

## **CROSS SECTION DATA FOR ELECTRON-IMPACT INELASTIC PROCESSES OF VIBRATIONALLY EXCITED MOLECULES OF HYDROGEN AND ITS ISOTOPES**

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An extensive cross section database for the electron-impact inelastic processes of vibrationally excited molecules of hydrogen and its isotopes is presented. The following inelastic processes are covered: electronic excitation (dissociative and nondissociative), direct ionization (dissociative and nondissociative), excitation-radiative decay vibrational excitation and dissociation, and dissociative electron attachment. The data have been compiled partly from the literature and partly generated theoretically for the present report. The data are presented in graphical form. The data are also presented by sufficiently accurate analytic fit functions. Mass-scaling relations are provided for cross section evaluation of those isotope molecules for which calculated data are not available. © 2001 Academic Press

Data files associated with this article may be found on IDEAL at <http://www.idealibrary.com/links/doi/10.1006/adnd.2000.0850/dat>.

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## 1. INTRODUCTION

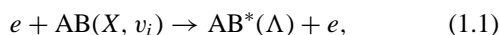
Electron-impact inelastic processes of vibrationally excited hydrogen molecules (or their isotopic variants) play a paramount role in the kinetics of a low-temperature hydrogenic plasma. This role is a consequence mainly of two specific features which characterize the inelastic processes (taking place via an electronic transition) of vibrationally ex-

cited molecules with respect to those involving ground state molecules: (i) the threshold for an inelastic process involving a vibrationally excited molecule decreases with increasing vibrational excitation of the molecule, and (ii) the cross section of the process increases (for some processes dramatically) with the increase of vibrational excitation of the

molecule. The electron-impact inelastic processes involving vibrationally excited hydrogen molecules play a critical role in multicusp magnetic plasmas ( $H^-/D^-$  ion sources) [1, 2] and in plasma kinetics of cold divertor regions of magnetic fusion devices [3]. For a consistent description of the phenomena taking place in such plasmas, in particular for modeling their radiative and transport properties, it is of critical importance to have a complete, and as accurate as possible, cross section database for the electron-impact (and other) collision processes. A large amount of cross section information on electron-impact processes of vibrationally excited molecular hydrogen and its isotopic variants has been generated in theoretical calculations in our laboratories and compared with the limited independently derived data available in literature. An attempt has recently been made to collect this information, and present it in a systematic manner and in a form appropriate for use in practical applications (e.g., plasma studies) [4]. In this paper we present in a more compact way the same information, illustrating in graphical form the cross section data, as a function of both incident electron energy and vibrational levels of the molecule. Scaling laws and relationships for some processes, which allow a rapid evaluation of cross section data or their extension to situations for which more reliable information is not available, are also provided. The numerical cross section data can be also accessed, in electronic form, as Supplementary Material (<http://www.idealibrary.com/links/doi/10.1006/adnd.2000.0850/dat>) in association with this article on IDEAL.

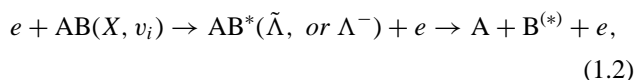
The electron-impact processes covered by the present article are as follows (A and B designate any hydrogen atom isotope):

—nondissociative electronic excitation,



(where  $X$  is the ground electronic state of the molecule  $AB$ ,  $\Lambda$  is the electronic state of the excited molecule  $AB^*$ , and  $v_i$  denotes the vibrational state of the initial electronic (ground) state);

—dissociative electronic excitation,



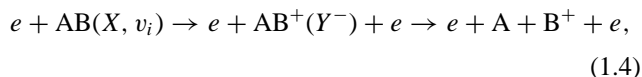
(where  $\tilde{\Lambda}$  is the continuum part of the bound electronic state  $\Lambda$ ,  $\Lambda^-$  denotes a repulsive electronic state, and A and  $B^{(*)}$  indicate the atomic dissociation products. B may also be in an excited electronic state);

—ionization



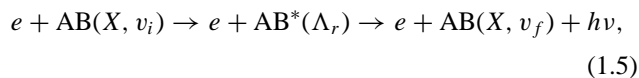
(where  $Y$  denotes a bound state of the ion  $AB^+$ );

—dissociative ionization,



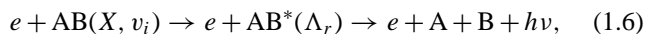
(where  $Y^-$  is a dissociative state of the ion  $AB^+$ );

—excitation-radiative decay vibrational excitation,

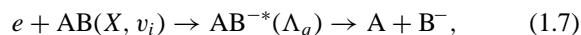


(where  $\Lambda_r$  is an electronic excited state that is radiatively coupled with the ground state  $X$ ,  $v_i, v_f$  are the initial and final vibrational quantum numbers);

—excitation-radiative decay dissociation,

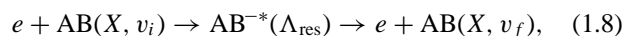


—dissociative electron attachment,



(where  $\Lambda_q$  is a quasi-stationary, resonant state).

Due to insufficient data information for the resonant excitation,



(where  $\Lambda_{\text{res}}$  is a resonant state of  $AB^-$ ), particularly for the heavier isotopic variants, this process has not been included in the present database.

When we do not differentiate between the dissociative and nondissociative channels of the excitation of a bound state  $\Lambda$ , we call the process simply electronic excitation, and refer to the sum of the corresponding dissociative and nondissociative cross sections as total excitation cross section. The processes (1.1)–(1.7) have been the subject of extensive theoretical (and a limited number of experimental) studies, and cross sections have been generated for many of the isotopic combinations of hydrogen. We have taken as a basis for the present database our previous publications, where the cross section data have been discussed and compared with any existing experiment and theory. The following publications have been considered:

- dissociative and nondissociative excitation: Refs. [5–10],
- dissociative ionization: Refs. [10–11],
- excitation-radiative decay processes: Refs. [12–13],
- dissociative electron attachment: Refs. [4, 14].

For the total excitation and dissociative ionization cross sections certain scaling relationships were established recently [8, 15, 16] both with respect to the vibrational quantum number and the isotope mass. The isotope effect in the dissociative electron attachment process has been known to exist from the early 1960s [17] and was recently discussed in more detail [18]. Although there is no clear physical basis for establishing a scaling relationship for the vibrational dependence of the dissociative electron attachment cross sections, they can be nevertheless expressed in a compact approximate analytic form [14].

The present article is organized as follows. In Section 2 we give a brief description of the various collision processes. In Section 3 we report a complete list of all the processes included in the paper, and in Section 4 we present the cross sections of specifically studied reactions by analytic-fit functions (with respect to their energy and vibrational quantum number dependence) and discuss the mass scaling relationships which should provide cross section information for the isotopic hydrogen molecule cases for which specific calculations have not been performed.

## 2. BRIEF DESCRIPTION OF COLLISION PROCESSES

In this section we comment briefly on the various electron-molecule collision processes included in this paper. For the theoretical methods used to evaluate the related cross sections and for the numerical details of the calculation, the reader is referred to the cited literature.

The corresponding potential energy curves for the considered molecular electronic states are shown in Fig. 1.

### 2.1. Excitation and Ionization

Electronic excitation processes by electron impact considered here involve molecules of hydrogen (or one of its isotopic variants) initially in a given vibrational level belonging to an  $\alpha_i$  electronic state. The molecule, after the collision, is left either in the bound vibrational manifold of the excited electronic state (see Process 1.1) or in the continuum one (Process 1.2). In this last case dissociation takes place. The *total cross section*  $\sigma_{v_i}^{\alpha_i \rightarrow \alpha_f}(E)$  for these processes is

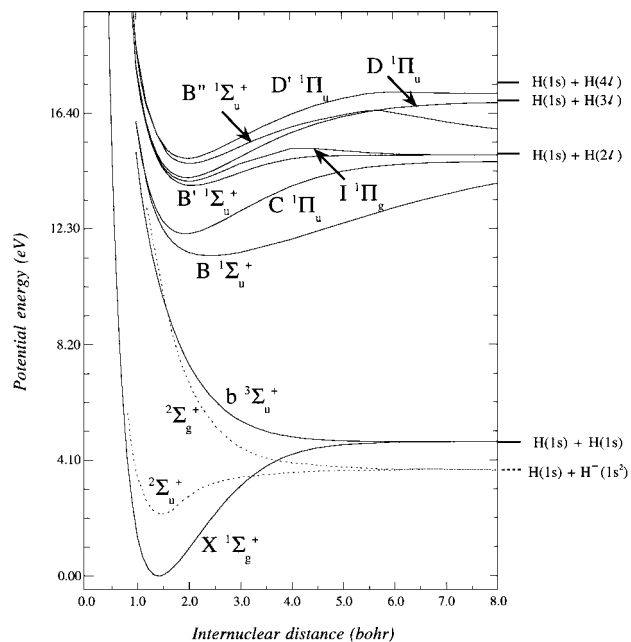


FIG. 1. Schematic potential energy diagram for the H<sub>2</sub> molecule.

defined as

$$\sigma_{v_i}^{\alpha_i \rightarrow \alpha_f}(E) = \sum_{v_f} \sigma_{v_i, v_f}^{\alpha_i \rightarrow \alpha_f}(E) + \int d\varepsilon \frac{d\sigma_{v_i, \varepsilon}^{\alpha_i \rightarrow \alpha_f}(E)}{d\varepsilon}, \quad (2.1)$$

where  $v_i$  and  $v_f$  indicate the quantum number of the vibrational levels belonging to  $\alpha_i$  and  $\alpha_f$  electronic states, respectively,  $\varepsilon$  is the energy of the continuum state of the  $\alpha_f$  electronic state, and  $E$  is the incident electron energy. The two terms on the right hand side of Eq. (2.1) represent the contributions to the total cross section coming, respectively, from the nondissociative (bound-to-bound) and dissociative (bound-to-continuum) excitations.

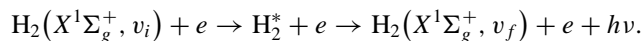
In the present paper the following singlet–singlet (optically allowed) transitions have been included:  $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ ,  $X^1\Sigma_g^+ \rightarrow C^1\Pi_u$ ,  $X^1\Sigma_g^+ \rightarrow B'^1\Sigma_u^+$ ,  $X^1\Sigma_g^+ \rightarrow D^1\Pi_u$ ,  $X^1\Sigma_g^+ \rightarrow B''^1\Sigma_u^+$ ,  $X^1\Sigma_g^+ \rightarrow D'^1\Pi_u$ ,  $B^1\Sigma_u^+ \rightarrow I^1\Pi_g$ . The states B', D, B'', D' are usually referred to as low-lying Rydberg states. All the transitions start from the ground state  $X^1\Sigma_g^+$ , except the last one which involves two excited electronic states. The related dissociative and total cross sections (the bound-to-bound non-dissociative cross sections can be obtained from (2.1) by subtraction) have been calculated as a function of both the incident energy and the initial vibrational quantum number  $v_i$ , by using the quantum-mechanical impact parameter method [5, 7, 8, 13, 19, 20].

Cross sections, obtained by using a semiclassical method [9, 21], are reported also for the singlet–triplet (optically forbidden) transition  $X^1\Sigma_g^+ \rightarrow b^3\Sigma_u$ , which is the main dissociative channel for the hydrogen molecule.

The same semiclassical method has been employed also for the evaluation of electron-impact dissociative and nondissociative ionization cross sections [10, 11]. The calculation has been performed for both the H<sub>2</sub> and D<sub>2</sub> molecules by considering the nondissociative ionization (1.3) through the  $^2\Sigma_g^+$  electronic state of the H<sub>2</sub><sup>+</sup> and D<sub>2</sub><sup>+</sup> molecules, and the dissociative ionization (1.4) occurring either through the repulsive part of the  $^2\Sigma_g^+$  state or through the completely repulsive state  $^2\Sigma_u^+$  of the molecular ion.

## 2.2. Excitation-Radiative Decay Vibrational Excitation and Dissociation

The excitation-radiative decay process (1.5), also known in plasma chemistry as the E-V process, can be explicitly sketched, for a hydrogen molecule, as



It can be regarded as a two-step process leading to vibrational excitation. The molecule, initially in its ground electronic state and in a given vibrational level  $v_i$ , is excited by electron impact to a singlet state, represented by H<sub>2</sub><sup>\*</sup>, which can radiatively decay again on the same vibrational manifold ( $v_f$ ), populating in particular the higher levels [22]. This is the main channel in negative ion sources leading to a strong non-Boltzmann vibrational distribution of the hydrogen plasma.

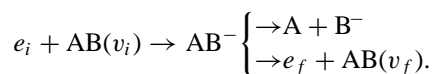
Dissociation can also occur for those molecules falling in the continuum branch of the ground electronic state.

Vibrational and dissociative excitation cross sections for this two-step process have been obtained for both H<sub>2</sub> and D<sub>2</sub> molecules [12, 13], including in the electron-impact excitation step (leading to H<sub>2</sub><sup>\*</sup> or D<sub>2</sub><sup>\*</sup> formation) both the  $B^1\Sigma_u^+$  and  $C^1\Pi_u$  singlet states.

## 2.3. Dissociative Electron Attachment

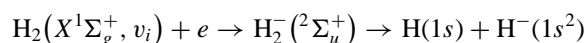
In the resonance model, the physics of the process of dissociative electron attachment to a molecule AB is described via the formation of a temporary bound state of the electron-molecule system [23, 24]. The electron in this molecular anion state AB<sup>−</sup> (also called the resonant state) can autodetach with a finite lifetime (related to the width,  $\Gamma$ , of the resonance), leaving behind a vibrationally excited neutral molecule. On the other hand, if the lifetime of the resonance is long enough, the anion AB<sup>−</sup> can dissociate into A + B<sup>−</sup>, leading to the process of dissociative electron attachment.

Thus, in a schematic sense one has



The final level with quantum number  $v_f$  can be either discrete (corresponding to vibrational excitation of the molecule) or could lie in the continuum (corresponding to dissociation of the molecule).

Specifically, for molecular hydrogen (and its heavier isotopic variants) the lowest resonant state is the  $^2\Sigma_u^+$  state of H<sub>2</sub><sup>−</sup> (see Fig. 1). This is a shape resonance, with the  $X^1\Sigma_g^+$  state of H<sub>2</sub> as its parent, for internuclear separations less than 3 a.u. The next higher resonant state of H<sub>2</sub><sup>−</sup> is the  $^2\Sigma_g^+$  state, but its contribution to the dissociative attachment at low energies can be neglected [25, 26]. In the present article we include the results obtained [4, 14] within the nonlocal version of the resonance model for the  $^2\Sigma_u^+$  resonant state of H<sub>2</sub><sup>−</sup> only, i.e., for the process



and for its other five isotopic versions (HD, HT, D<sub>2</sub>, DT, and T<sub>2</sub>).

The computational procedure is somewhat involved and is described elsewhere [27, 28].

## 3. CROSS SECTION DATA

The calculated cross sections data refer to the electron impact inelastic processes given in Table A. Each process is labeled by a Roman number plus a, b, c, d, e, f to indicate H<sub>2</sub>, D<sub>2</sub>, T<sub>2</sub>, DT, HD, and HT, respectively. The corresponding data tables, accessible as downloadable files on IDEAL (<http://www.idealibrary.com/links/doi/10.1006/adnd.2000.0850/dat>), are identified using the same classification labels.

## 4. ANALYTICAL FITS OF THE DATA AND SCALING RELATIONSHIPS

In this section we give analytical fits of the numerical cross section data for some of the transitions discussed in the previous sections and also provide some “vibrational” and “mass” scaling relationships, which permit a rapid evaluation of the cross sections as a function of the vibrational quantum number as well as an extension of the present results to other hydrogen isotopes for which cross section data are not available.

The vibrational energy eigenvalues for all isotopic variants of H<sub>2</sub>, useful in the scaling and fits relationships, are given in Table B.

**TABLE A**  
List of Electron Impact Inelastic Processes

Process	Identification label
<b>Dissociative excitation</b>	
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B^1\Sigma_u^+) + e \rightarrow 2H + e$	Ia
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B^1\Sigma_u^+) + e \rightarrow 2D + e$	Ib
$T_2(X^1\Sigma_g^+, v_i) + e \rightarrow T_2(B^1\Sigma_u^+) + e \rightarrow 2T + e$	Ic
$DT(X^1\Sigma_g^+, v_i) + e \rightarrow DT(B^1\Sigma_u^+) + e \rightarrow D + T + e$	Id
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(C^1\Pi_u) + e \rightarrow 2H + e$	IIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(C^1\Pi_u) + e \rightarrow 2D + e$	IIb
$T_2(X^1\Sigma_g^+, v_i) + e \rightarrow T_2(C^1\Pi_u) + e \rightarrow 2T + e$	IIc
$DT(X^1\Sigma_g^+, v_i) + e \rightarrow DT(C^1\Pi_u) + e \rightarrow D + T + e$	IId
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B'^1\Sigma_u^+) + e \rightarrow 2H + e$	IIIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B'^1\Sigma_u^+) + e \rightarrow 2D + e$	IIIb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(D^1\Pi_u) + e \rightarrow 2H + e$	IVa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(D^1\Pi_u) + e \rightarrow 2D + e$	IVb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B''^1\Sigma_u^+) + e \rightarrow 2H + e$	Va
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B''^1\Sigma_u^+) + e \rightarrow 2D + e$	Vb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(D'^1\Pi_u) + e \rightarrow 2H + e$	VIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(D'^1\Pi_u) + e \rightarrow 2D + e$	VIb
$H_2(B^1\Sigma_u^+, v_i) + e \rightarrow H_2(I^1\Pi_g) + e \rightarrow 2H + e$	VIIa
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(b^3\Sigma_u^+) + e \rightarrow 2H + e$	VIIIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(b^3\Sigma_u^+) + e \rightarrow 2D + e$	VIIIb
<b>Total excitation</b>	
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B^1\Sigma_u^+) + e$	IXa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B^1\Sigma_u^+) + e$	IXb
$T_2(X^1\Sigma_g^+, v_i) + e \rightarrow T_2(B^1\Sigma_u^+) + e$	IXc
$DT(X^1\Sigma_g^+, v_i) + e \rightarrow DT(B^1\Sigma_u^+) + e$	IXd
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(C^1\Pi_u) + e$	Xa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(C^1\Pi_u) + e$	Xb
$T_2(X^1\Sigma_g^+, v_i) + e \rightarrow T_2(C^1\Pi_u) + e$	Xc
$DT(X^1\Sigma_g^+, v_i) + e \rightarrow DT(C^1\Pi_u) + e$	Xd
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B'^1\Sigma_u^+) + e$	XIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B'^1\Sigma_u^+) + e$	XIb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(D^1\Pi_u) + e$	XIIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(D^1\Pi_u) + e$	XIIb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B''^1\Sigma_u^+) + e$	XIIIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B''^1\Sigma_u^+) + e$	XIIIb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(D'^1\Pi_u) + e$	XIVa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(D'^1\Pi_u) + e$	XIVb
$H_2(B^1\Sigma_u^+, v_i) + e \rightarrow H_2(I^1\Pi_g) + e$	XVa
<b>Dissociative ionization</b>	
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^+(X^2\Sigma_g^+) + 2e$ $\rightarrow H + H^+ + 2e$	XVIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2^+(X^2\Sigma_g^+) + 2e$ $\rightarrow D + D^+ + 2e$	XVIb
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^+(^2\Sigma_u^+) + 2e$ $\rightarrow H + H^+ + 2e$	XVIIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2^+(^2\Sigma_u^+) + 2e$ $\rightarrow D + D^+ + 2e$	XVIIb
<b>Nondissociative ionization</b>	
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2^+(X^2\Sigma_g^+) + 2e$	XVIIIb

**TABLE A—Continued**

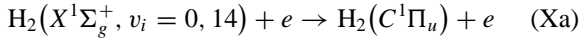
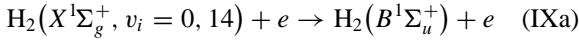
Process	Identification label
<b>Excitation-radiative decay vibrational excitation</b>	
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^*(B^1\Sigma_u^+, C^1\Pi_u) + e$ $\rightarrow H_2(X^1\Sigma_g^+, v_f) + e + h\nu$	XIXa1–15
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2^*(B^1\Sigma_u^+, C^1\Pi_u) + e$ $\rightarrow D_2(X^1\Sigma_g^+, v_f) + e + h\nu$	XIXb1–8
<b>Excitation-radiative decay dissociation</b>	
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^*(B^1\Sigma_u^+, C^1\Pi_u)$ $+ e \rightarrow H_2(X^1\Sigma_g^+) + e + h\nu$ $\downarrow$ $H + H + e$	XXa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2^*(B^1\Sigma_u^+, C^1\Pi_u)$ $+ e \rightarrow D_2(X^1\Sigma_g^+) + e + h\nu$ $\downarrow$ $D + D + e$	XXb
<b>Dissociative electron attachment</b>	
$H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^-(^2\Sigma_u^+) \rightarrow H + H^-$	XXIa
$D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2^-(^2\Sigma_u^+) \rightarrow D + D^-$	XXIb
$T_2(X^1\Sigma_g^+, v_i) + e \rightarrow T_2^-(^2\Sigma_u^+) \rightarrow T + T^-$	XXIc
$DT(X^1\Sigma_g^+, v_i) + e \rightarrow DT^-(^2\Sigma_u^+) \rightarrow D + T^-$	XXId
$HD(X^1\Sigma_g^+, v_i) + e \rightarrow HD^-(^2\Sigma_u^+) \rightarrow H + D^-$	XXIe
$HT(X^1\Sigma_g^+, v_i) + e \rightarrow HT^-(^2\Sigma_u^+) \rightarrow H + T^-$	XXIf

**TABLE B**  
Vibrational Energies (eV) for Nonrotational States of Hydrogen Molecule and Its Isotopic Variants taken from Ref. [30]

$v_i$	H <sub>2</sub>	D <sub>2</sub>	T <sub>2</sub>	HD	HT	DT
0	0.269621	0.191437	0.156698	0.233935	0.220739	0.174955
1	0.785643	0.562637	0.462281	0.684342	0.646680	0.515117
2	1.272478	0.919064	0.757944	1.112742	1.053012	0.842929
3	1.730734	1.260982	1.043845	1.519570	1.440112	1.158600
4	2.160789	1.588593	1.320108	1.905130	1.808254	1.462292
5	2.562770	1.902047	1.586839	2.269597	2.157612	1.754136
6	2.936514	2.201432	1.844114	2.612993	2.488243	2.034220
7	3.281535	2.486772	2.091988	2.935174	2.800074	2.302590
8	3.596933	2.758012	2.330482	3.235814	3.092897	2.559235
9	3.881305	3.015025	2.559587	3.514346	3.366335	2.804102
10	4.132594	3.257592	2.779258	3.769939	3.619805	3.037081
11	4.347968	3.485377	2.989420	4.001410	3.852505	3.257992
12	4.523470	3.697942	3.189955	4.207173	4.063305	3.466576
13	4.653525	3.894680	3.380690	4.385146	4.250775	3.662508
14	4.730414	4.074808	3.561412	4.532532	4.413019	3.845342
15		4.237378	3.731847	4.645552	4.547566	4.014501
16		4.381146	3.891630	4.719242	4.651099	4.169322
17		4.504592	4.040336		4.719374	4.308939
18		4.605719	4.177461			4.432312
19		4.682042	4.302368			4.538137
20		4.730468	4.414316			4.624762
21			4.512393			4.690197
22			4.595471			4.731982
23			4.662200			
24			4.710992			

#### 4.1. Electronic Excitation

Total cross sections for the processes



and the corresponding ones for D<sub>2</sub> (IXb, Xb), have been put in analytical form [29] by using the following expressions ( $E_{\min}$  and  $\bar{E}$  are defined below).

$$\underline{X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+ \text{ transition}}$$

For  $E_{\min} \leq E \leq \bar{E}$

$$\sigma_{v_i}^{X \rightarrow B}(E) = c_1 x e^{(-c_2 x)} + c_4 x^{c_5}, \quad (4.1)$$

where  $x = E - c_3$ .

