Transitions between excited electronic states of H$_2$ molecules by electron impact

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We present theoretical integral and differential cross sections for transitions produced by electron collision with an excited H$_2$ molecule ($c^3\Pi_u$ and $a^3\Sigma_g^{(+)}$) obtained with the Schwinger multichannel method in a four-state approximation. We also present the transition rates obtained with these cross sections. The results indicate the importance of these scattering processes in modeling H$_2$ discharge. [S1050-2947(98)02210-0]

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I. INTRODUCTION

In the last 10 years, theoretical studies of electron-molecule collision process have made important progress. Presently we have several methods [1–3] able to study the electron-molecule with all the complexity of the many-body problem. The use of pseudopotentials has opened up the possibility of studying molecules with hundreds of electrons [4,5]. There is strong motivation to study the electron-molecule collision problem. It is interesting from the many-body point of view (control of approximations) but also their results can be used in many applied problems. For instance, processes based on cold plasmas are crucial steps to fabrication of electronic devices. In these low-temperature plasmas, the collision processes between electron and molecules play a key role in the formation and destruction of the various plasma species. Applications of plasma processing have been developed largely empirically, partially due to the lack of a detailed understanding of the fundamental atomic and molecular collision processes in such a system [6].

Studies of electron-excited molecule collision are rare, despite many applications [6–8]. Almost all studies [9] are related to experimental or theoretical aspects of the dissociative attachment processes of H$_2$ and CO. There is one study on the superelastic collision of electrons with vibrationally excited N$_2$ [10] and another for O$_2$ on the $a^1\Delta_g \rightarrow b^1\Sigma_g^+$ electronic transition [11]. Even for atoms the number of studies involving collision of electrons against electronically excited targets is very small [12].

Recently two publications, Celiberto *et al.* [13] and Sartori *et al.* [14], addressed the problem of calculating electron–excited-state molecule cross sections. There are several motivations to study electron-excited molecule collisions. For instance, the present analysis of plasma transport coefficient does not include the presence of excited (vibrationally or electronically) states. In recent work, Capitelli

et al. [15] have show the importance of the electron-excited molecule cross section to determine electron energy distribution function of H$_2$ plasma. [16]

In this paper we use the Schwinger multichannel method [2] to calculate cross section and transition rates related with the electron collision with excited H$_2$ molecules. The calculation is performed in a four-state approximation and our study includes the following transitions: $a^3\Sigma_g^{(+)} \rightarrow a^3\Sigma_g^{(+)}$, $a^3\Sigma_g^{(+)} \rightarrow b^3\Sigma_g^{(+)}$, $a^3\Sigma_g^{(+)} \rightarrow c^3\Pi_u$ and $c^3\Pi_u \rightarrow a^3\Sigma_g^{(+)}$, $c^3\Pi_u \rightarrow b^3\Sigma_g^{(+)}$, $c^3\Pi_u \rightarrow c^3\Pi_u$. The majority of the H$_2$ molecule excited states is short lived. As a result the population of these excited states is small and scattering processes from these states are not important. Our choice of the excited states was driven by the metastability of $c^3\Pi_u$ [17,18] and quasimetastability of $a^3\Sigma_g^{(+)}$ [19]. The $c^3\Pi_u(v=0, K=0)$ is located at 29 635 cm^{-1} below the ionization limit and the $a^3\Sigma_g^{(+)}(v=0, K=0)$ is located at 29 344 cm^{-1} below the ionization. Although these two states are close in energy, they have different equilibrium positions. In a glow discharge Catherinot *et al.* [19] measured a $a^3\Sigma_g^{(+)}(v=0, J=2)$ population as high as 5% of the total. They attributed this population enhancement as due to energy transfer collision with the $c^3\Pi_u$. Such high excited state population should have important contributions to understanding the plasma stationary properties.

In our previous publication [14] we have presented integral cross sections for electron collision with a H$_2$ molecule in the $c^3\Pi_u$ state. In this paper, we present further information about these collisions processes and a similar study for transitions out of the ($a^3\Sigma_g^{(+)}$) state. In addition to differential cross sections (DCS), we also present calculated transition rates for processes starting at an excited state. Our transitions rates are several orders of magnitude larger than those obtained with the molecule in the ground state.

