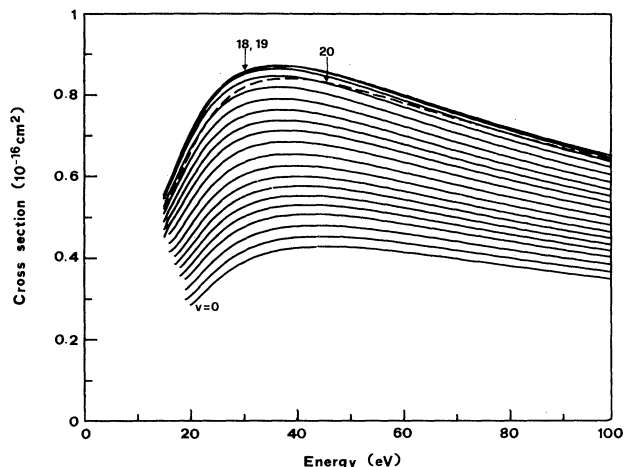
FIG. 9. Same as Fig. 5 but for the process $D_2(X \ ^1\Sigma_g^+, \ v_i = 0\text{–}20) + e \rightarrow D_2(C \ ^1\Pi_u^+) + e$.

From the preceding discussion of the behavior of the cross sections in the framework of the impact-parameter approximation, we may conclude that a knowledge of the dependence of the electronic transition dipole moment on internuclear distance can represent a valid heuristic tool to understand, from a qualitative point of view, the dependence of the total cross sections on the initial vibrational state.

V. CONCLUSIONS

In this paper we have presented complete sets of cross sections for the excitation $X \rightarrow B$ and $X \rightarrow C$ in the H_2 and D_2 systems. The $v = 0$ cross sections are in good agreement with the theoretical calculations, being, however, two times greater than the experimental results.

This discrepancy has been recently discussed by Hiskes [26], who calculated the cross sections for the process:

$$e + H_2(X \ ^1\Sigma_g^+, v_i) \rightarrow e + H_2(\text{singlet states})$$

$$\rightarrow e + H_2(X \ ^1\Sigma_g^+, v_f) + h\nu \ .$$
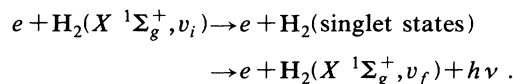
In addition, the calculations of Buckman and Phelps [27] based on the deconvolution of H_2 transport properties as well as the crude calculations based on the Gryzinski approximation without any corrections [2(a)] confirm the present data. Therefore it is very difficult to explain the discrepancy between theoretical and experimental results (see also the discussion of Gibson et al. [16]). Further theoretical and experimental work will be welcome to shed light on this problem.

The main result of our investigations lies in the trend of the cross sections as a function of the vibrational quantum number, which is different from both the results of Refs. [2(a)] and [26]. In this last case the differences arise only for the $X \rightarrow C$ state transition.

In conclusion we can say that the present method of calculation seems to yield accurate values of cross sections for high vibrational levels and can represent a powerful tool for calculating complete sets of cross sections to be used in plasma modeling.

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