For  $E \geq \bar{E} + 1 \text{ eV}$

$$\begin{aligned} \sigma_{v_i}^{X \rightarrow B}(E) &= \frac{c_6}{x} \left( \frac{x-1}{x+1} \right)^{c_{10}} \left[ c_7 + c_8 \left( 1 - \frac{1}{2x} \right) \ln(c_9 + \sqrt{x-1}) \right], \end{aligned} \quad (4.2)$$

where  $x = E/\Delta E$ .

$$\underline{X^1\Sigma_g^+ \rightarrow C^1\Pi_u \text{ transition}}$$

For  $E_{\min} \leq E \leq \bar{E}$

$$\sigma_{v_i}^{X \rightarrow C}(E) = c_1 x e^{(-c_2 x)} + c_4 x^{c_5} + c_6 x e^{(-c_7 x)}, \quad (4.3)$$

where  $x = E - c_3$ .

For  $E \geq \bar{E} + 1 \text{ eV}$

$$\begin{aligned} \sigma_{v_i}^{X \rightarrow C}(E) &= \frac{c_8}{x^{c_{13}}} \left( \frac{x-1}{x+1} \right)^{c_{12}} \left[ c_9 + c_{10} \left( 1 - \frac{1}{2x} \right) \ln(c_{11} + \sqrt{x-1}) \right], \end{aligned} \quad (4.4)$$

where  $x = E/\Delta E$ .

The energy is expressed in eV and the cross section in Å<sup>2</sup>.

Expressions (4.1) and (4.3) have been used to properly smooth out the small maximum arising in the cross sections for low incident energies ( $E \leq \bar{E}$ ) and which is an artifact of

the computational method. The parameter  $E_{\min}$  is very close to the threshold energy, so that for  $E < E_{\min}$  the cross section is assumed to be zero. Far from the threshold ( $E > \bar{E} + 1 \text{ eV}$ ) the cross sections have been fitted by using the expressions (4.2) and (4.4), where  $x$  is defined in terms of transition energy  $\Delta E$ . The cross sections in the energy range  $\bar{E} < E < \bar{E} + 1 \text{ eV}$  can be obtained by interpolation.

All the parameters  $\bar{E}$ ,  $E_{\min}$ , and  $\Delta E$  depend on the vibrational quantum number  $v_i$ . Their values, together with the fitting coefficients  $c_i$  and the percentage rms deviation (i.e., the root mean square (rms) average of the relative deviations of the fitted from the calculated values in %) are given in Tables I–IV.

A vibrational scaling law for the total cross sections of processes (IXa) and (Xa) can be obtained from the equations of the impact-parameter method and can be written as [6, 15]

$$\sigma_{v_i}^{X \rightarrow \alpha_f}(x) = \tilde{\sigma}^{X \rightarrow \alpha_f}(x) \frac{1}{|\Delta E^{X \rightarrow \alpha_f}(R_{v_i})|^\gamma}, \quad (4.5)$$

where  $x = E/\Delta E^{X \rightarrow \alpha_f}(R_{v_i})$  is the *reduced energy* and  $R_{v_i}$  is the largest classical turning point for the  $v_i$ th vibrational level.  $\tilde{\sigma}^{X \rightarrow \alpha_f}(x)$  is a “shape function,” practically independent of the mass, obtained by an averaging procedure [15], which includes, through  $x$ , the dependence of the total cross section on the incident energy.  $\gamma$  is a numerical exponent, set to 3 for  $X \rightarrow B$  and to 2 for  $X \rightarrow C$  transition.

The shape function  $\tilde{\sigma}^{X \rightarrow \alpha_f}(x)$  is expressed in analytical form as [6, 15]

$$X \rightarrow B \quad \tilde{\sigma}^{X \rightarrow B}(x) = \frac{1}{x} [c_1 e^{-c_2 \cdot x} + c_3 \ln(c_4 \cdot x)] \quad (4.6)$$

$$X \rightarrow C \quad \tilde{\sigma}^{X \rightarrow C}(x) = c_1 e^{-c_2 \cdot x} + c_3 \ln(c_4 \cdot x). \quad (4.7)$$

The fitting coefficients  $c_i$  ( $i = 1, 4$ ) are given in Table C. The transition energies  $\Delta E^{X \rightarrow \alpha_f}(R_{v_i})$ , defined as the difference (evaluated at the classical turning point  $R_{v_i}$ ) between the potential energies for the two electronic states involved in the transition, are given in Table D.

**TABLE C**  
Fitting Coefficient for the Function  $\tilde{\sigma}^{X \rightarrow \alpha_f}(x)$

	$\tilde{\sigma}^{X \rightarrow B}(x)$	$\tilde{\sigma}^{X \rightarrow C}(x)$
$c_1$	4926.0 (Å <sup>2</sup> · eV <sup>3</sup> )	−172.49 (Å <sup>2</sup> · eV <sup>2</sup> )
$c_2$	1.9586	0.74392
$c_3$	2312.2 (Å <sup>2</sup> · eV <sup>3</sup> )	27.212 (Å <sup>2</sup> · eV <sup>2</sup> )
$c_4$	0.82802	0.014272

**TABLE D**

$X \rightarrow B$  and  $X \rightarrow C$  Vertical Transition Energies  $\Delta E$  (eV) for the H<sub>2</sub> Molecule as a Function of the Vibrational Quantum Number  $v_i$

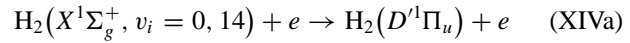
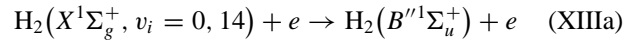
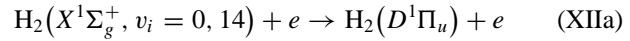
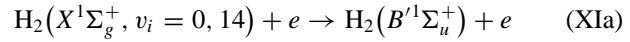
$v_i$	$\Delta E(X \rightarrow B)$	$\Delta E(X \rightarrow C)$
0	11.61	12.28
1	10.75	11.61
2	10.13	11.12
3	9.62	10.81
4	9.19	10.53
5	8.81	10.30
6	8.48	10.12
7	8.21	9.97
8	7.97	9.86
9	7.80	9.80
10	7.68	9.78
11	7.64	9.79
12	7.70	9.88
13	7.94	10.01
14	9.11	10.21

Total cross sections for processes (IXb, IXc, IXd) and (Xb, Xc, Xd) for the other isotopic variants can be obtained by using Eq. (4.5) as well. The required transition energies can be obtained from the corresponding ones for the H<sub>2</sub> molecule, by applying a mass-scaling law based on the correspondence among the vibrational eigenvalues for the various isotopes [8]. According to this scaling law, the  $v_i$ th vibrational level for a given isotope should have the same energy eigenvalue as a pseudo-vibrational level of the hydrogen molecule whose (noninteger) quantum number  $v'$  is [6, 8]

$$v' = \sqrt{\frac{\mu_{H_2}}{\mu_I}} v_i \quad (4.8)$$

and where  $\mu_{H_2}$  and  $\mu_I$  represent the reduced mass for the hydrogen molecule and the isotopic variant, respectively. The vertical transition energy for the “level”  $v'$ , equal to the  $\Delta E(R_{v_i})$  for the isotope, can be obtained by linear interpolation of the data given in Table D.

The vibrational scaling for the processes



has the form [8]

$$\begin{aligned} \sigma_{v_i}^{X \rightarrow \alpha_f}(x) = & \sigma_{v_i=1}^{X \rightarrow \alpha_f}(x) \left[ \frac{\Delta E_{v_i=1}}{\Delta E_{v_i}} \right]^{(1+c_1 v_i^{c_2})(c_3+(2/x)^{c_4})} \\ & \times \left\{ c_5 + c_6 v_i + \left( \frac{c_7}{x^{c_8}} + c_9 \right) v_i^2 + c_{10} v_i^3 \right. \\ & \left. + \left( \frac{c_{11}}{x^{c_8}} + c_{12} \right) v_i^4 \right\}, \end{aligned} \quad (4.9)$$

where  $\Delta E_{v_i}$  is the transition energy for  $v_i$ th vibrational level and  $x = E/\Delta E_{v_i}$ . Equation (4.9) gives the total cross section for each vibrational level in terms of the  $v_i = 1$  total cross section  $\sigma_{v_i=1}^{X \rightarrow \alpha_f}(x)$ . This last quantity, together with the  $v_i = 0$  cross section, can be obtained in analytical form as [8]

$$\sigma_{v_i=0,1}^{X \rightarrow \alpha_f}(x) = \frac{1}{x} [a_1 e^{-a_2 x} + a_3 \ln(a_4 x)]. \quad (4.10)$$

The fitting coefficients  $a_i$  ( $i = 1, 4$ ) and the transition energies, entering Eq. (4.9), for  $v_i = 0, 1$  for the XIa–XIVa processes, are given in Table E, while the coefficients  $c_i$  are listed in Table F.

Total cross sections for the isotopic variants can also be obtained by using Eq. (4.9) by replacing  $v_i$  by  $v'$ , calculated from Eq. (4.8), and by evaluating the transition energies at the classical turning point of the “ $v'$ th” level for the given isotope [8, 31].

**TABLE E**

Fitting Coefficients  $a_i$  and Transition Energies  $\Delta E_{v_i}$  for the  $v_i = 0, 1$  H<sub>2</sub> Cross Sections

	$X \rightarrow B'$		$X \rightarrow D$		$X \rightarrow B''$		$X \rightarrow D'$	
	$v_i = 0$	$v_i = 1$	$v_i = 0$	$v_i = 1$	$v_i = 0$	$v_i = 1$	$v_i = 0$	$v_i = 1$
$a_1(\text{\AA}^2)$	−0.0828	−0.114	−0.0399	−0.0507	0.586	0.529	0.278	0.288
$a_2$	0.387	0.371	0.456	0.419	1.678	1.238	1.867	1.544
$a_3(\text{\AA}^2)$	0.187	0.215	0.0694	0.0776	0.310	0.361	0.127	0.145
$a_4$	1.334	1.352	1.494	1.514	0.794	0.698	0.781	0.703
$\Delta E_{v_i}$ (eV)	14.85	13.09	15.67	13.86	14.99	13.35	15.66	14.04

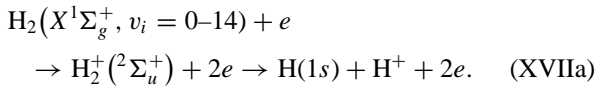


**TABLE F**  
Scaling Relation  $c_i$  Coefficients

Coefficient	$X \rightarrow B'$	$X \rightarrow D$	$X \rightarrow B''$	$X \rightarrow D'$
$c_1$	0.0	$2.93 \times 10^{-3}$	0.0	$1.1 \times 10^{-4}$
$c_2$	0.0	2.25	0.0	3.6
$c_3$	2.0	1.0	$-2.0 \times 10^{-1}$	0.55
$c_4$	0.0	0.20	0.0	0.26
$c_5$	1.1	1.0	1.1	1.0
$c_6$	$-1.3 \times 10^{-1}$	0.0	$-1.3 \times 10^{-1}$	0.0
$c_7$	$1.94 \times 10^{-2}$	0.0	$1.26 \times 10^{-2}$	0.0
$c_8$	$7.0 \times 10^{-1}$	0.0	$5.0 \times 10^{-1}$	0.0
$c_9$	$2.42 \times 10^{-2}$	0.0	$3.44 \times 10^{-2}$	0.0
$c_{10}$	$-3.2 \times 10^{-3}$	0.0	$-5.4 \times 10^{-3}$	0.0
$c_{11}$	$-1.08 \times 10^{-4}$	0.0	$-9.20 \times 10^{-5}$	0.0
$c_{12}$	$1.36 \times 10^{-4}$	0.0	$2.55 \times 10^{-4}$	0.0

#### 4.2. Dissociative Ionization

Equation (4.5) can also be used to describe the cross section for the dissociative ionization process [11, 16]



The  $\gamma$ -exponent in Eq. (4.5) equals 2.18 in this case. The transition energies at the classical turning point are given in Table G. The shape function has the form [16],

$$\tilde{\sigma}^{X \rightarrow ^2\Sigma_u^+}(x) = \frac{c_1}{x} \left( \frac{x-1}{x} \right)^{c_2} (1 + c_3 \ln x), \quad (4.11)$$

where  $c_1 = 20013 \text{ (}\text{\AA}^2\text{eV}^\gamma\text{)}$ ,  $c_2 = 2.63323$ , and  $c_3 = 0.57363$ .

Cross sections for the other isotopic variants can be obtained by using once again Eq. (4.8) for evaluating the transition energies and by assuming the shape function, given by Eq. (4.11), as independent of the mass.

#### 4.3. Dissociative Electron Attachment

For all six isotopic versions of H<sub>2</sub> the attachment cross sections show a peak at the threshold and a rapid reduction in magnitude as the electron energy is increased above the threshold  $E_{\text{th}}$ . The attachment cross sections can be fitted

**TABLE H**

Threshold Energy  $E_{\text{th}}$  (eV) and Peak Cross Section ( $\text{\AA}^2$ ), as a Function of the Initial Vibrational Quantum Number  $v_i$ , for Dissociative Electron Attachment to Vibrationally Excited H<sub>2</sub> and Its Isotopic Variants

$v_i$	H <sub>2</sub>		HD		HT	
	$E_{\text{th}}$	$\sigma_{\text{peak}}$	$E_{\text{th}}$	$\sigma_{\text{peak}}$	$E_{\text{th}}$	$\sigma_{\text{peak}}$
0	3.73	1.65 (-05)	3.76	1.57 (-06)	3.78	5.35 (-07)
1	3.21	5.54 (-04)	3.31	6.52 (-05)	3.35	2.30 (-05)
2	2.73	7.92 (-03)	2.88	1.13 (-03)	2.95	4.34 (-04)
3	2.27	6.33 (-02)	2.48	1.16 (-02)	2.56	4.76 (-03)
4	1.84	3.22 (-01)	2.09	7.56 (-02)	2.19	3.39 (-02)
5	1.44	1.16 (+00)	1.73	3.36 (-01)	1.84	1.66 (-01)
$v_i$	D <sub>2</sub>		DT		T <sub>2</sub>	
	$E_{\text{th}}$	$\sigma_{\text{peak}}$	$E_{\text{th}}$	$\sigma_{\text{peak}}$	$E_{\text{th}}$	$\sigma_{\text{peak}}$
0	3.81	3.11 (-08)	3.82	3.36 (-09)		
1	3.44	1.52 (-06)	3.48	2.04 (-07)	3.54	1.39 (-08)
2	3.08	3.33 (-05)	3.16	5.07 (-06)	3.25	3.89 (-07)
3	2.74	4.28 (-04)	2.84	7.67 (-05)	2.96	6.61 (-06)
4	2.41	3.70 (-03)	2.54	7.64 (-04)	2.68	7.78 (-05)
5	2.10	2.37 (-02)	2.25	5.46 (-03)	2.41	6.66 (-04)
6	1.80	1.08 (-01)	1.97	2.91 (-02)	2.16	4.17 (-03)
7					1.91	2.09 (-02)

with high accuracy to the expression

$$\sigma_{\text{DA}}(E) = \sigma_{\text{peak}} \exp[-(E - E_{\text{th}})/E_0], \quad (4.12)$$

where  $\sigma_{\text{peak}}$  is the cross section value at the threshold and  $E_0$  is a fitting parameter. The parameter  $E_0$  has the value, in eV, 0.45, 0.39, 0.36, 0.32, 0.30, and 0.28 for H<sub>2</sub>, HD, HT, D<sub>2</sub>, DT, and T<sub>2</sub> respectively.  $\sigma_{\text{peak}}$  and  $E_{\text{th}}$  are given in Table H.

Assuming a Maxwellian distribution for electron energies, the rate of electron attachment can be written in terms of an analytical expression of the form

$$k(\langle E \rangle) = \left( \frac{27}{\pi} \frac{\langle E \rangle}{m} \right)^{1/2} \sigma_{\text{peak}} \exp \left( -\frac{3E_{\text{th}}}{2\langle E \rangle} \right) \times \left[ \left( \frac{3}{2} + \frac{\langle E \rangle}{E_0} \right)^{-2} + \frac{E_{\text{th}}}{\langle E \rangle} \left( \frac{3}{2} + \frac{\langle E \rangle}{E_0} \right)^{-1} \right], \quad (4.13)$$

where  $\langle E \rangle = 3kT/2$  and  $T$  is the electron temperature.

**TABLE G**  
Transition Energies  $\Delta E_{v_i}$  (eV) for the Dissociative Ionization of H<sub>2</sub> Molecule, Evaluated at the Classical Turning Point of the  $v_i$ th Vibrational Level of the Electronic Ground State

$v_i$	0	1	2	3	4	5	6	7	8	9	10	11	12	13
$\Delta E_{v_i}$	30.6	27.4	25.2	23.4	21.9	20.6	19.6	18.5	17.6	16.7	16.0	15.4	14.8	14.2

### Acknowledgment

This work has been partially supported by MURST (Project 9903102919–004).

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## EXPLANATION OF GRAPHS

GRAPHS I–VIII.	Dissociative Excitation Cross Sections
GRAPHS IX–XV.	Total Excitation Cross Sections
GRAPHS XVI, XVII.	Dissociative Ionization Cross Sections
GRAPH XVIII.	Non-Dissociative Ionization Cross Sections
GRAPH XIX.	Excitation-Radiative Decay Vibrational Excitation Cross Sections
GRAPH XX.	Excitation-Radiative Decay Dissociation Cross Sections
GRAPH XXI.	Dissociative Electron Attachment Cross Sections

The calculated cross sections, for a given process as indicated at the top of each graph, are plotted for all vibrational levels of the molecule as a function of incident electron energy

The cross sections are expressed in  $\text{\AA}^2$  and the energy in eV.

$v_i$	initial vibrational quantum number of the molecule
$v_f$	final vibrational quantum number of the molecule

Graphs are labeled with the same identification Roman numeral as in Table A, with a, b, c, d, e, and f (here given in parentheses inside each graph) referring to  $\text{H}_2$ ,  $\text{D}_2$ ,  $\text{T}_2$ ,  $\text{DT}$ ,  $\text{HD}$ , and  $\text{HT}$ , respectively.

Each graph for the radiative decay process in hydrogen (XIXa) and deuterium (XIXb) refers to a given value of initial vibrational quantum number  $v_i$ , while each cross section curve is identified by the final vibration quantum number  $v_f$ . The value  $v_f = v_i$ , corresponding to the largest cross section, is explicitly indicated in the plot. For the  $\text{H}_2$  molecule, cross section data are given for  $v_i = 0\text{--}14$ , for the  $\text{D}_2$  molecule they are available only for  $v_i = 0, 5, 7, 10, 14, 15, 17, 20$ .

## EXPLANATION OF TABLES

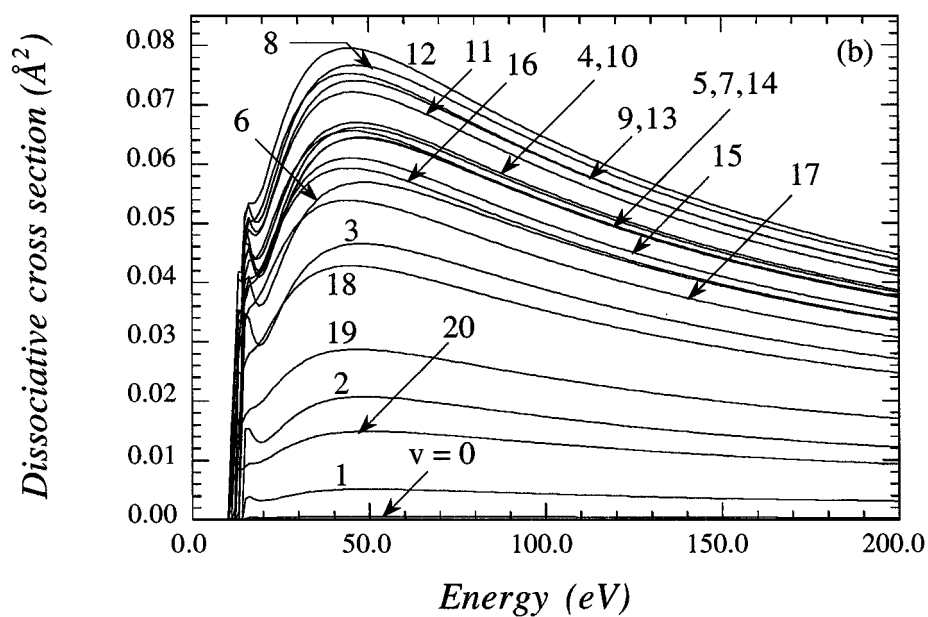
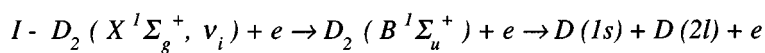
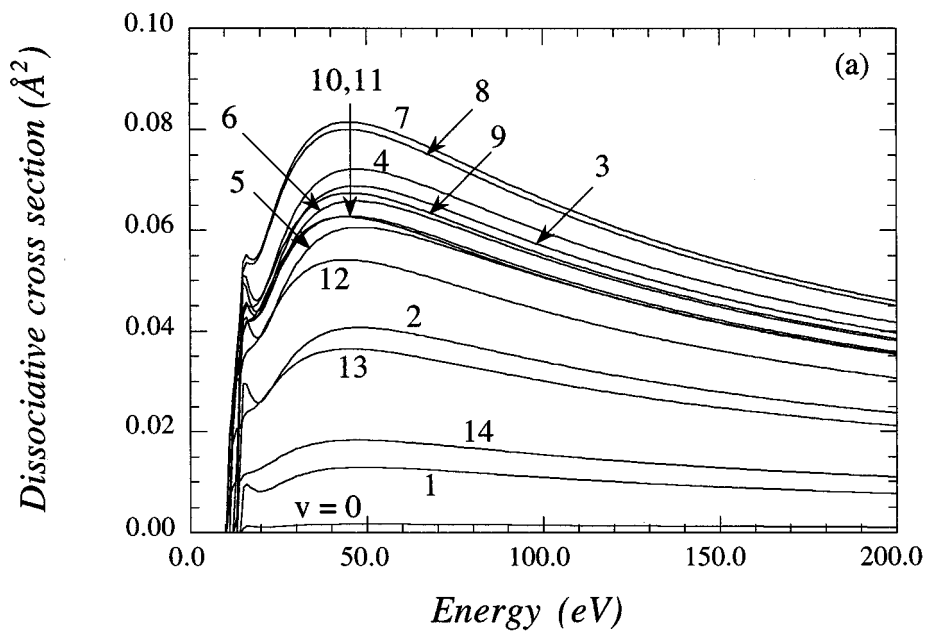
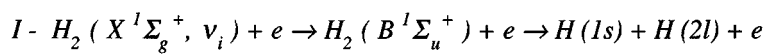
TABLE I.	Energy Parameters and Fitting Coefficients for the Process $\text{H}_2(X^1\Sigma_g^+, v_i) + e \rightarrow \text{H}_2(B^1\Sigma_u^+) + e$
TABLE II.	Energy Parameters and Fitting Coefficients for the Process $\text{H}_2(X^1\Sigma_g^+, v_i) + e \rightarrow \text{H}_2(C^1\Pi_u) + e$
TABLE III.	Energy Parameters and Fitting Coefficients for the Process $\text{D}_2(X^1\Sigma_g^+, v_i) + e \rightarrow \text{D}_2(B^1\Sigma_u^+) + e$
TABLE IV.	Energy Parameters and Fitting Coefficients for the Process $\text{D}_2(X^1\Sigma_g^+, v_i) + e \rightarrow \text{D}_2(C^1\Pi_u) + e$

Energy parameters and fitting coefficients, entering in Eqs. (4.1)–(4.4), are tabulated for the total excitation processes IXa, Xa, IXb, and Xb and for each vibrational level,  $v_i$ .