Our paper develops as follows. In Sec. II we present essential features of the SMC method and how it is used in the case of transition between excited states. In Sec. III we present the basis set used and the results. We close our paper by discussing possible effects in modeling discharge environments due to the present calculated transition rates.

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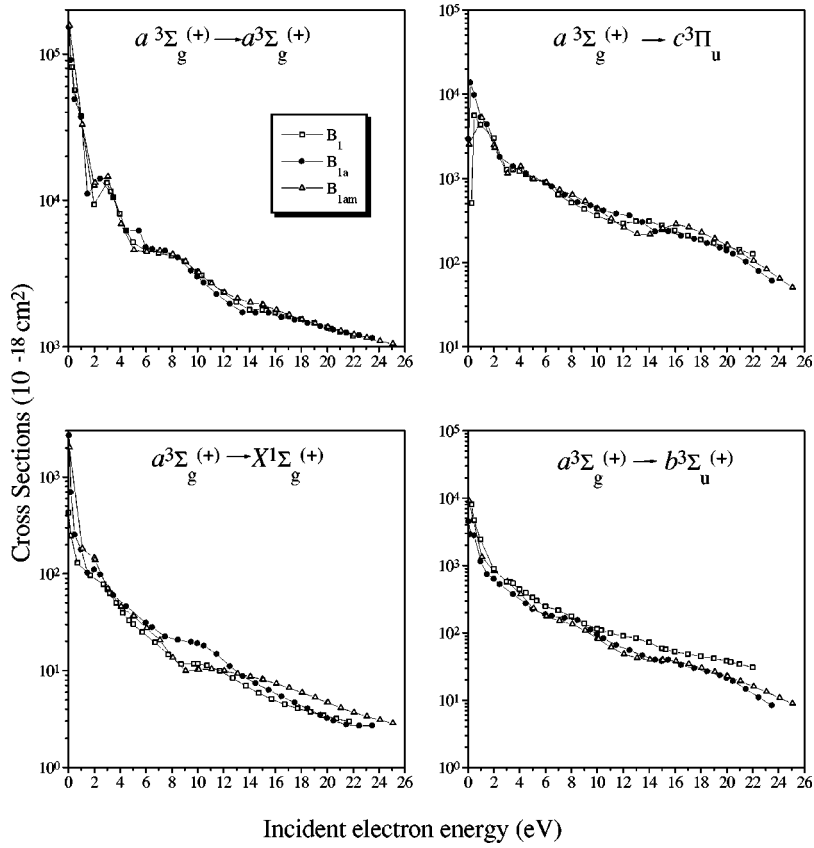[‡]Electronic address: maplima@ifi.unicamp.br

FIG. 1. Electronic transition integrated cross sections of an excited H_2 molecule for the $a^3\Sigma_g \rightarrow a^3\Sigma_g^{(+)}$, $a^3\Sigma_g \rightarrow c^3\Pi_u$, $a^3\Sigma_g \rightarrow b^3\Sigma_u^{(+)}$, and $a^3\Sigma_g \rightarrow X^1\Sigma_g^{(+)}$ transitions. Open squares: target description of type 1 for $R_{H\text{-}H}=1.4a_0$; closed circles: target description of type 1 for $R_{H\text{-}H}=1.96a_0$; open triangles: target description of type 2 for $R_{H\text{-}H}=1.96a_0$. For target descriptions, see text.

II. THEORY

We summarize the development of the SMC method [2] as follows. The Hamiltonian for the collision system can be written as

$$H=H_N+T_{N+1}+V=H_0+V, \qquad (1)$$

where H_N is the target Hamiltonian, T_{N+1} is the kinetic energy operator for the continuum electron, and V is the potential between the continuum electron and the target. In this formalism a variational stable expression for the scattering amplitude is given by

$$f_{\vec{k}_f\vec{k}_i}=-\frac{1}{2\pi}\sum \langle S_{\vec{k}_f}|V|\psi_m\rangle[d^{-1}]_{mn}\langle\psi_n|V|S_{\vec{k}_i}\rangle, \qquad (2)$$

where d_{mn} is given by

$$d_{mn}=\langle\psi_m|A^{(+)}|\psi_n\rangle \qquad (3)$$

and $A^{(+)}$ is

$$A^{(+)}=\frac{1}{2}(PV+VP)-VG_P^{(\pm)}V+\frac{1}{N}\left[\hat{H}-\frac{N}{2}(\hat{H}P+P\hat{H})\right]. \qquad (4)$$