$\Delta E$	transition energy (eV)
$\bar{E}$	upper energy limit (eV) for Eqs. (4.1) and (4.3)
$E_{\min}$	lower energy limit (eV) for Eqs. (4.1) and (4.3)
rms deviation%	root mean square deviation for fitting procedure (see text)
$c_i$	fitting coefficients for Eqs. (4.1)–(4.4)

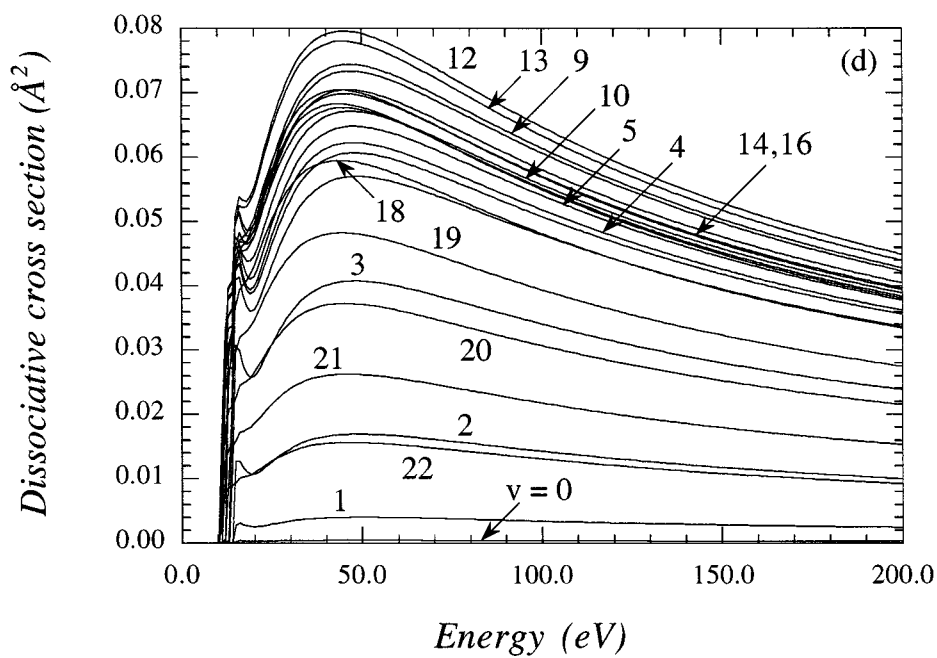
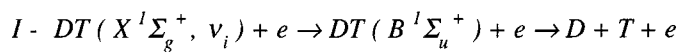
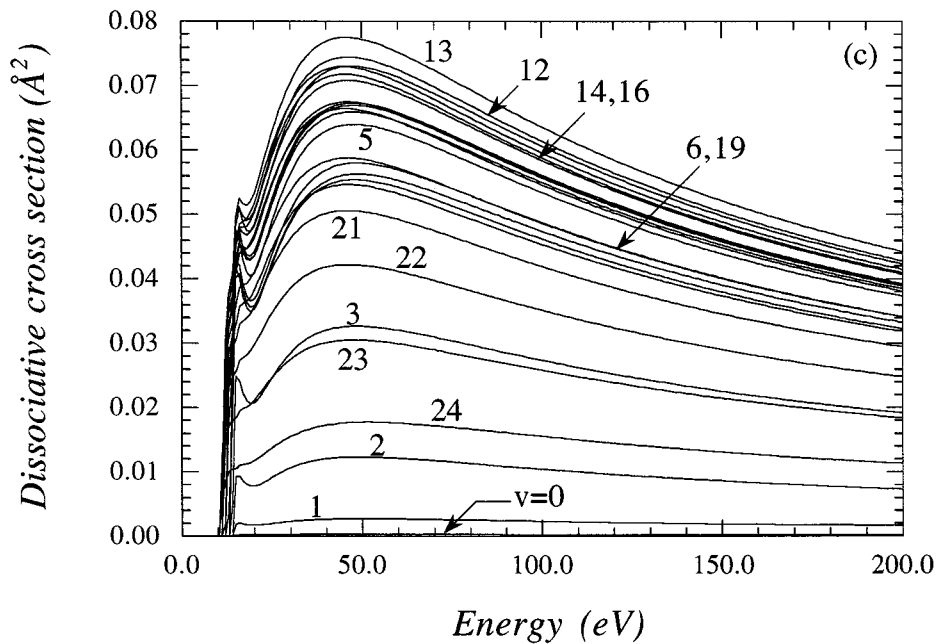
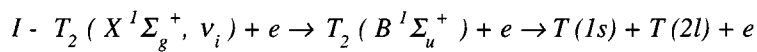
## GRAPH I. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



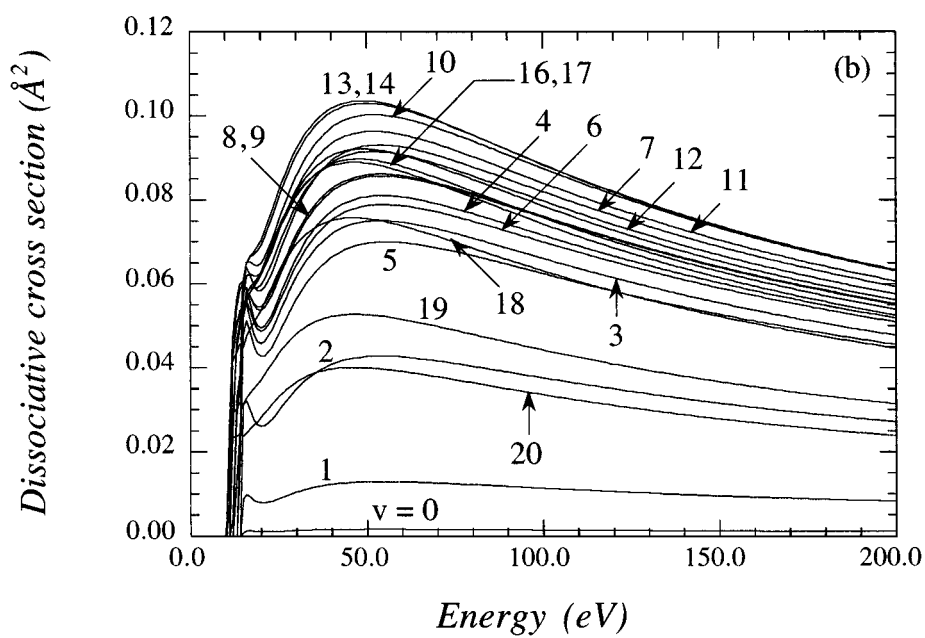
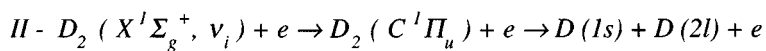
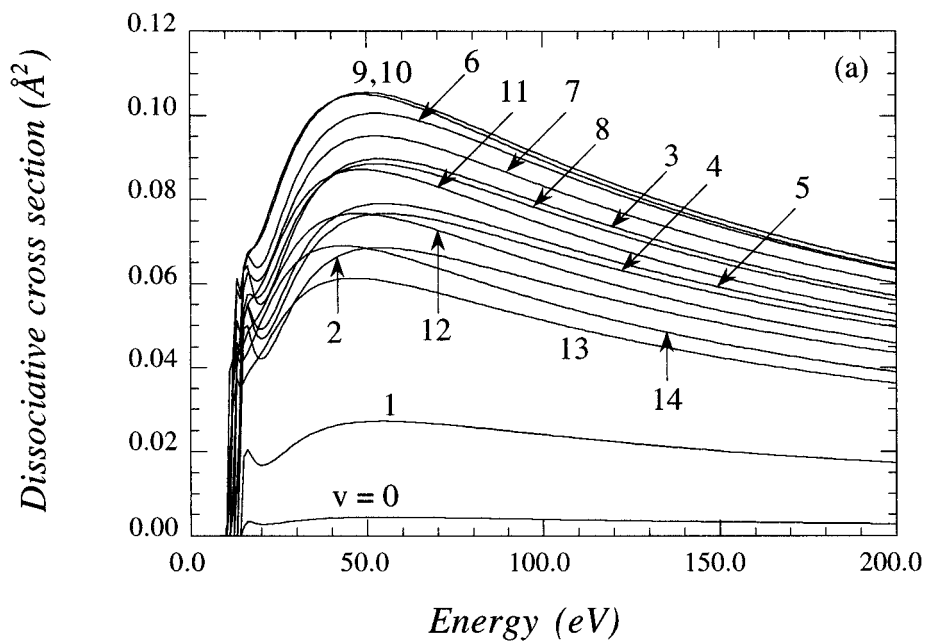
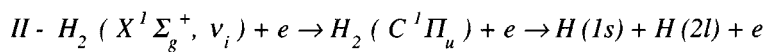
## GRAPH I. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



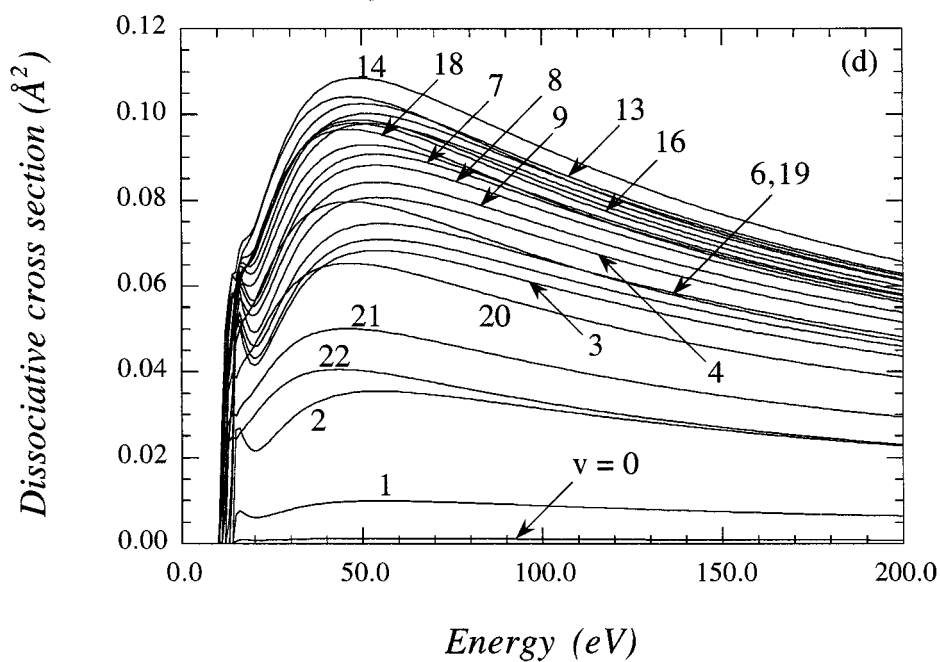
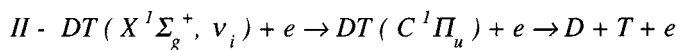
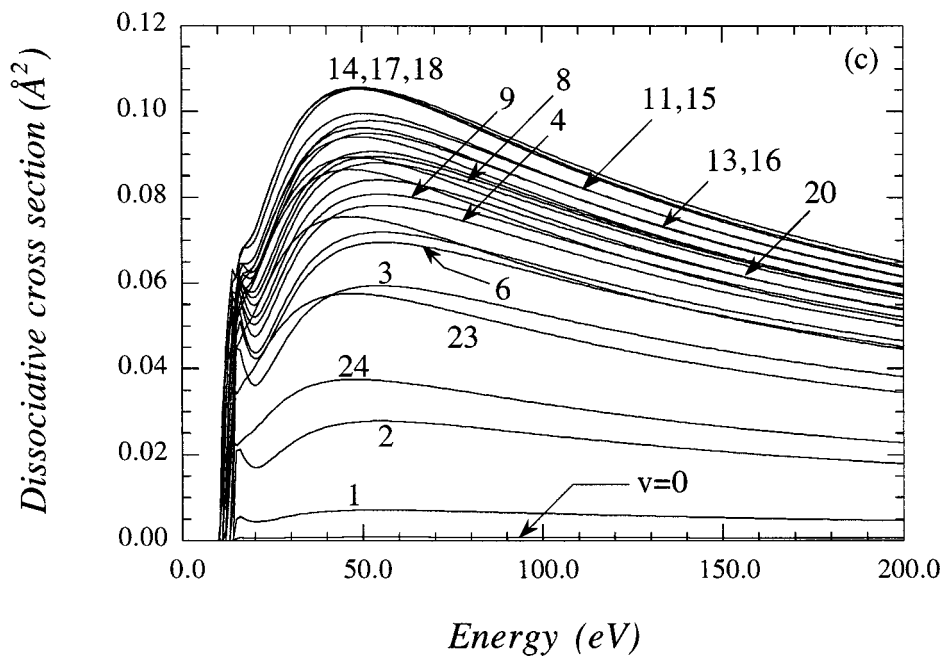
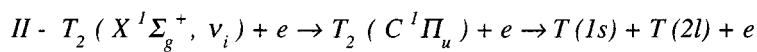
## GRAPH II. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



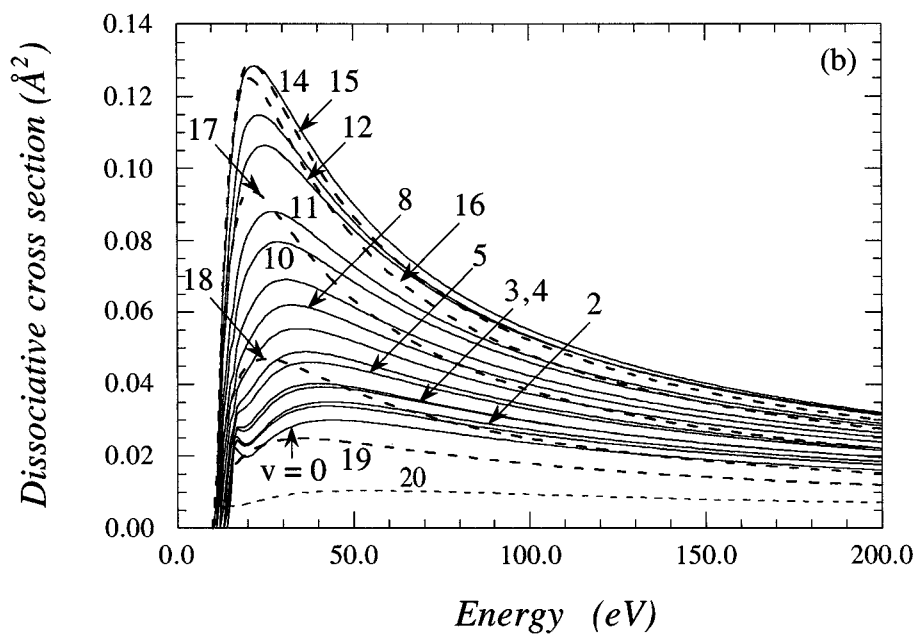
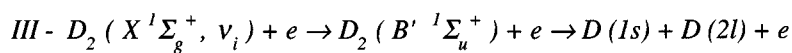
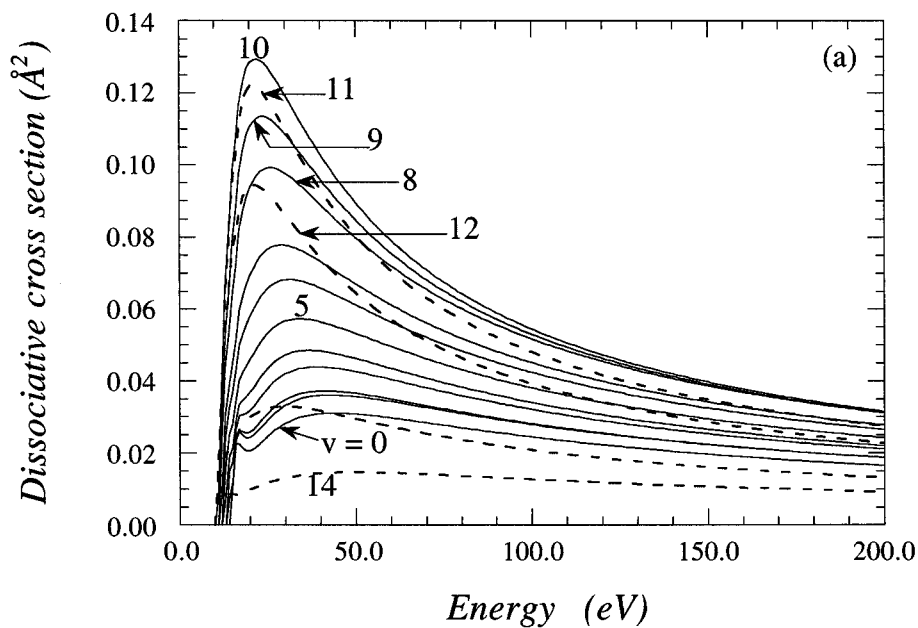
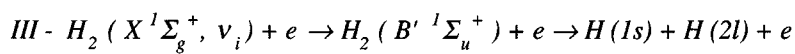
## GRAPH II. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



## GRAPH III. Dissociative Excitation Cross Sections

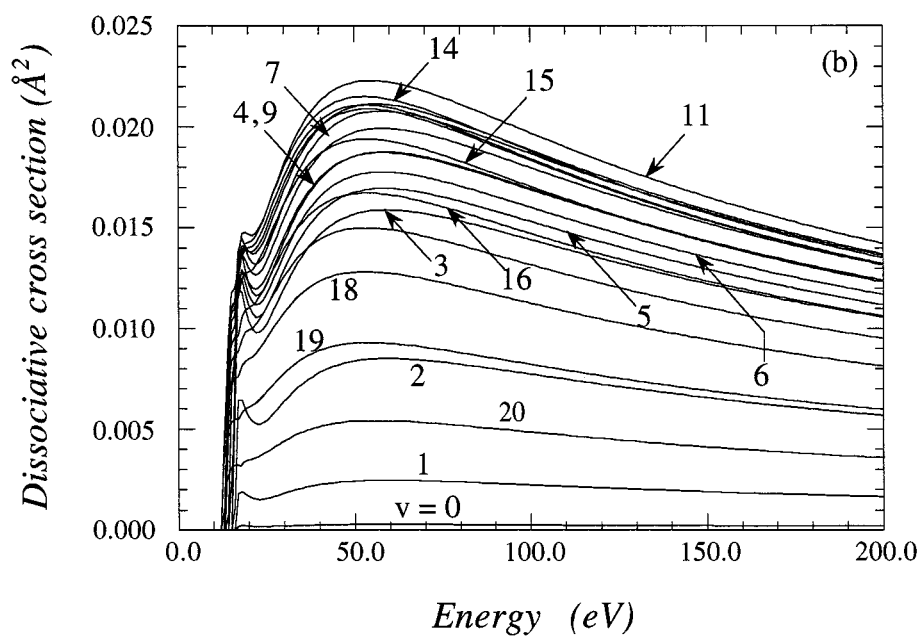
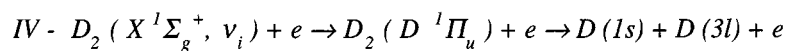
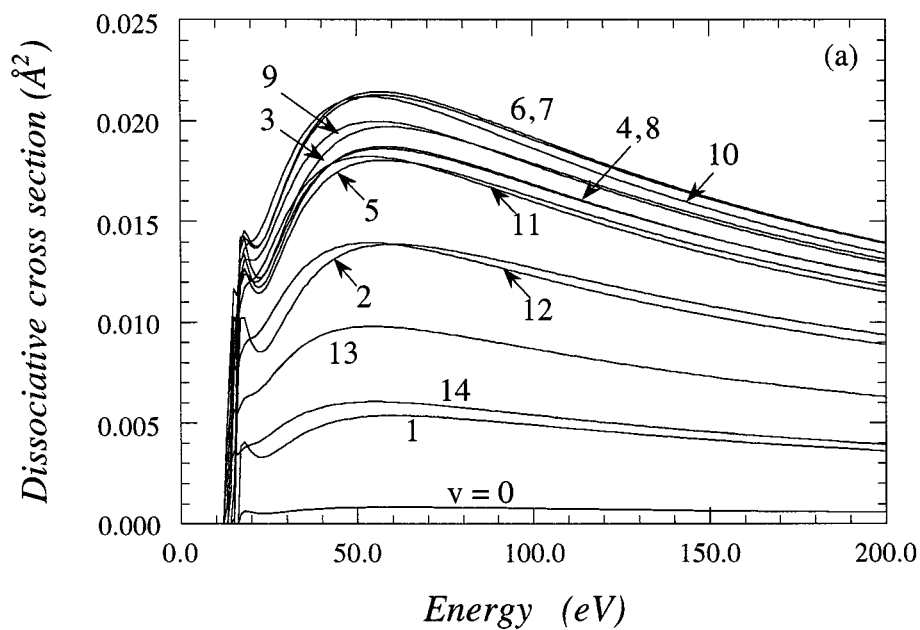
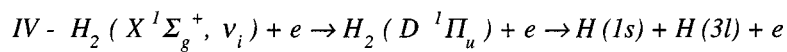
See page 171 for Explanation of Graphs





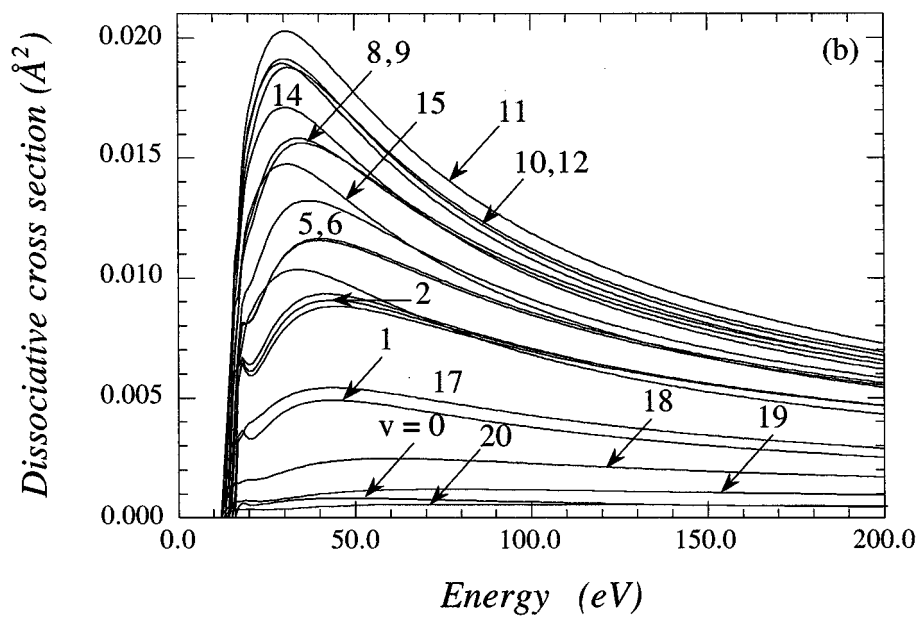
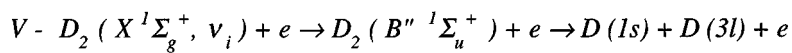
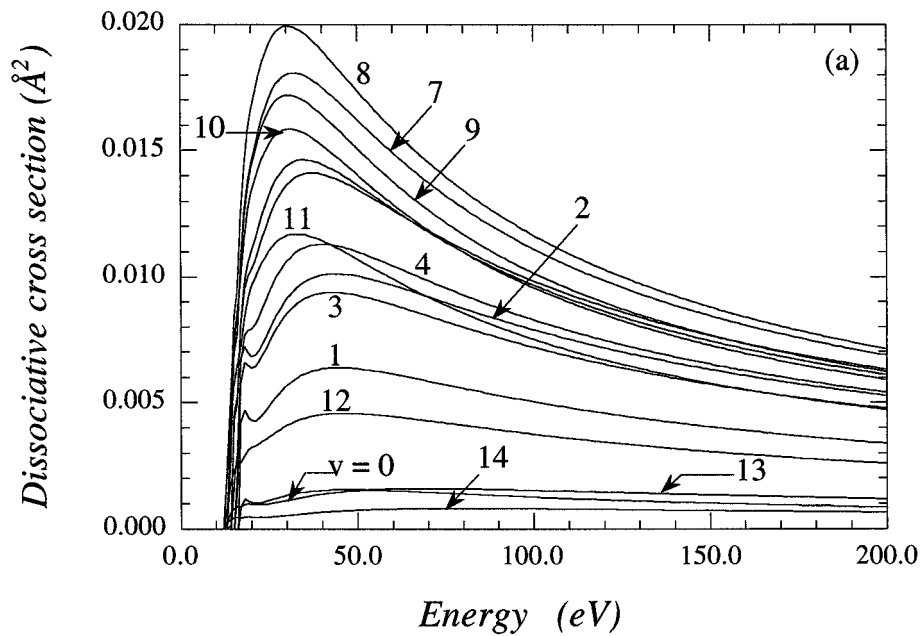
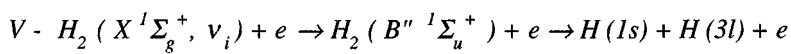
## GRAPH IV. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



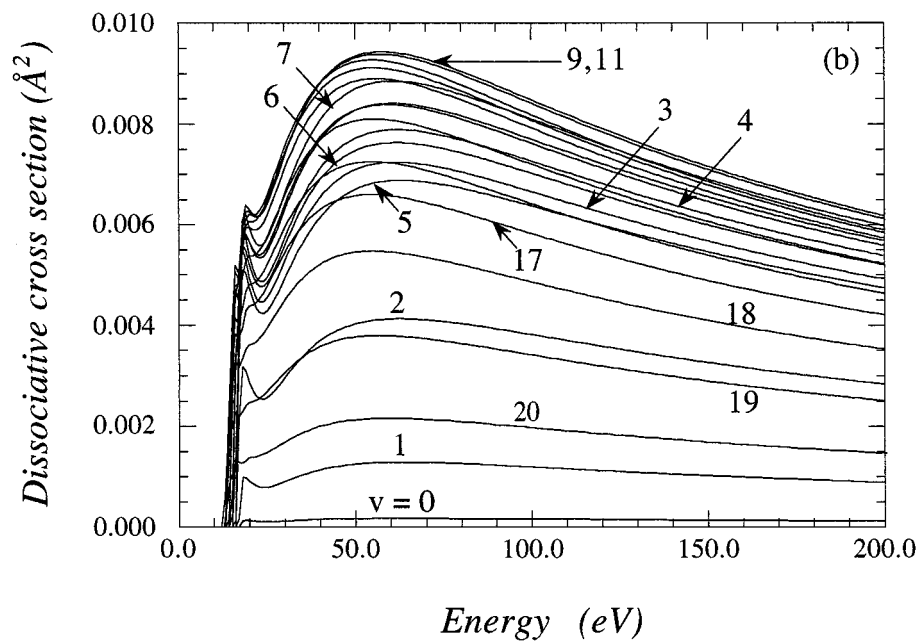
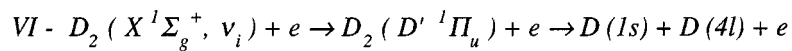
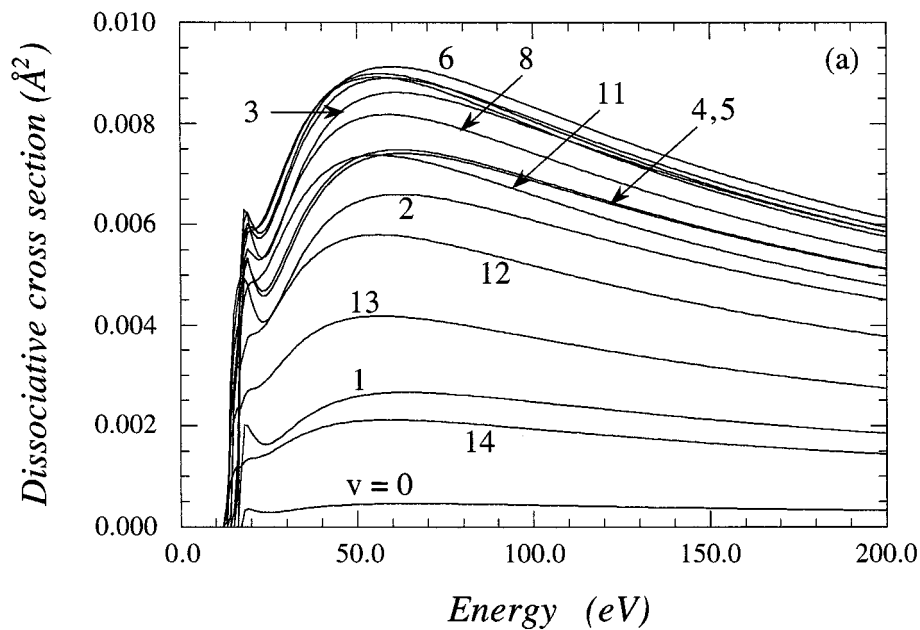
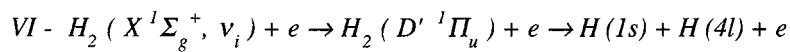
## GRAPH V. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



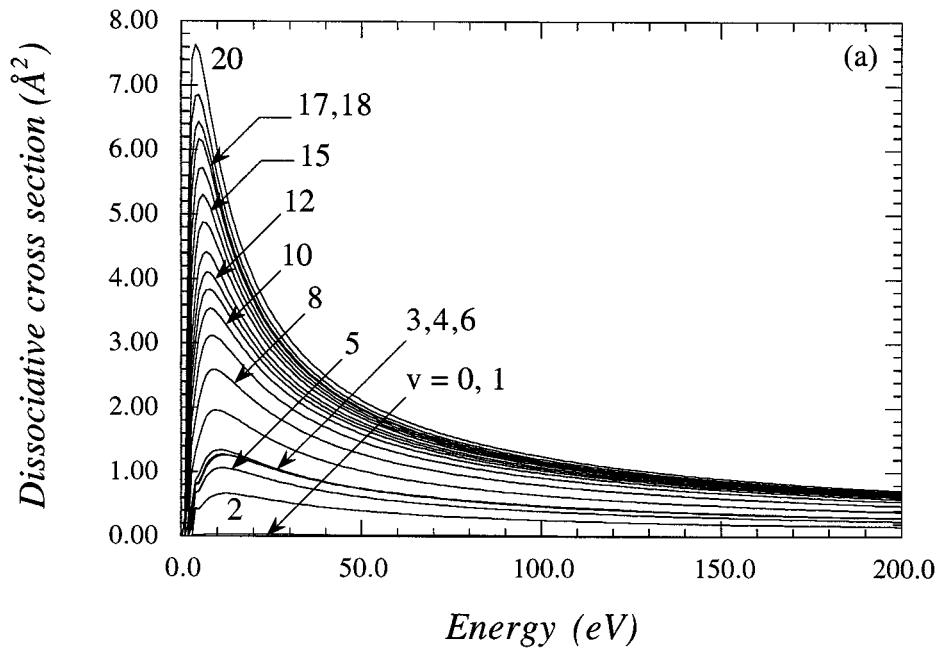
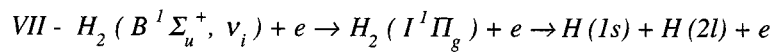
## GRAPH VI. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



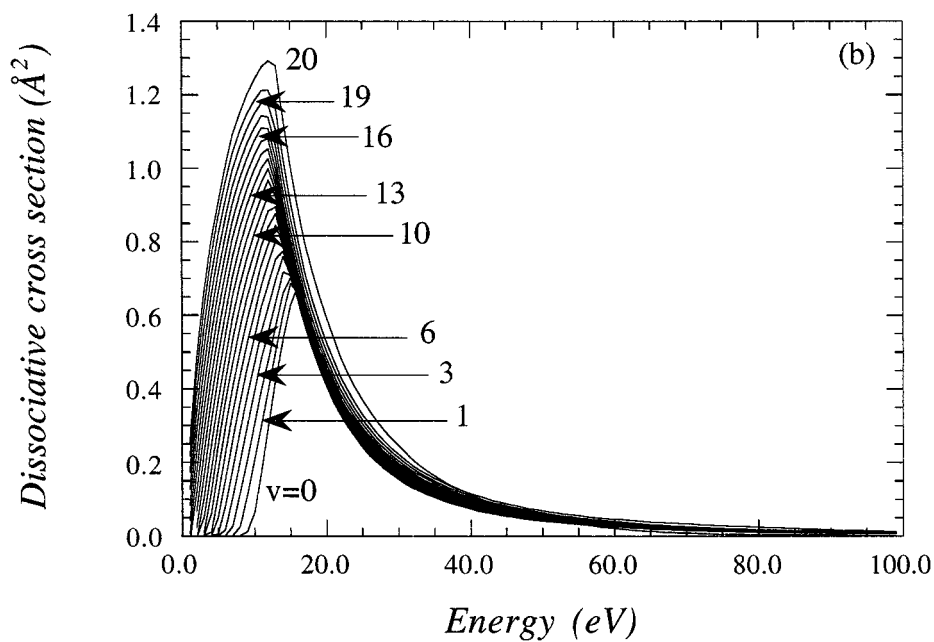
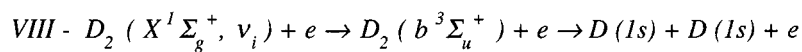
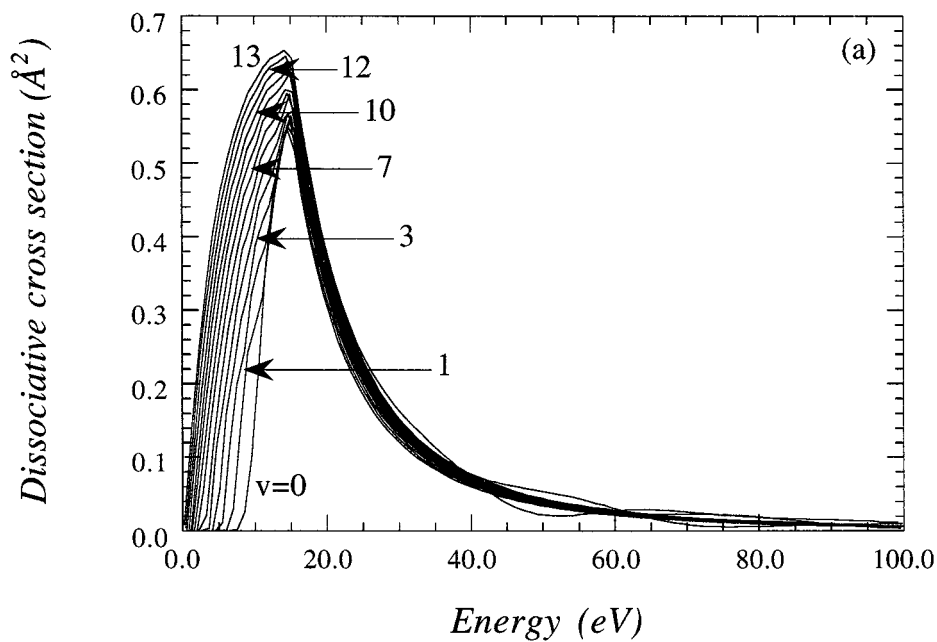
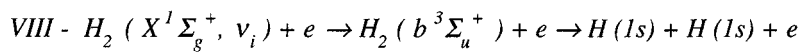
## GRAPH VII. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



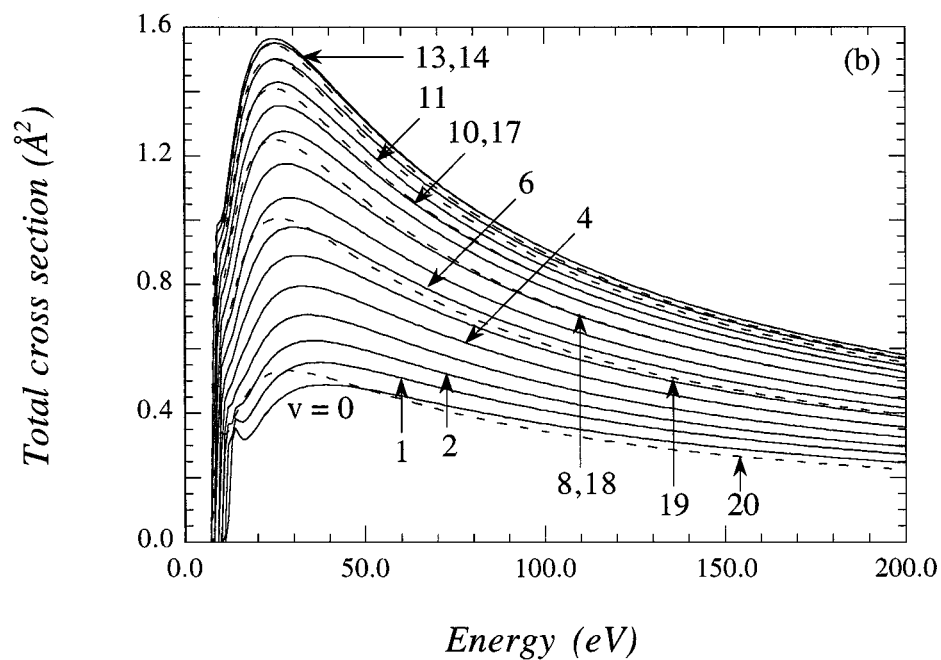
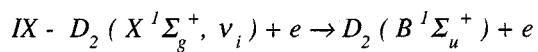
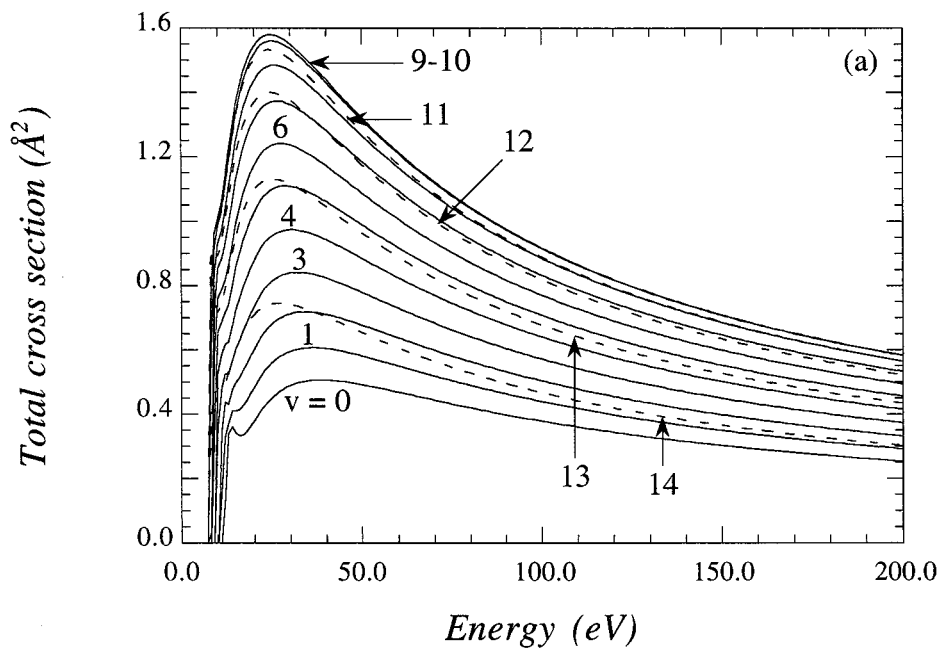
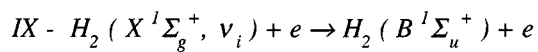
## GRAPH VIII. Dissociative Excitation Cross Sections

See page 171 for Explanation of Graphs



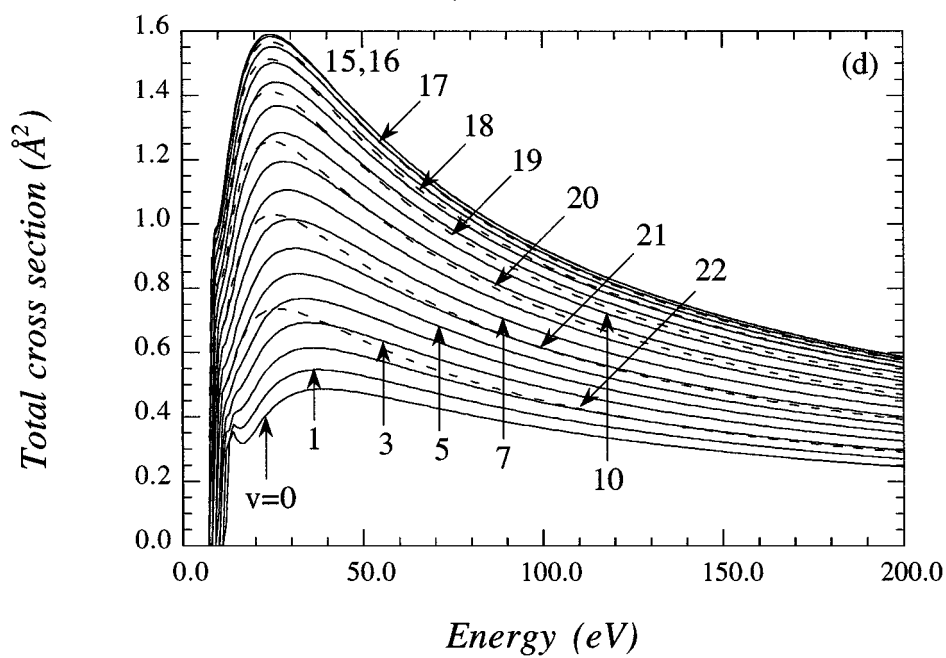
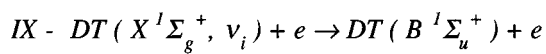
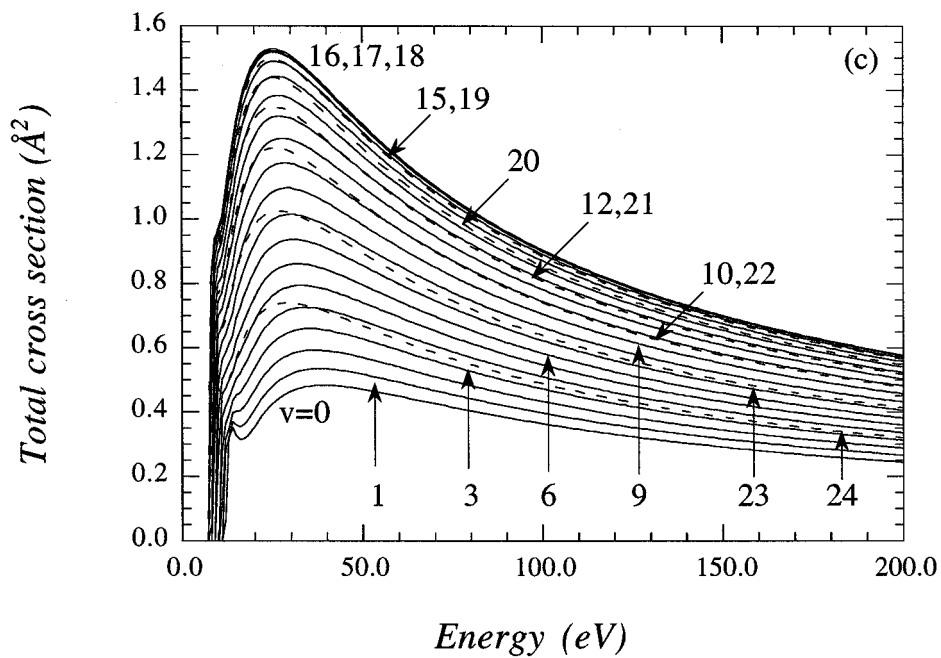
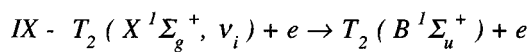
## GRAPH IX. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