In these equations $S_{\vec{k}_i}$ is a product of a target state and a plane wave, Ψ_m is an $(N+1)$-electron Slater determinant (or combination of them) in which the variational trial function is expanded, $\hat{H}$ is the total energy minus the full Hamiltonian of the system, N is the total number of electrons in the target, P is a projector onto the open electronic target states, and $G_P^{(+)}$ is the Green's function projected on this P space.

The scattering problem of an electron and an excited molecule is similar to the electron-open-shell molecule scattering [20]. In particular the spin problem can be simplified in the same way. The scattering amplitude can be written as

$$f_{m_i,M_i;m_f,M_f}(i\rightarrow f)=\sum_{S,M_S} C^{1/2\,S_i S}_{m_i M_i M_S} C^{1/2\,S_f S}_{m_f M_f M_S} f^{(2S+1)}(i\rightarrow f), \qquad (5)$$

where $C^{S_1\,S_2\,S_3}_{m_1\,m_2\,m_3}$ are Clebsch-Gordan coefficients $(m_i,\ M_i)$ and $(m_f,\ M_f)$ are the initial and the final spin components of the continuum electron and the molecule. i and f are the state quantum numbers other then the spin components. For collision between unpolarized target and electron the cross sections is

$$\frac{d\sigma(i\rightarrow f)}{d\Omega}=\frac{1}{2(2S_i+1)}\frac{k_f}{k_i}\sum_S (2S+1)|f^{(2S+1)}(i\rightarrow f)|^2. \qquad (6)$$
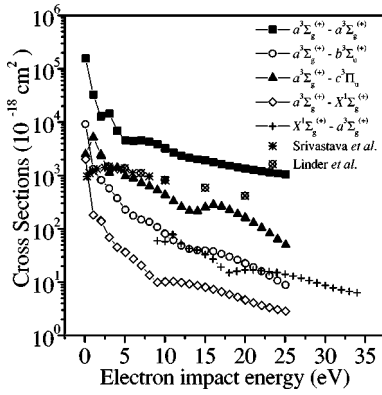
FIG. 2. Electronic transition cross sections of an excited H_2 molecule: closed squares, $a^3\Sigma_g \rightarrow a^3\Sigma_g^{(+)}$; open circles, $a^3\Sigma_g \rightarrow b^3\Sigma_u^{(+)}$; closed triangles, $a^3\Sigma_g \rightarrow c^3\Pi_u$; open diamonds, $a^3\Sigma_g \rightarrow X^1\Sigma_g^{(+)}$; plusses, $X^1\Sigma_g^{(+)} \rightarrow c^3\Pi_u$; stars, experimental total cross sections out of the $X^1\Sigma_g^{(+)}$ state of Srivastava et al.; asterisk, experimental total cross sections out of the $X^1\Sigma_g^{(+)}$ state of Linder et al. We used target description (see text) of type 2 for $R_{H-H} = 1.96a_0$.

III. STATES, BASIS SET, AND RESULTS

A. States and basis set

Our calculations have been carried out within the framework of the fixed-nuclei and Frank-Condon approximation. In the SMC method the expansion basis set is formed by (N+1)-particle Slater determinants, Ψ_m, constructed from a chosen set of target states (these states are multiplied by a set of one-particle virtual orbitals and each product is made antisymmetric). A subset of the target states defines the level of coupling of the electronic states through the projector P. In this calculation both P and Ψ_m include the ground state $X^1\Sigma_g^{(+)}$, the $c^3\Pi_u$, the $a^3\Sigma_g^{(+)}$, and the $b^3\Sigma_u^{(+)}$ states. Our choice of states was driven by our goal, to study the electron collision with H_2 molecule at $a^3\Sigma_g^{(+)}$ and the $c^3\Pi_u$ states. One criterion to choose states in strong coupling calculations is the description of the static polarizability [21] of the initial state of the target. In our case, we are interested in the electron scattering process out of triplet states so we included only one singlet state, the ground state $X^1\Sigma_g^{(+)}$. The other