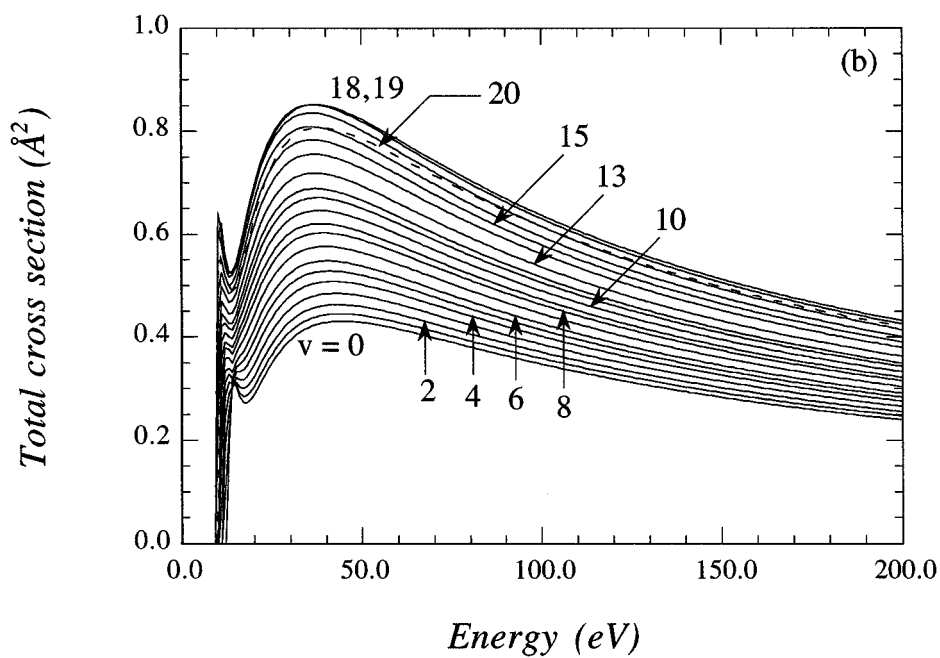
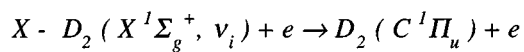
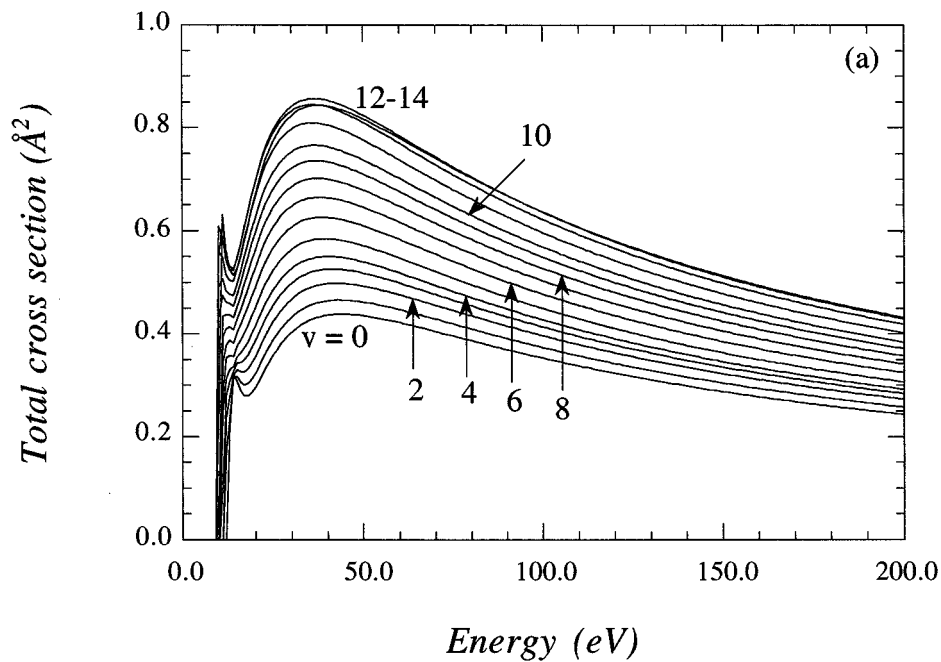
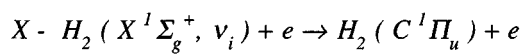
## GRAPH IX. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



## GRAPH X. Total Excitation Cross Sections

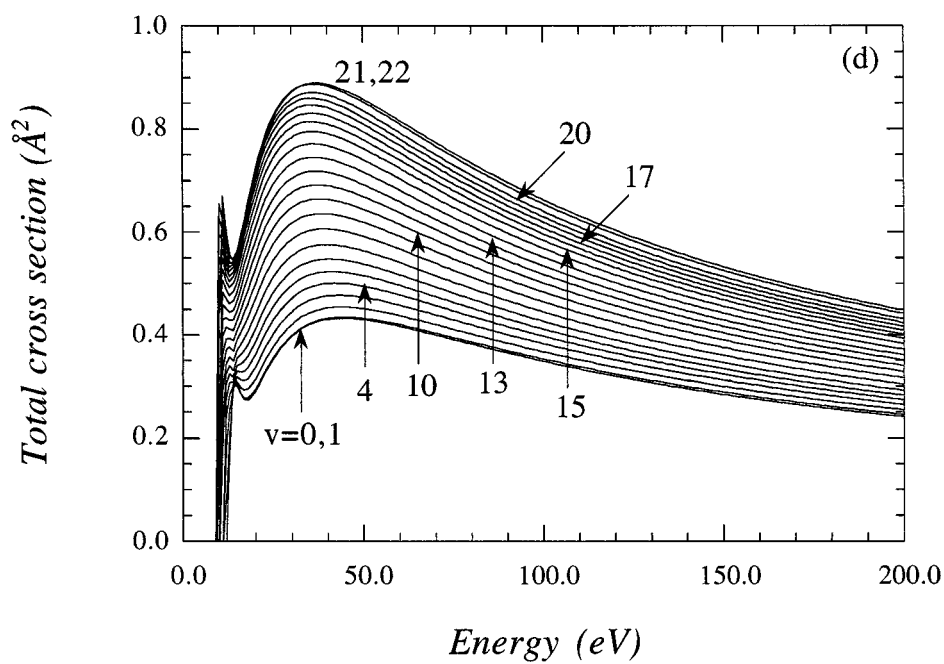
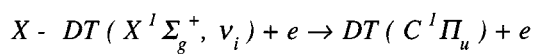
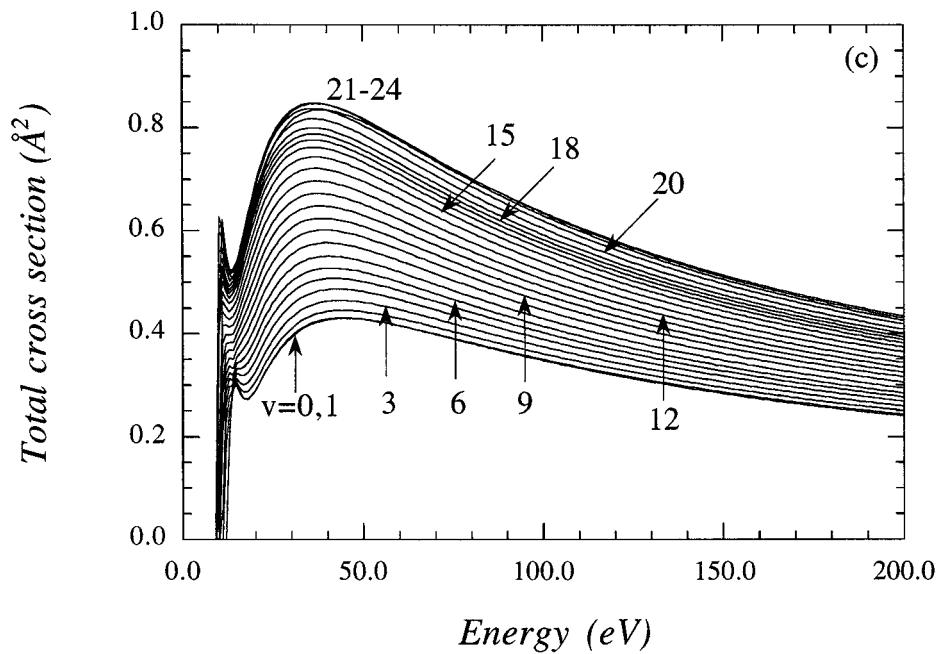
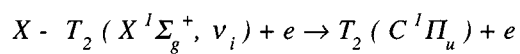
See page 171 for Explanation of Graphs





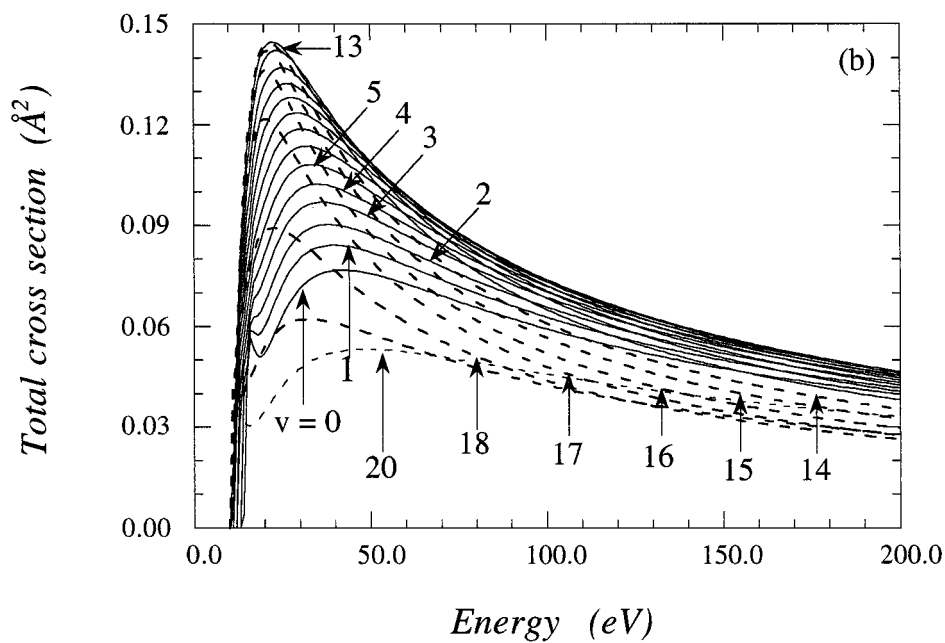
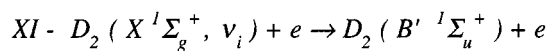
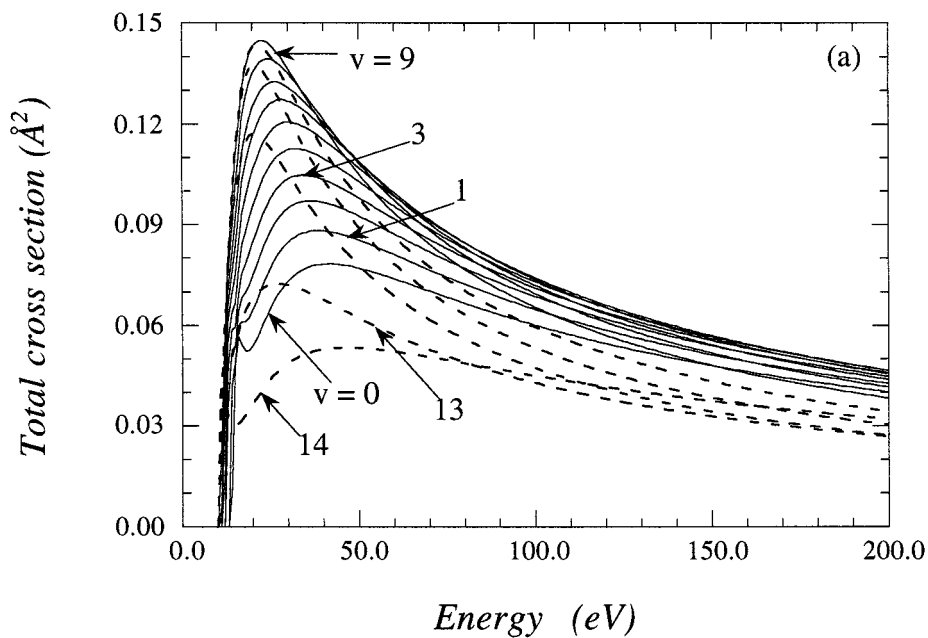
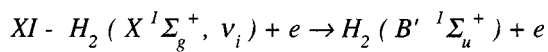
## GRAPH X. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



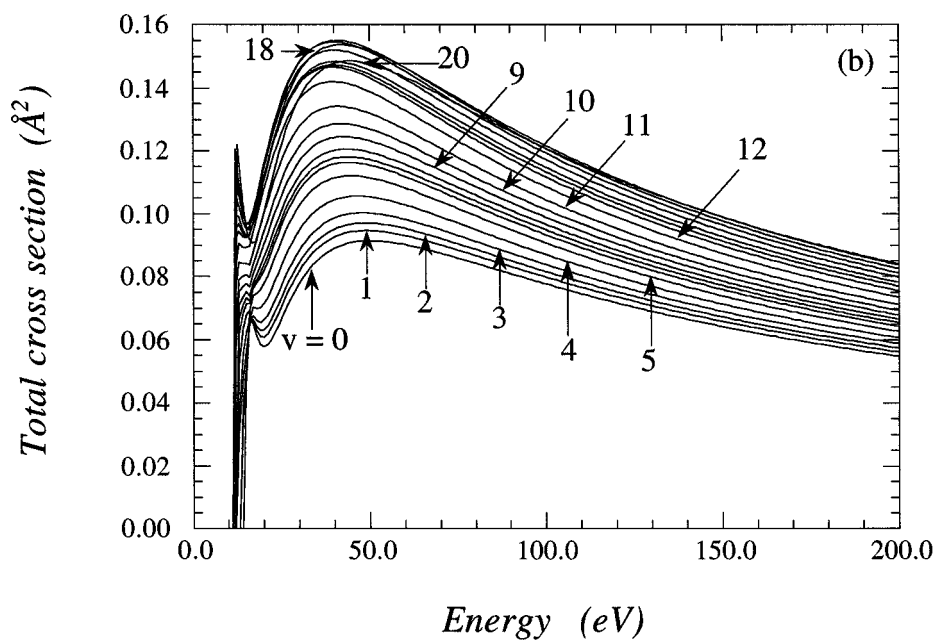
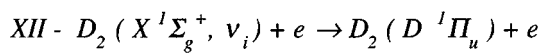
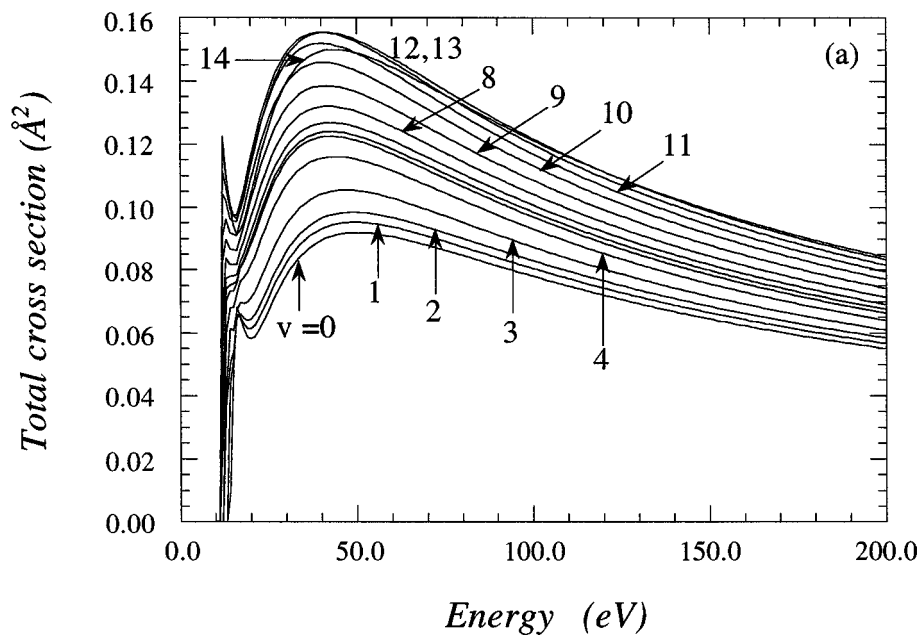
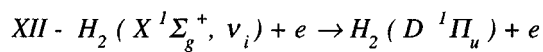
## GRAPH XI. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



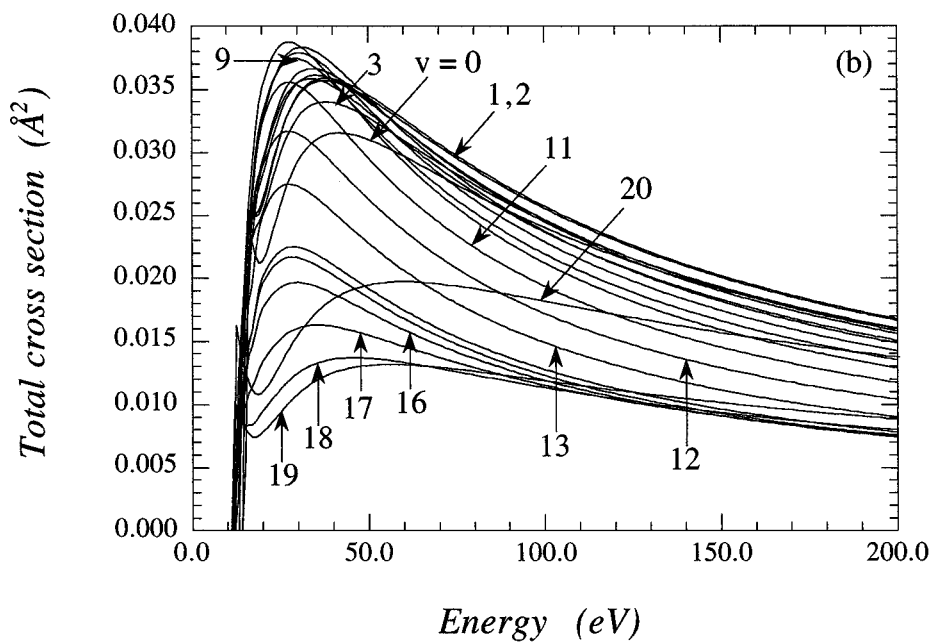
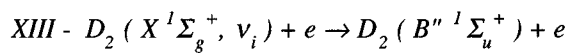
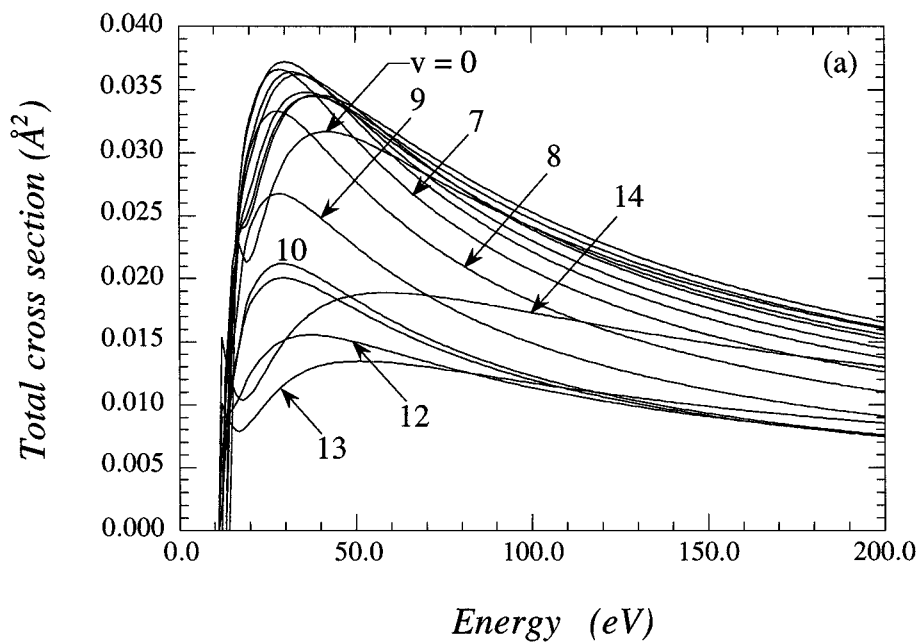
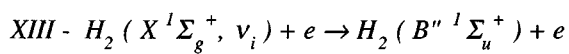
## GRAPH XII. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



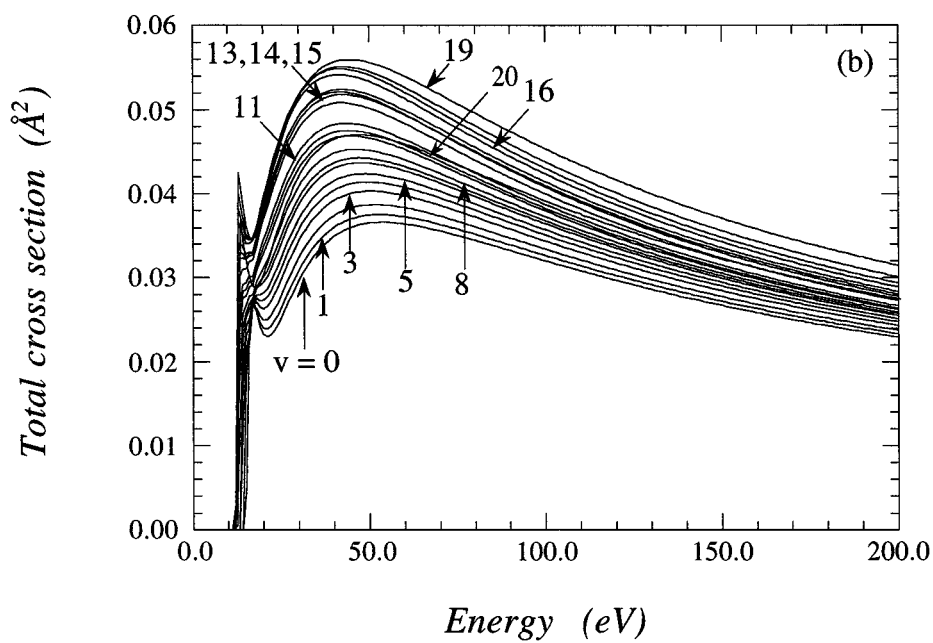
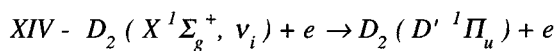
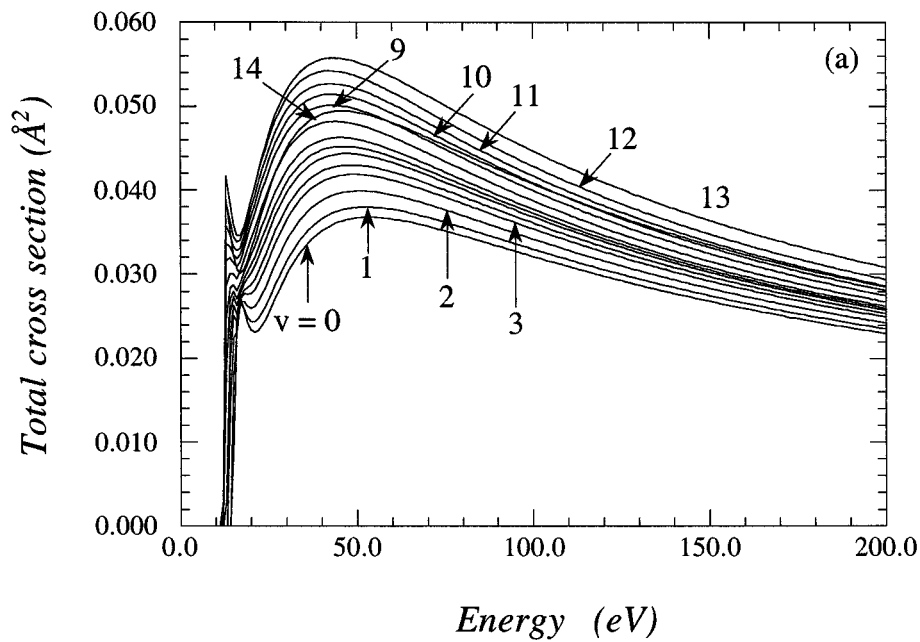
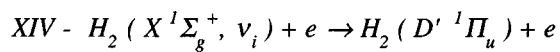
## GRAPH XIII. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



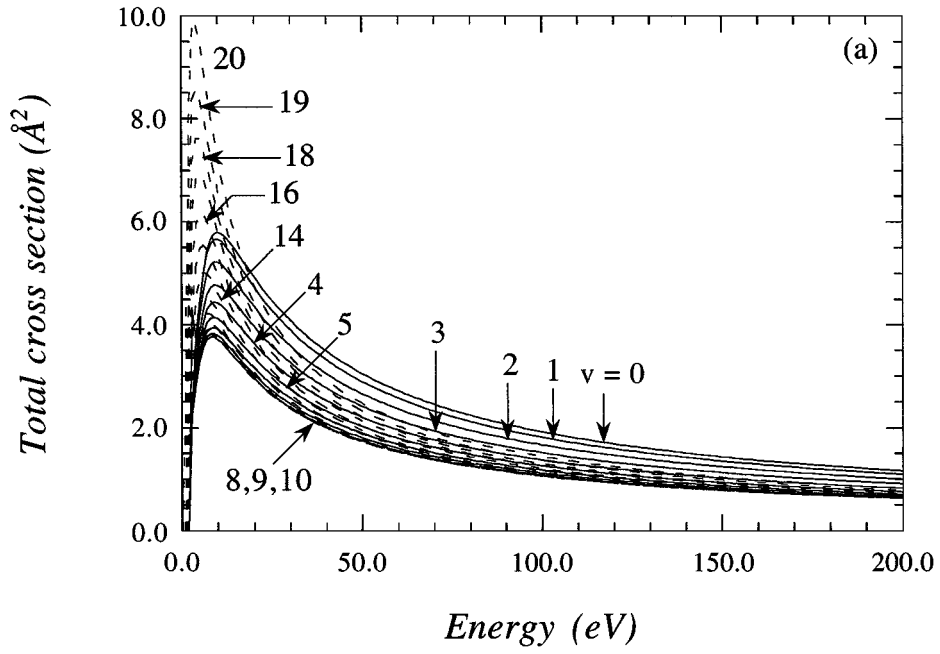
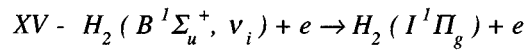
## GRAPH XIV. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



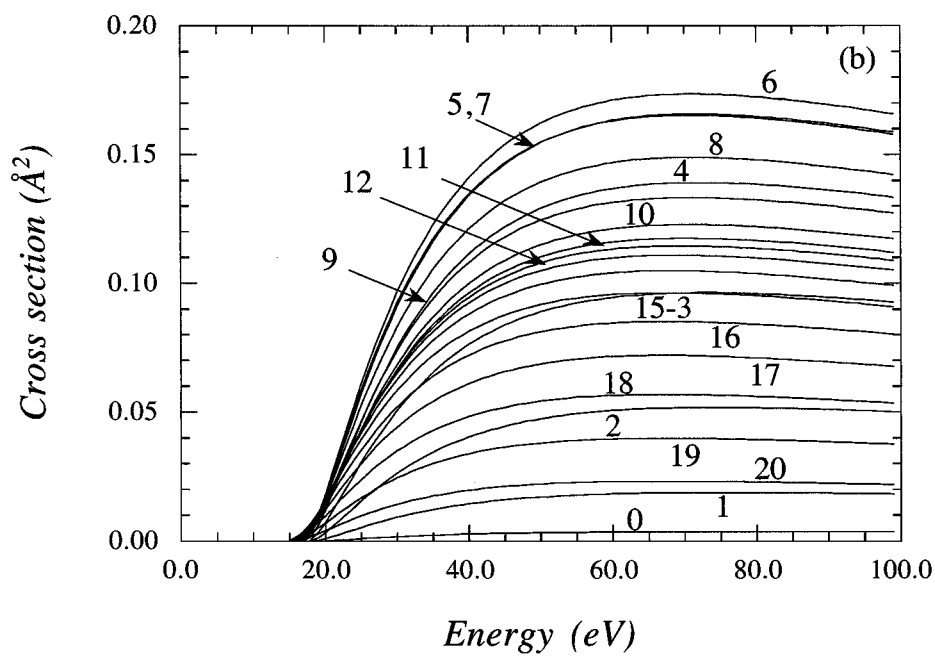
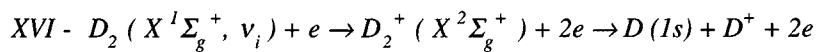
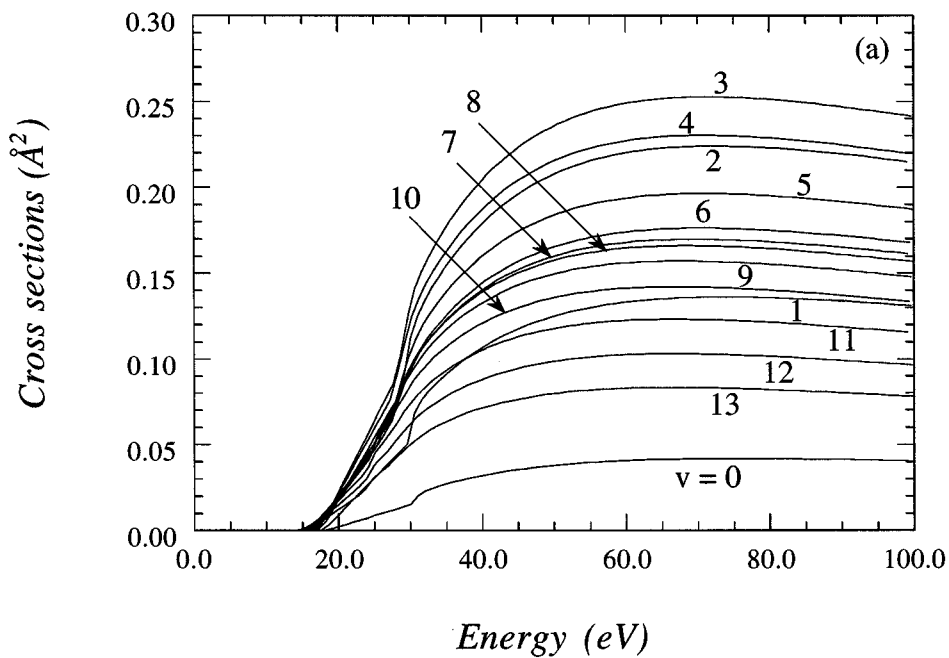
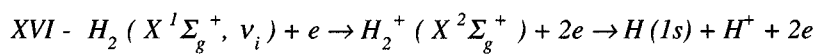
## GRAPH XV. Total Excitation Cross Sections

See page 171 for Explanation of Graphs



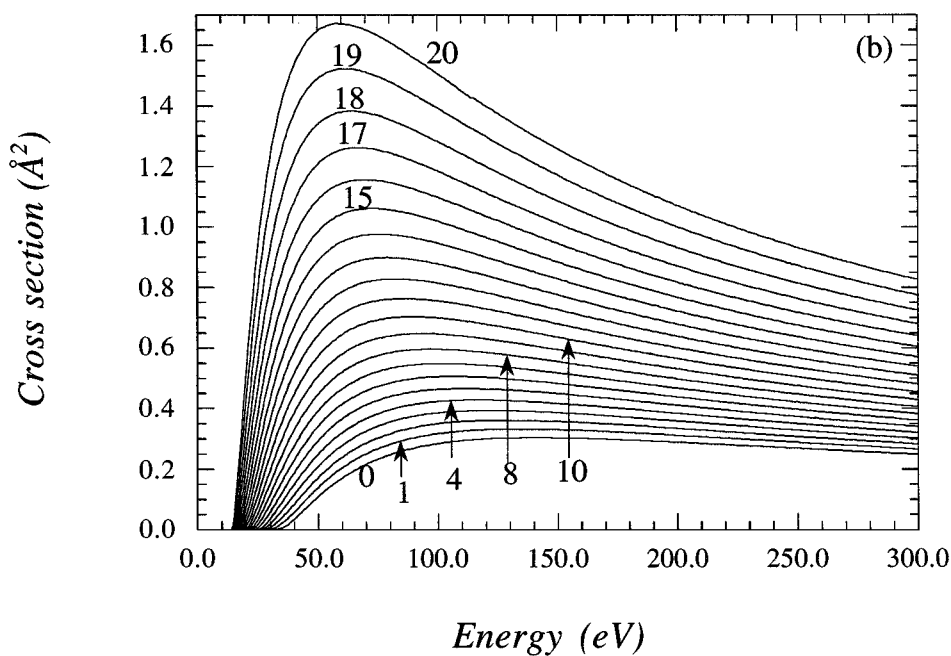
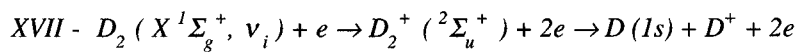
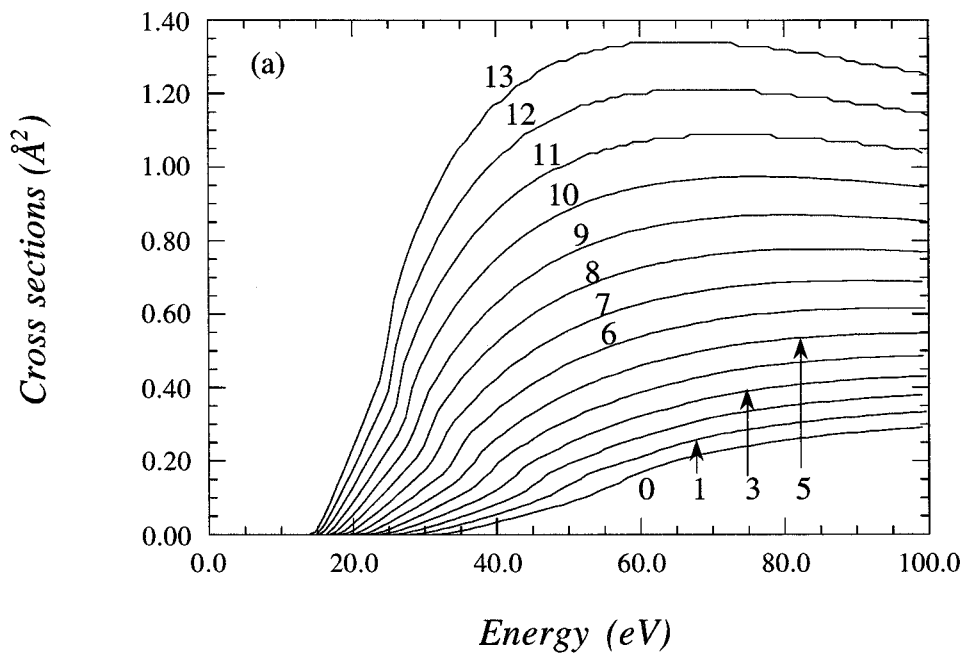
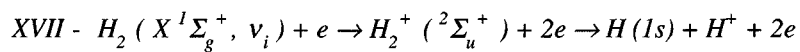
## GRAPH XVI. Dissociative Ionization Cross Sections

See page 171 for Explanation of Graphs



## GRAPH XVII. Dissociative Ionization Cross Sections

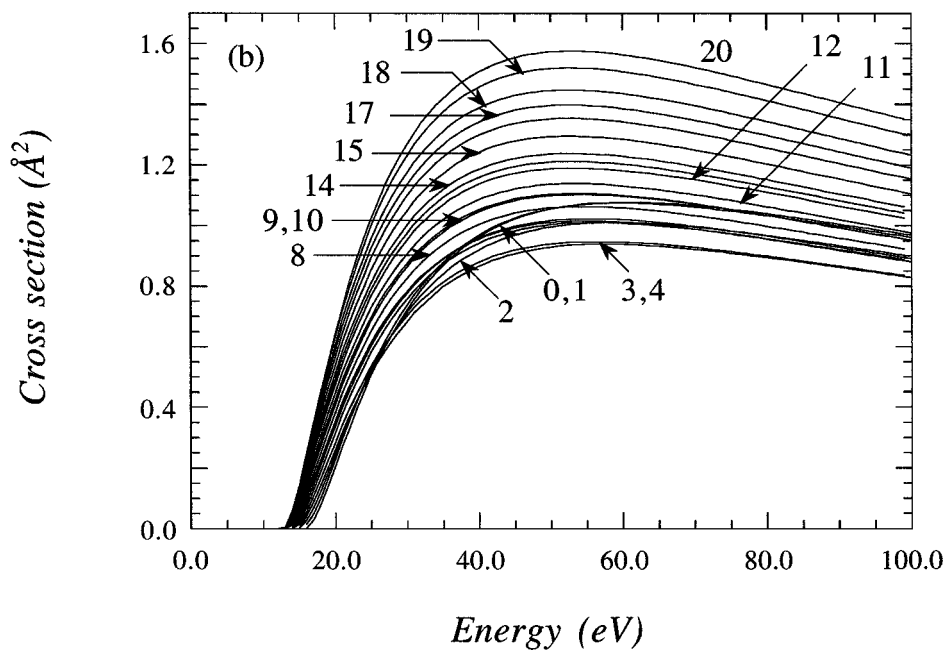
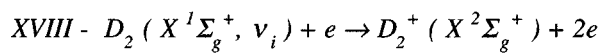
See page 171 for Explanation of Graphs





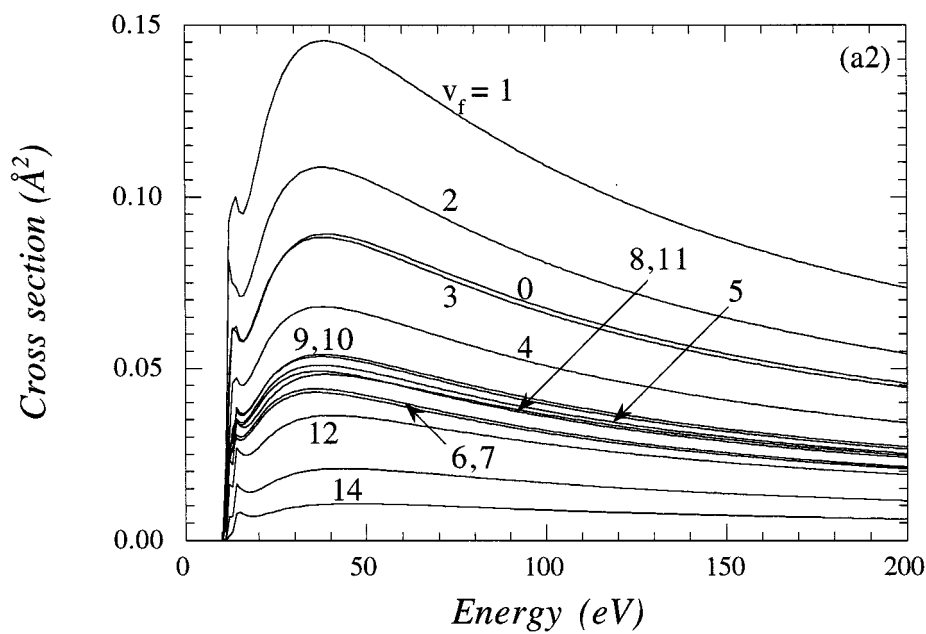
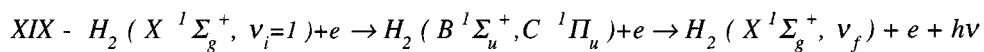
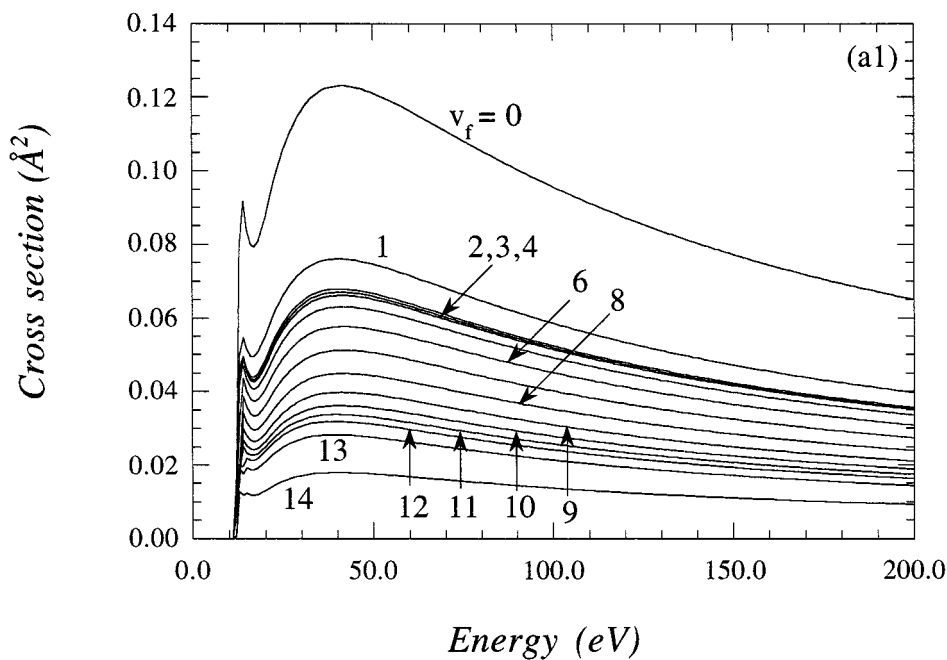
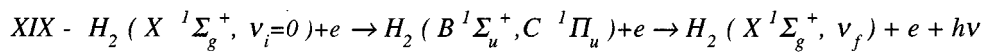
## GRAPH XVIII. Non-Dissociative Ionization Cross Sections

See page 171 for Explanation of Graphs



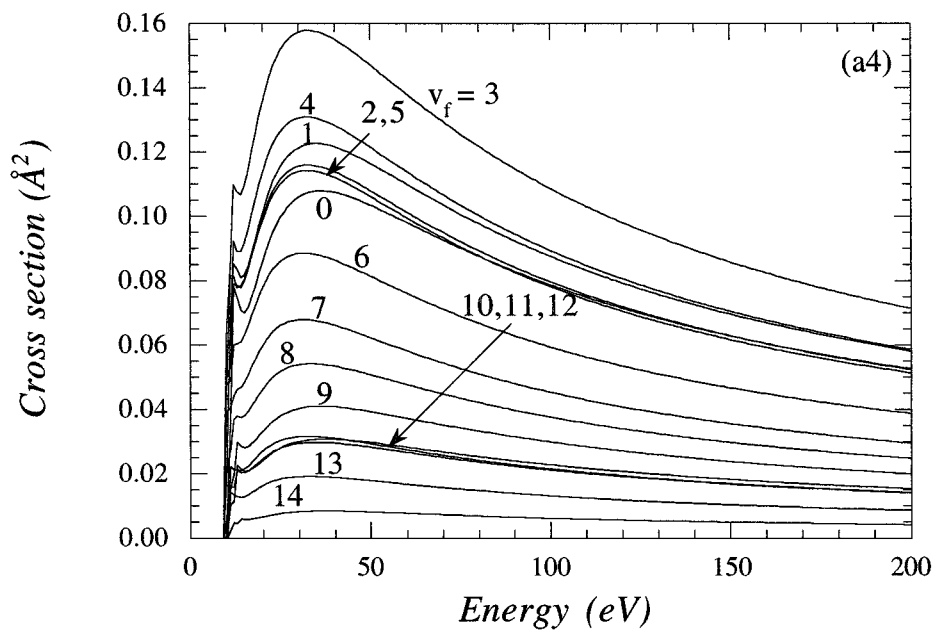
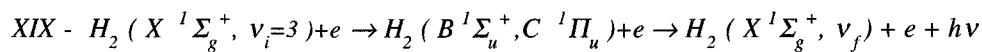
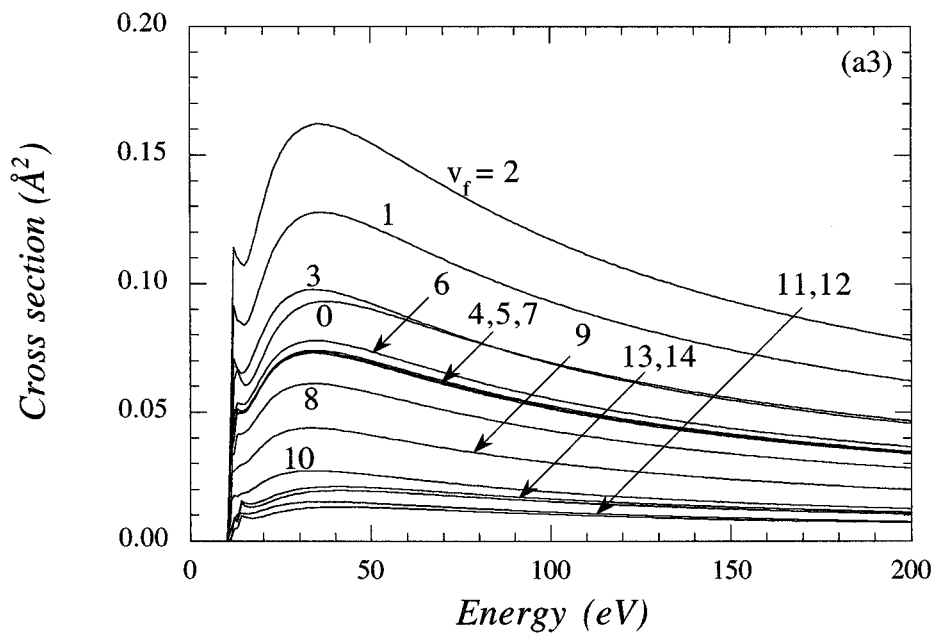
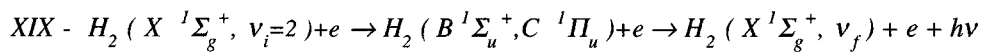
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