state present is the $b^3\Sigma_u^{(+)}$, chosen by its optical coupling with $a^3\Sigma_g^{(+)}$. The $a^3\Sigma_g^{(+)}$ and the $c^3\Pi_u$ states are optically coupled and are initial states in this work. Experimental results for static polarizability are limited for the ground state of atomic species [22] and as far as we know it has not been determined for our excited states. However, we expect that a large part is included because $a^3\Sigma_g^{(+)}$ and $c^3\Pi_u$ are very close in energy and this amplifies their importance for the static polarization. The inclusion of $b^3\Sigma_u^{(+)}$ is also important because it is a dissociative state and a source of fast H atoms.

Our basis set is made of $6s6p1d$ [23] Cartesian Gaussian functions on each atom of H. This set of functions is used to perform several SCF calculations. The minimum of the potential energy curve is in general different for each molecular state. For H_2 the internuclear separation at this minimum is $1.96a_0$ for $c^3\Pi_u$, $1.868a_0$ for the $a^3\Sigma_g^{(+)}$, and $1.4a_0$ for the $X^1\Sigma_g^{(+)}$ state [24]. To assess the influence of internuclear separation on the fixed-nuclei calculated cross sections we perform bound state calculations for each internuclear distances. Target states were obtained in following ways: type B_1 is obtained by converging the self-consistent-field (SCF) wave function of the $X^1\Sigma_g^{(+)}$ at the ground-state equilibrium separation. Then we diagonalize the V_{N-1} potential to obtain the improved virtual orbitals (IVO) [25]. Types B_{1a} and B_{1c} are obtained with the same procedure but with the internuclear separation of the $a^3\Sigma_g^{(+)}$ and $c^3\Pi_u$ respectively. Type B_{1cm}, is obtained by converging the SCF wave function of the $c^3\Pi_u$ (B_{1cm}) using the internuclear separation for this excited state. Then we calculate the triplet coupled IVO's with the $1\sigma_g$ orbital. Type (B_{1am}) SCF is obtained with the $a^3\Sigma_g^{(+)}$, and calculating the triplet coupled IVO's with the $1\sigma_g$ orbital of the ''a'' state kept frozen.

Table I shows the vertical excitation energies (out of the $X^1\Sigma_g^{(+)}$) to the upper states using these basis. For comparison we also include experimental excitation energies [24]. There are highly accurate theoretical calculation for the potential energy curves of all states included in our calculation ($X^1\Sigma_g^{(+)}$, $b^3\Sigma_u^{(+)}$, and $a^3\Sigma_g^{(+)}$ by Kolos and Wolniewicz [26,27], and the $c^3\Pi_u$ by Bwowne [28]). However, we use much simpler descriptions of the target states (Hartree-Fock level) and, as we will see, slight differences in these descriptions give similar scattering results,

State	B_1 (eV)	B_{1a} (eV)	B_{1am} (eV)	B_{1c} (eV)	B_{1cm} (eV)	Expt (eV)
$a^3\Sigma_g^{(+)}$	12.029	10.515	8.939	10.271	8.948	11.98
$c^3\Pi_u$	12.310	10.578	9.028	10.301	8.971i	11.96
$b^3\Sigma_u^{(+)}$	9.978	6.481	5.337	5.868	4.919	

B. Results and discussion

In Fig. 1 we present results of calculated integral cross sections for the four possible transitions out of the $a^3\Sigma_g^{(+)}$ state. For each excited state we used three different approximations for the target wave functions: B_1, B_{1a}, and B_{1am} for

the excitation from $a^3\Sigma_g^{(+)}$ and B_1, B_{1c}, and B_{1cm} for the excitation from $c^3\Pi_u$. Similar to our previous $c^3\Pi_u$ calculations, the results show little dependence on the target wave-function approximation. These results suggest that the effect of the internuclear separation and the choice of differ-
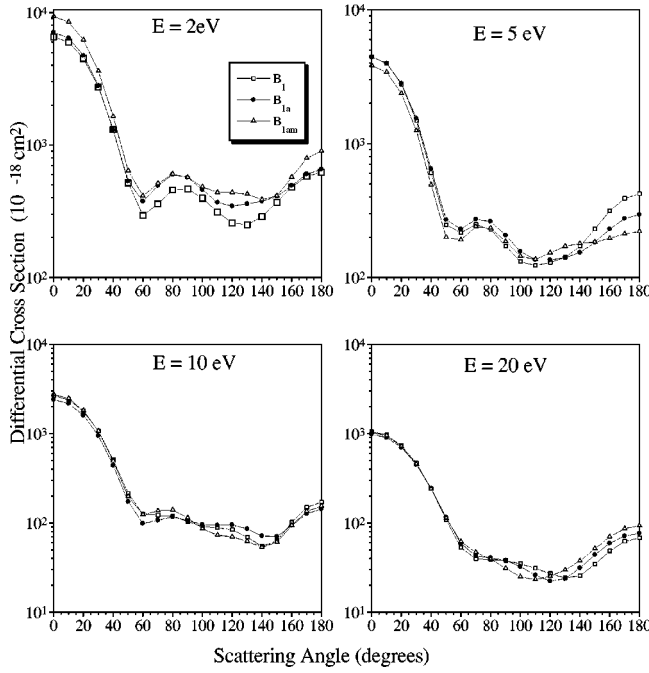
FIG. 3. Differential cross sections for elastic $a^3\Pi_u \to a^3\Pi_u$ for the three descriptions of target.

ent $V_{(N-1)}$ potential does not produce important effects on the calculated integral cross sections. In Figure 2 we present integral cross sections for excitation out the $a^3\Sigma_g^{(+)}$ with the basis B_{1am}. For comparison we also include experimental cross sections [29,30] for transitions out of the $X^1\Sigma_g^{(+)}$ state. Elastic cross section of the $a^3\Sigma_g^{(+)}$ are significantly larger than that of the ground state.

In Figs. 3, 4, and 5 we present calculated differential cross sections (DCS) for processes out of the $a^3\Sigma_g^{(+)}$ at incident electron energies of 2, 5, 10, and 20 eV. They include the
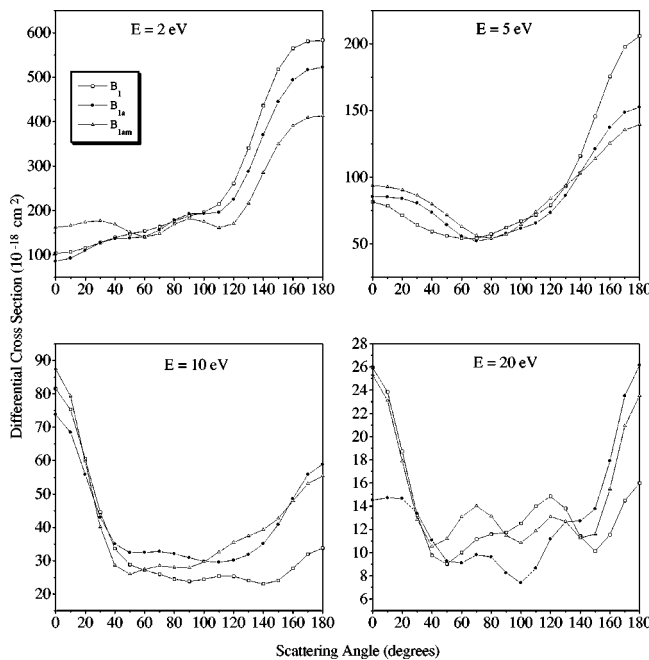

FIG. 4. Differential cross sections for $a^3\Sigma_g^{(+)} \to c^3\Pi_u$ for the three descriptions of target.