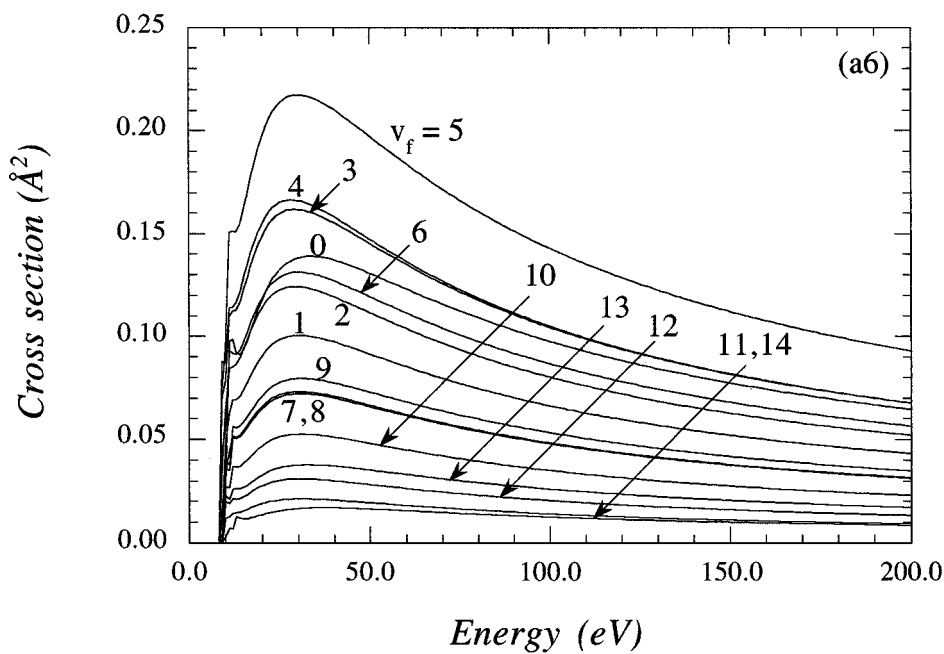
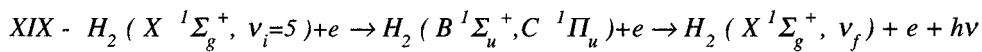
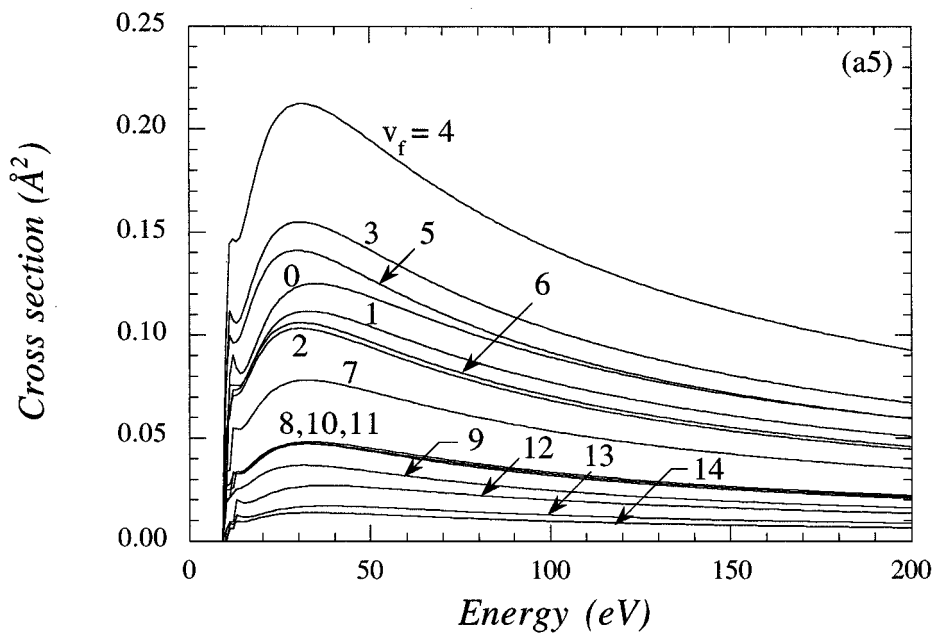
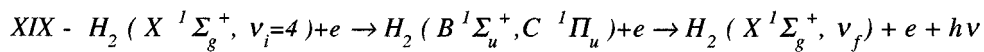
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



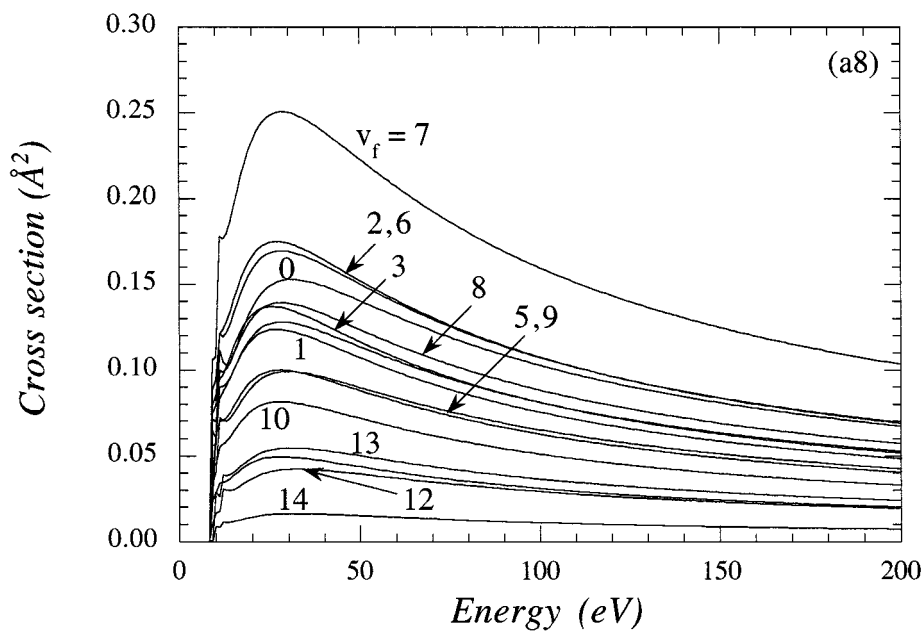
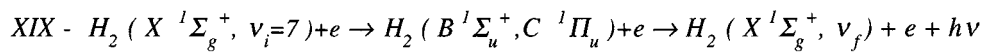
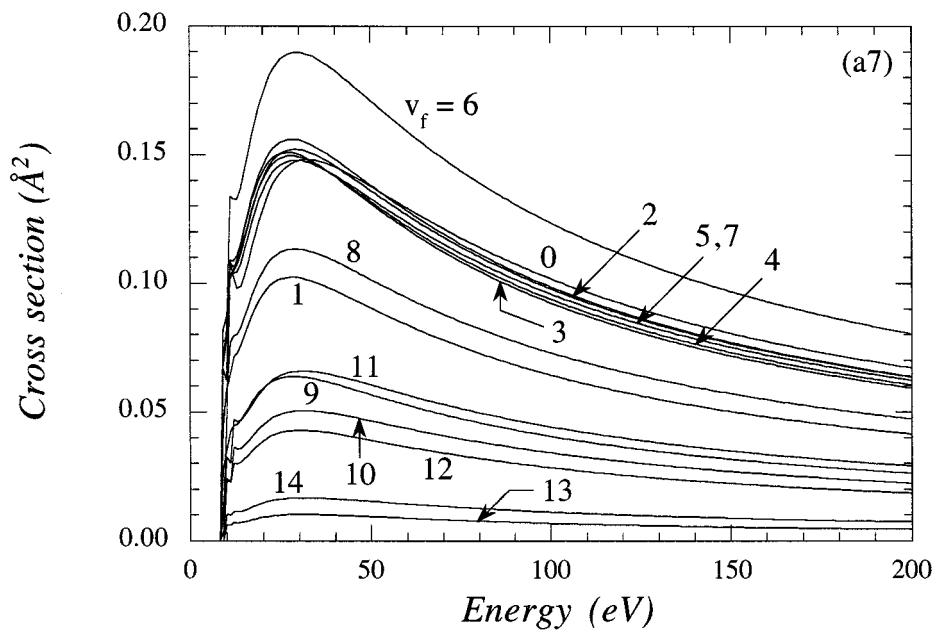
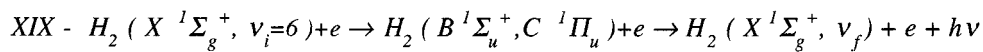
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



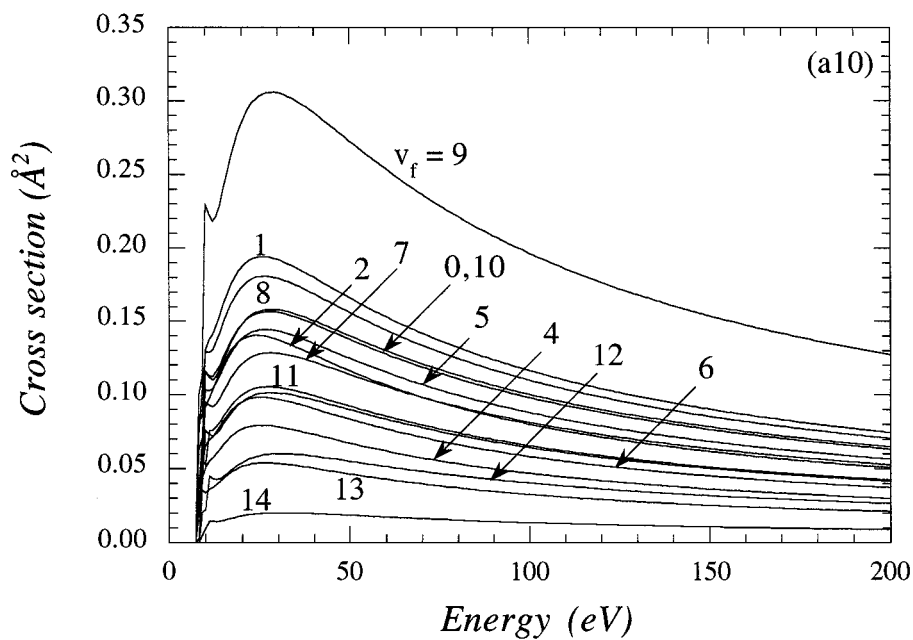
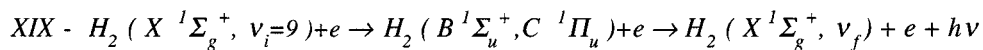
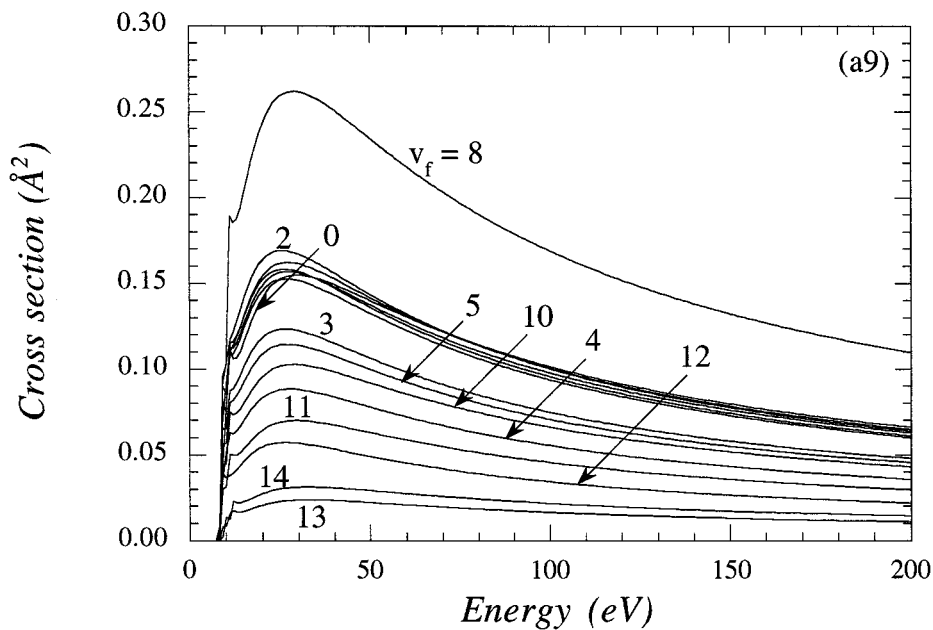
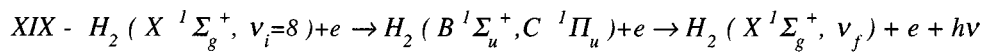
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



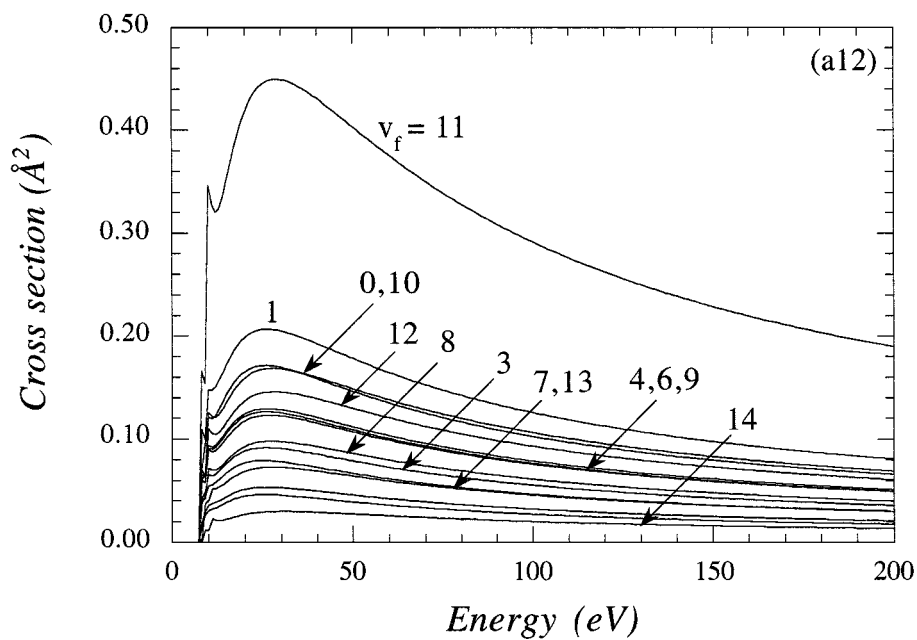
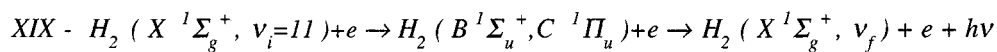
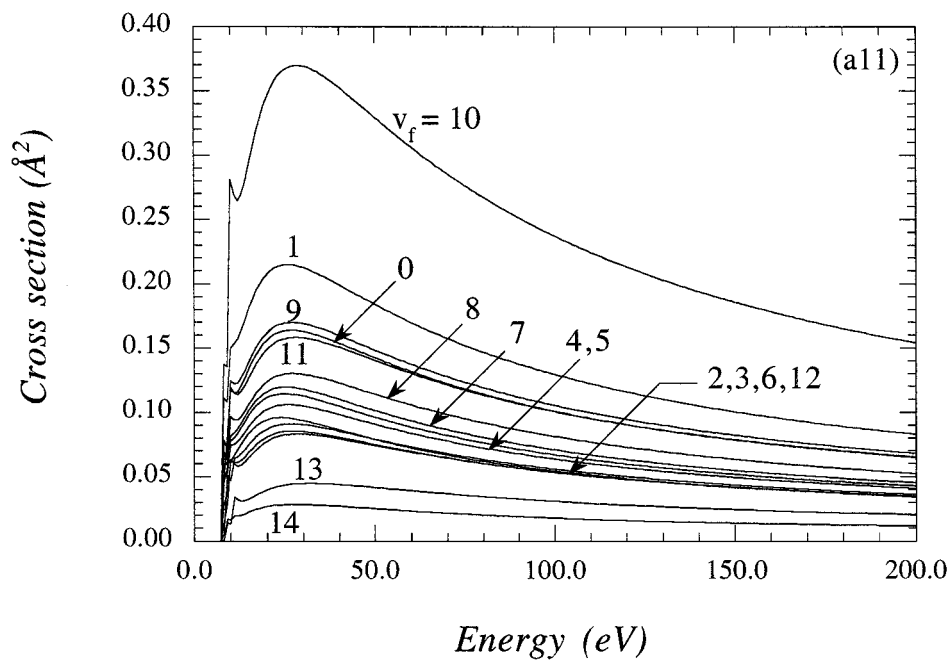
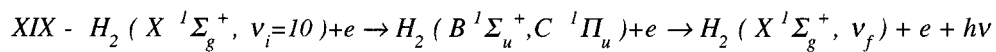
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



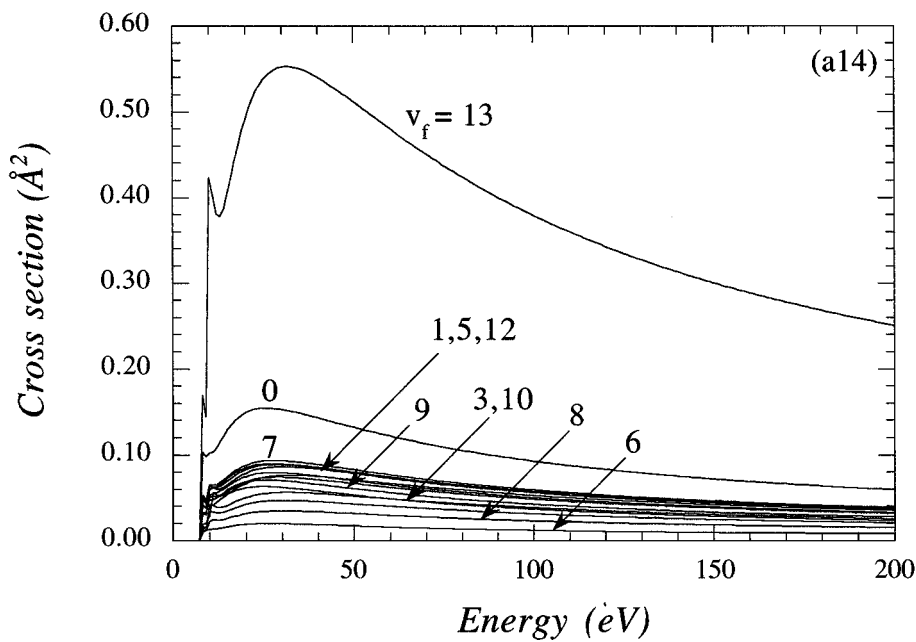
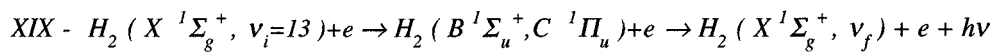
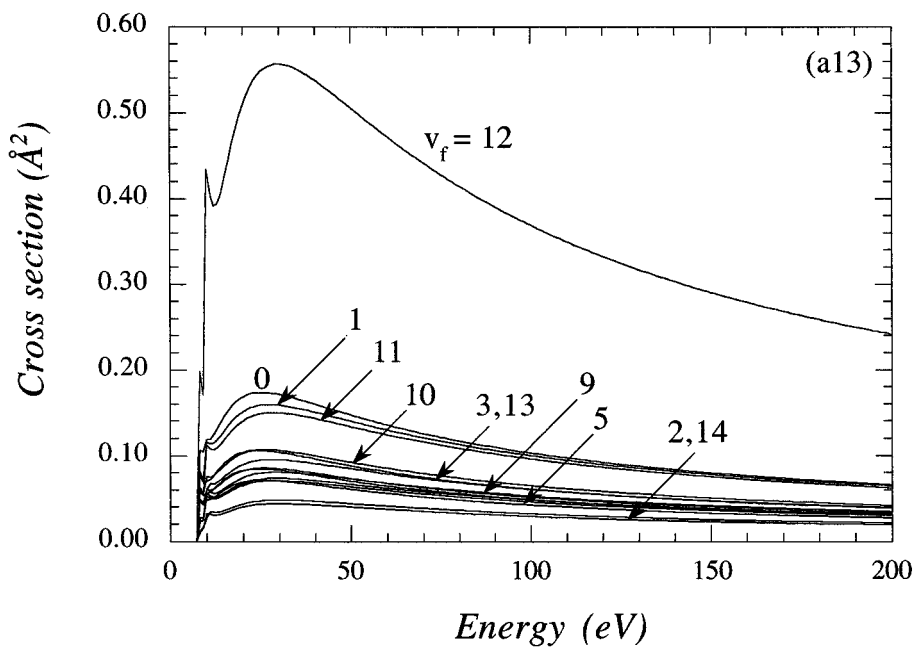
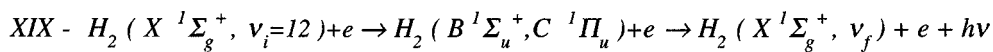
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