$a^3\Sigma_g^{(+)} \to a^3\Sigma_g^{(+)}$, $a^3\Sigma_g^{(+)} \to c^3\Pi_u$, and $a^3\Sigma_g^{(+)} \to b^3\Sigma_u^{(+)}$ transitions, respectively. For DCS, the effect of the internuclear distance and V_{N-1} potential depends on the transition. For the elastic $a^3\Sigma_g^{(+)} \to a^3\Sigma_g^{(+)}$ transition, as the incident energy increases the behavior of the cross sections at small scattering angles ($\leqslant 60$) becomes almost identical for all approximations. We attribute the differences seen at small energies and small scattering angles to polarization effects. Our calculation includes only two optically coupled states with $^3\Sigma_g^{(+)}$, so only a fraction of the polarizability is included. For atoms Christophorou and Illenbergeri [12] have shown the correlation between total cross section and the static polarizability. The differences in the large angular region can be attributed to short-range potentials as the exchange interaction. We use a frozen core description of the molecular target and as a result our short-range correlation comes through Ψ_m. The use of different internuclear distances and molecular states should affect the exchange interaction and polarization description, especially at low energies. For the $a^3\Sigma_g^{(+)} \to b^3\Sigma_u^{(+)}$ and $a^3\Sigma_g^{(+)} \to c^3\Pi_u$ transitions, the differences are more pronounced than those in the elastic cases. In the small angular region these differences can be attributed to the fact that each basis furnishes a different oscillator strength (long range interaction) for each transition.

In Figs. 6 and 7 we show calculated DCS for transitions $c^3\Pi_u \to c^3\Pi_u$ and $c^3\Pi_u \to b^3\Sigma_u^{(+)}$ with basis B_{1c} and B_{1cm}. Our elastic result displays little dependence with the basis set except at 10 eV. The superelastic transition $c^3\Pi_u \to b^3\Sigma_u^{(+)}$ also shows little dependence with the the chosen basis. Compared with previous case, the calculation for this transition is much less sensitive. This may be related to the fact that these states are not optically connected. Our results show that, in general, the elastic transitions are much less sensitive to the choice of basis sets, which probably is due to the overwhelming influence of the one-body potential. On the other hand, transitions between different states depend on the nature of the transition (if it is dipole allowed or not, if is mainly due to exchange interactions or not, or if it is sensitive to polarization effects).

Our results show that transitions between excited molecular states have a larger cross section when compared with ground-state elastic cross section. In addition, the excitation energy between excited states is smaller than those between ground and excited states. As a result for a given electron energy distribution there will be many more electrons able to perform transitions out of the excited state than out of the ground state. We can say that excited-state–to-excited state transitions probe the low-energy electron distribution function, which can not affect the ground-state—excited-state transitions. However, all this can be expressed through a quantity called transition rate defined as

$$K_{i \to f}(T) = \left(\frac{2}{\mu}\right)^{1/2} \int \sigma_{i \to f}(E)\sqrt{E}f(E)dE, \qquad (7)$$

where we assume a Maxwellian distribution $f(E)$ for the electrons and $\sigma_{i \to f}(E)$ is the integrated cross section for the transition $i \to f$.

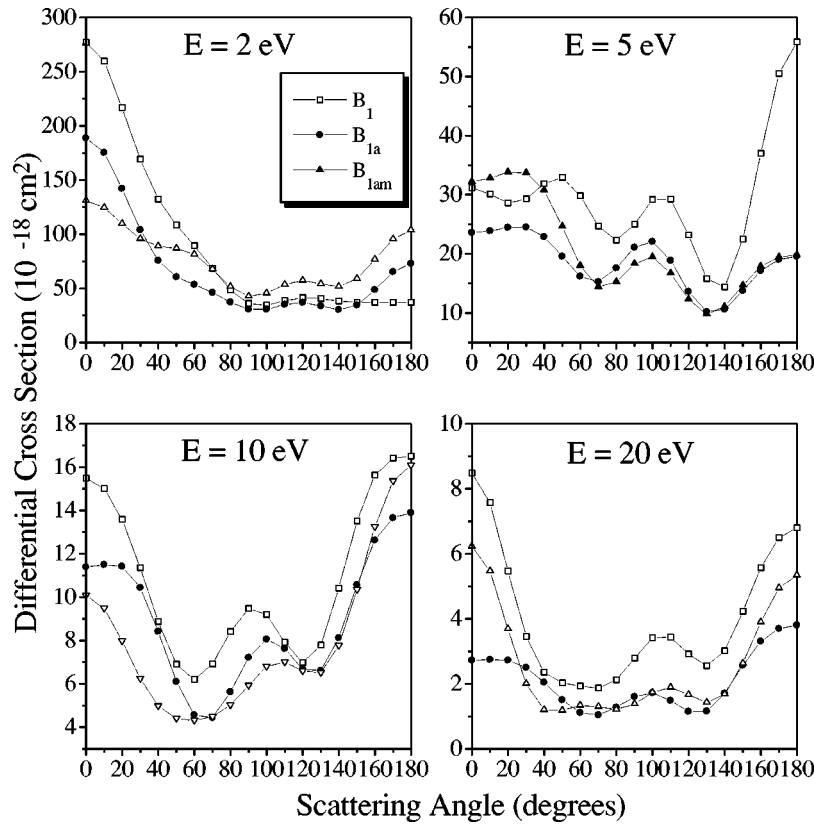Figures 8 and 9 show our calculated transition rates. Here we can see the combined effect of larger cross-section and

FIG. 5. Differential cross sections for $a^3\Sigma_g^{(+)} \rightarrow b^3\Sigma_u^{(+)}$ for the three descriptions of target.

lower excitation energy producing transition rates between excited states orders of magnitude larger than those corresponding to ground to excited states. The net effect is even more important at lower temperatures where the low-energy part of the electron distribution function is more important. At these temperatures the excitation energy (E_{ex}) plays a

crucial role. The integral for $K_{i \rightarrow f}(T)$ is performed only to those electrons with energy $E \geqslant E_{ex}$. E_{ex} for ground to excited state is of the order of 12 eV, for excitation out of the $c^3\Pi_u$ and $a^3\Sigma_g^{(+)}$, E_{ex} is either very small ($c^3\Pi_u \leftrightarrow a^3\Sigma_g^{(+)}$), or null (for elastic scattering and superelastic transition). As a result only a very small fraction of
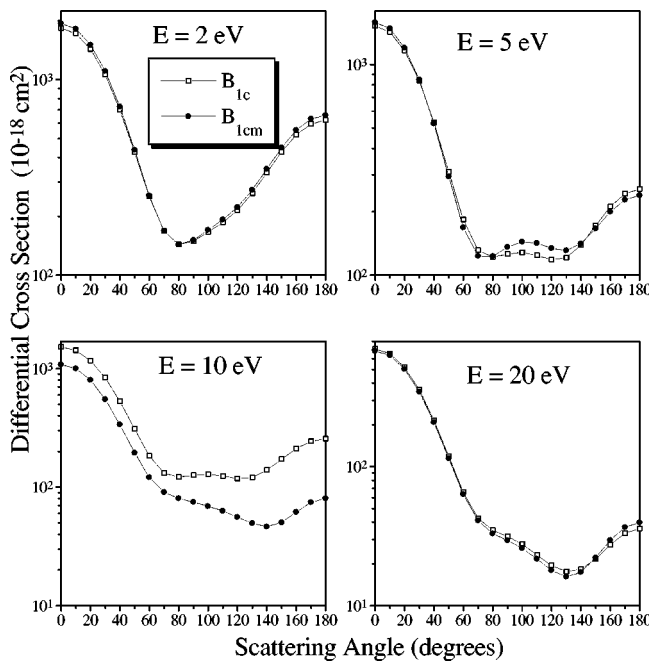

FIG. 6. Differential cross sections for $c^3\Pi_u \rightarrow c^3\Pi_u$ for the basis representation B_{1c} (open squares) and B_{1cm} (closed circles).
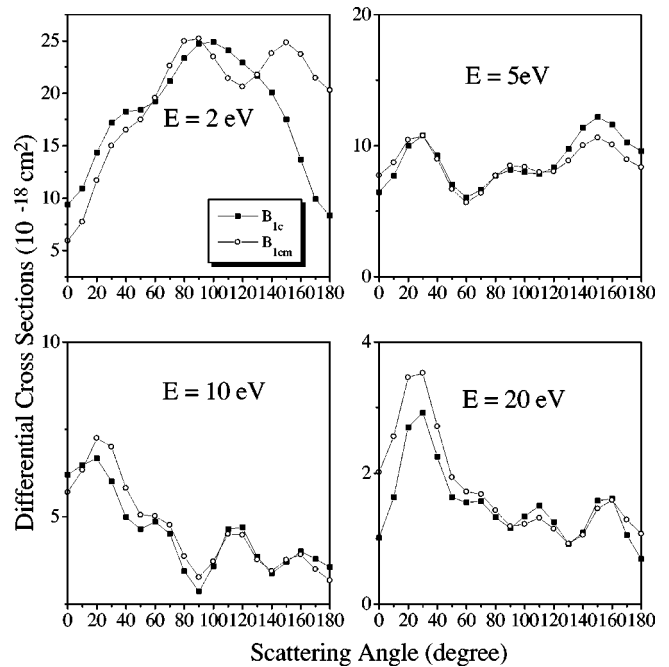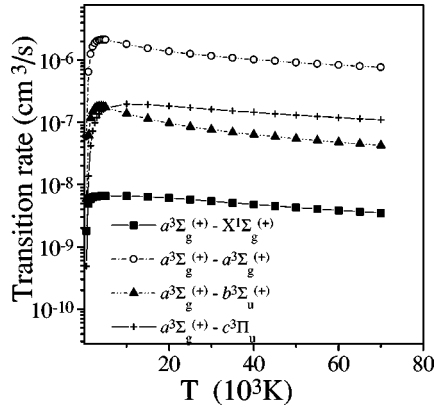

FIG. 7. Differential cross sections for $c^3\Pi_u \rightarrow b^3\Sigma_u^{(+)}$ for the basis representation B_{1c} (open squares) and B_{1cm} (closed circles).

FIG. 8. Transition rates for excitation from the $a^3\Sigma_g^{(+)} \to X^1\Sigma_g^{(+)}$ (closed squares); $a^3\Sigma_g^{(+)} \to a^3\Sigma_g^{(+)}$ (open circles); $a^3\Sigma_g^{(+)} \to b^3\Sigma_u^{(+)}$ (closed triangles); $a^3\Sigma_g^{(+)} \to c^3\Pi_u$ (crosses).

FIG. 9. Transition rates for excitation from the $c^3\Pi_u \to c^3\Pi_u$ (closed squares); $c^3\Pi_u \to c^3\Pi_u$ (open circles); $c^3\Pi_u \to b^3\Sigma_u^{(+)}$ (closed triangles).

the electrons are energy allowed to produce excitation out of the ground state but almost all electrons can produce the other transitions.

The calculated transition rates suggest important processes in a H_2 discharge. For example, the $c^3\Pi_u$ is a metastable state with 1-ms lifetime, then it has a transition probability of 10^3 s^{-1}. In a collisional-radiative model [31], electron depopulation of this state will be important when $n_e K_{i \to f}$ is of the same order of magnitude [13]. Our calculated transition rates indicate that this will occur for electron density of 10^{10} cm^{-3}. For the $a^3\Sigma_g^{(+)}$ with a lifetime of 10^{-8} s, the required electron density is of 10^{15} cm^{-3}.

IV. CONCLUSION

We calculated differential and integrated cross section and the corresponding transition rates. Our results suggest
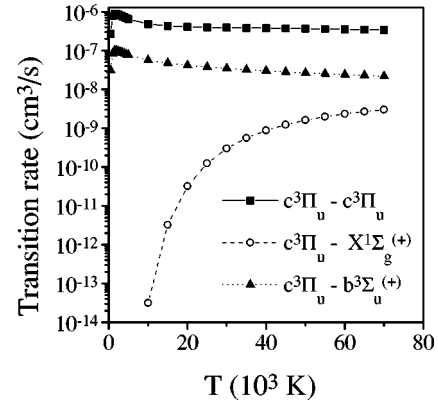
the importance of electron collision with an excited molecule at electron densities greater than 10^{10} cm^{-3}. The lack of experimental and other theoretical results limit further comparison with our results. However, our results support further analysis on the lines suggested by Capitelli [15] on the importance of excited states on the electron energy distribution function as well as inclusion of these processes on future analysis of transport coefficients.

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