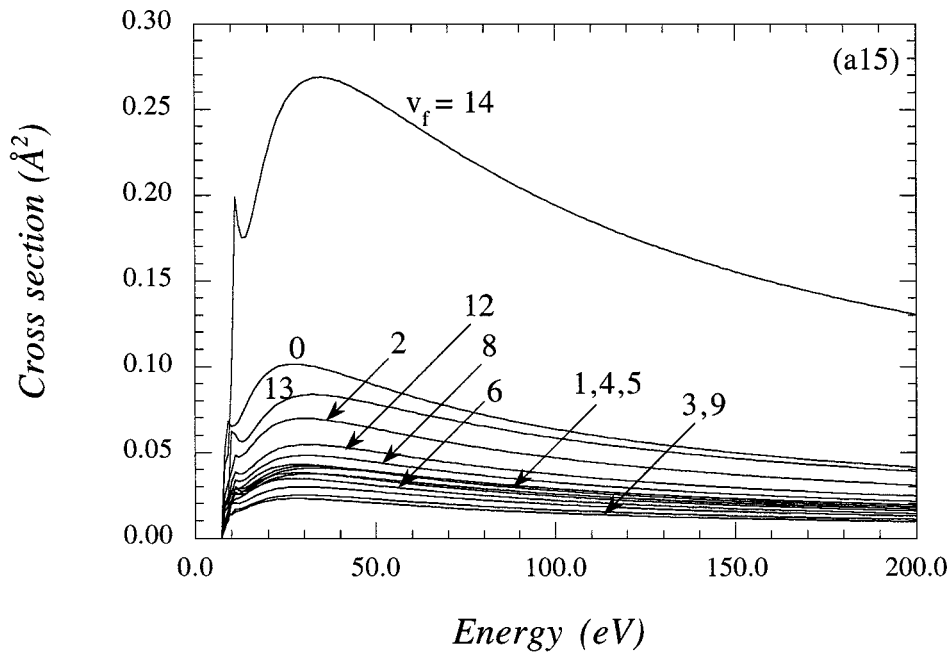
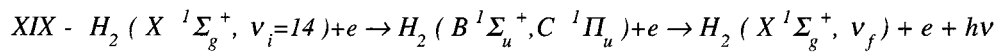
See page 171 for Explanation of Graphs





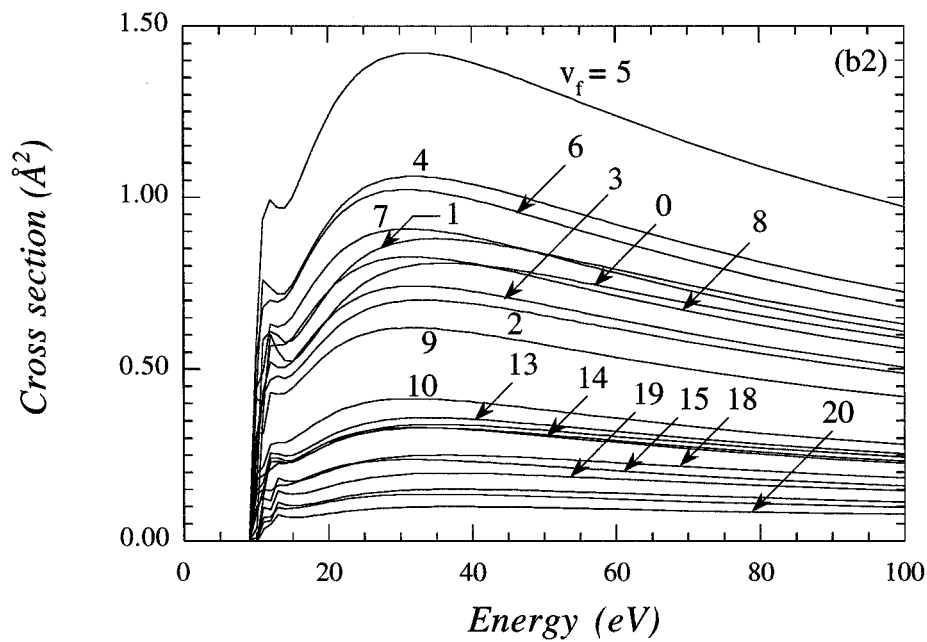
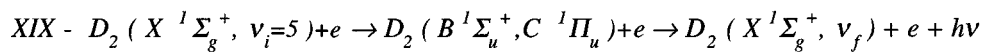
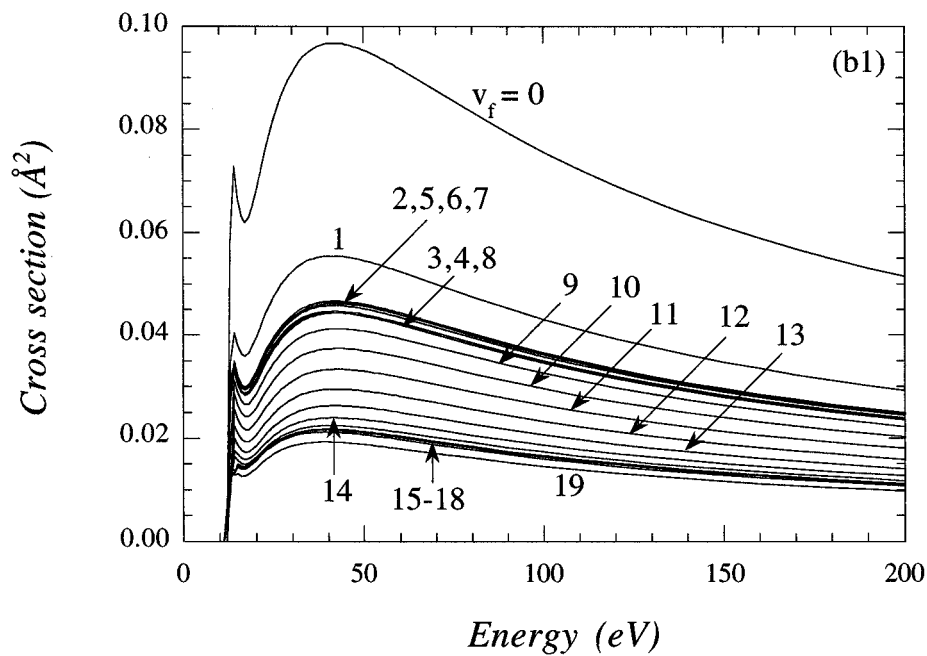
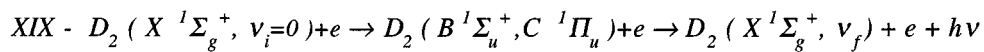
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



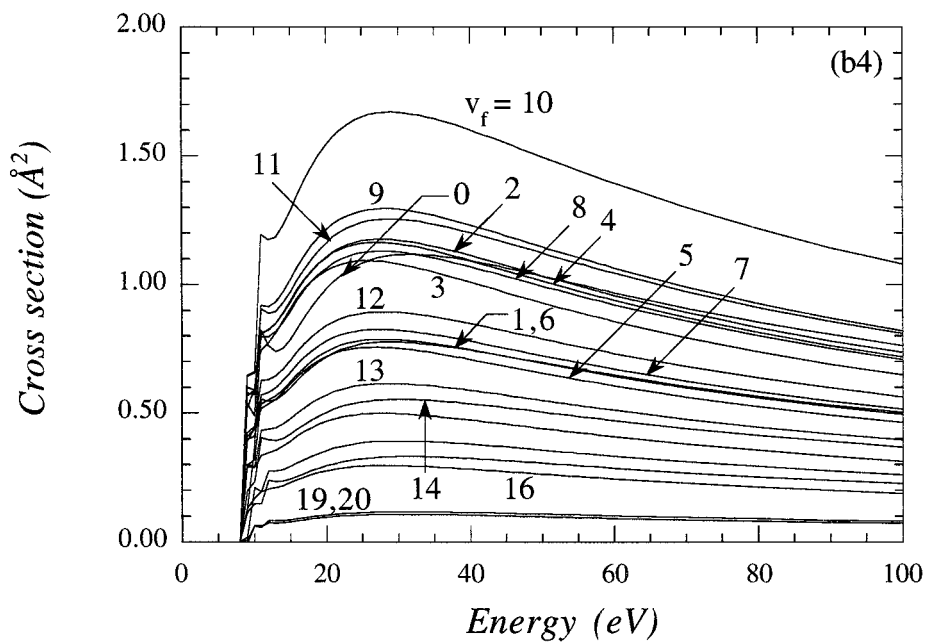
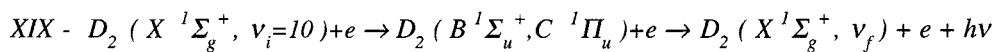
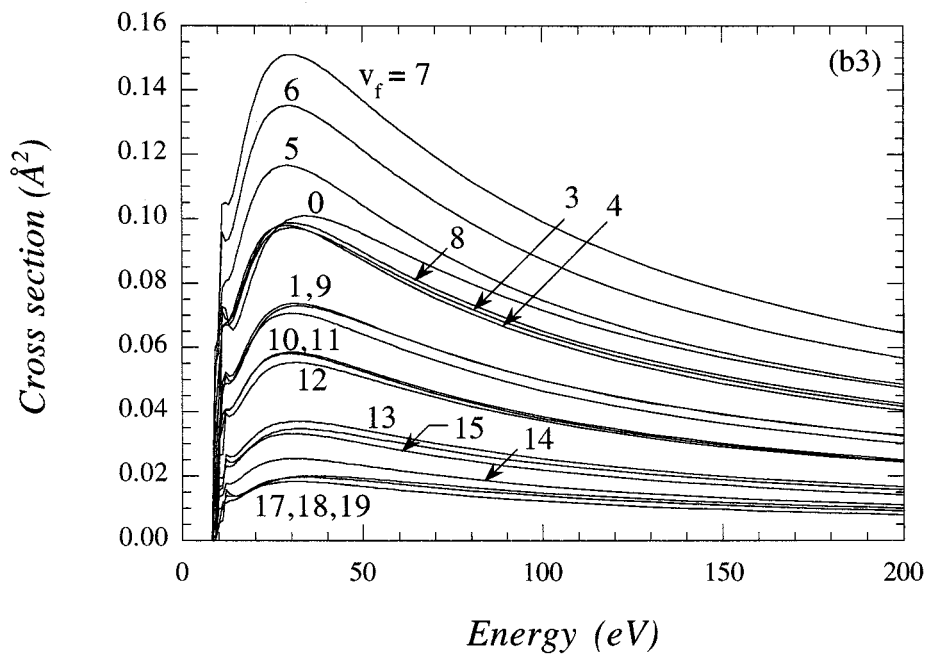
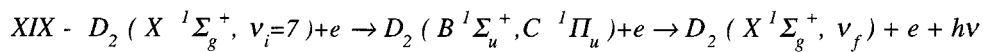
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



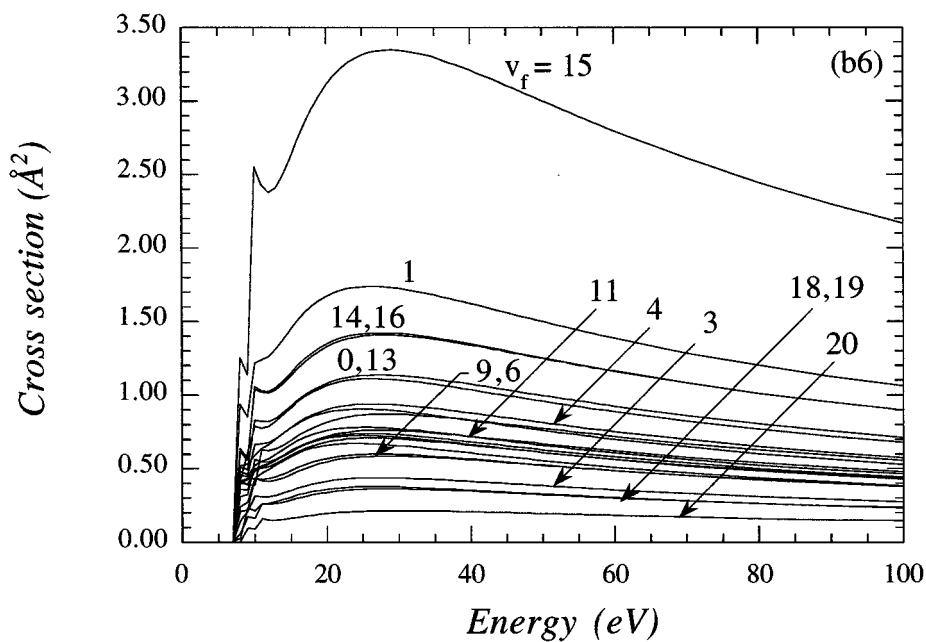
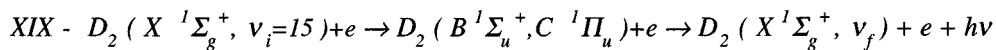
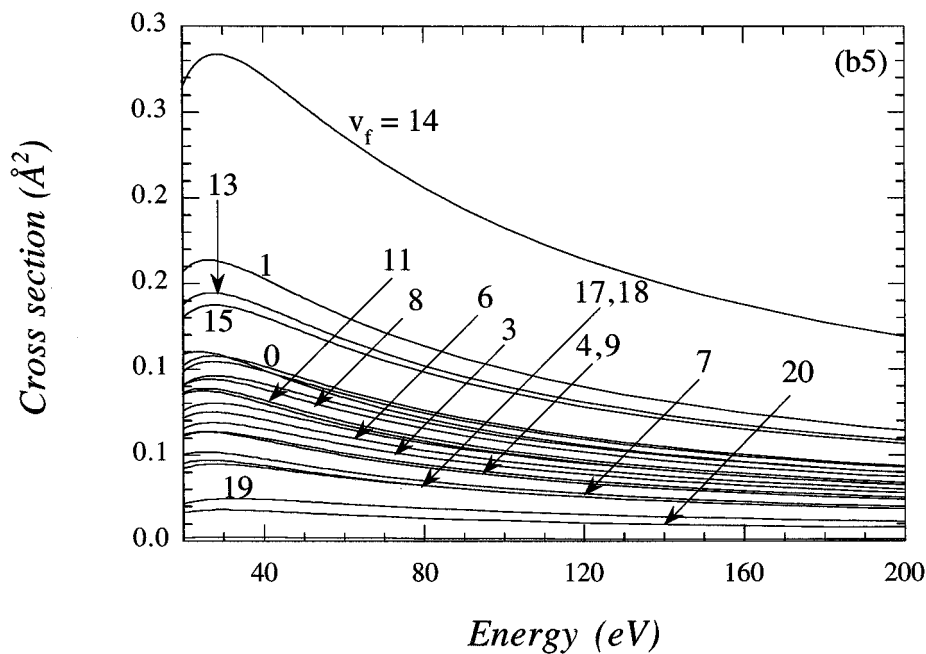
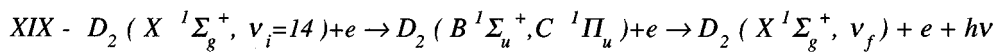
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



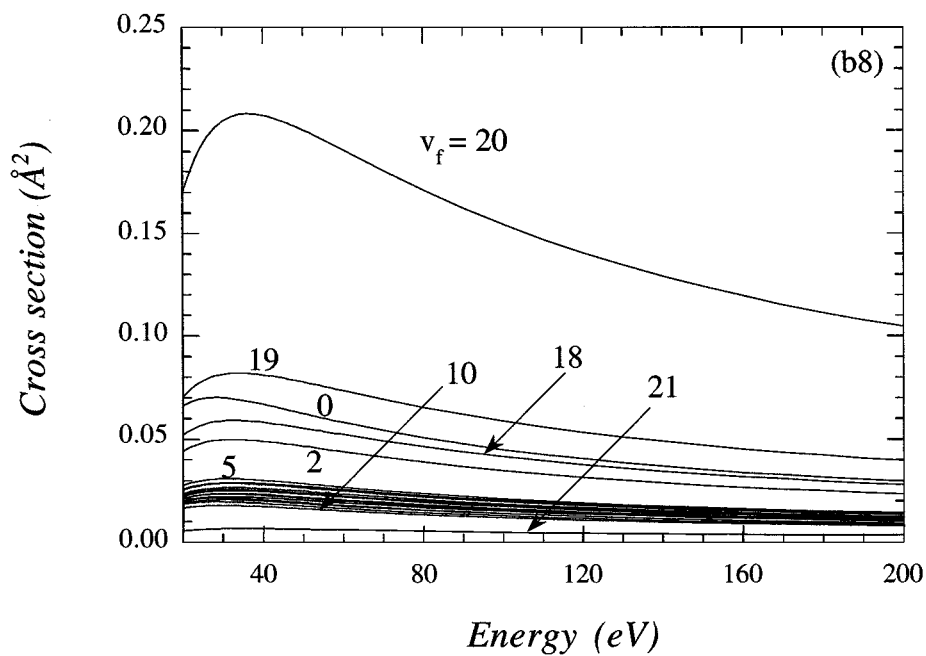
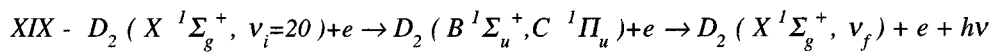
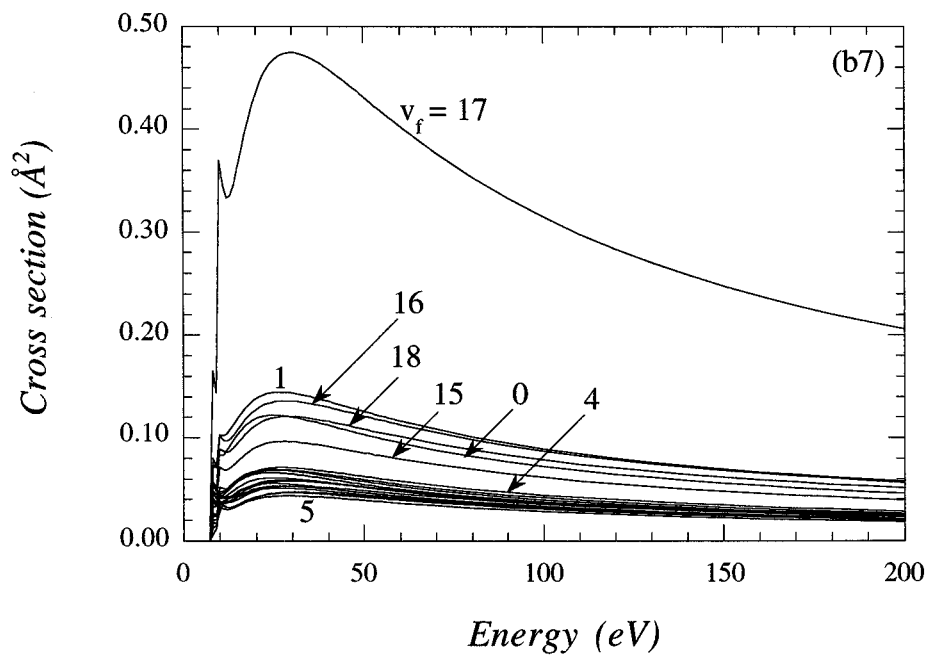
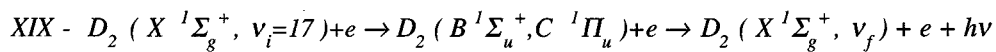
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs



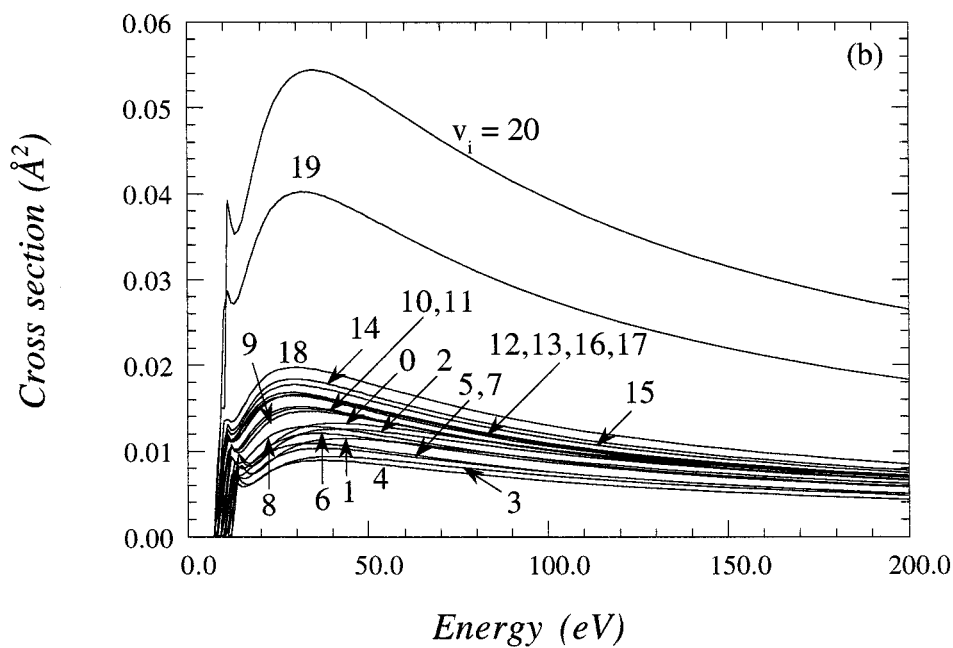
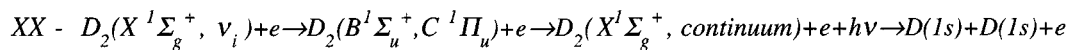
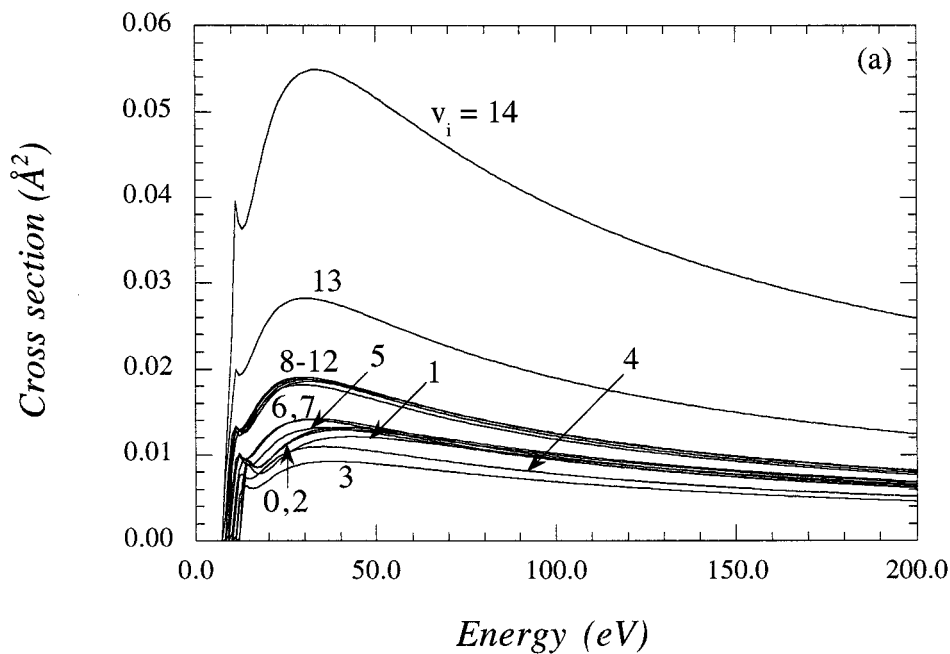
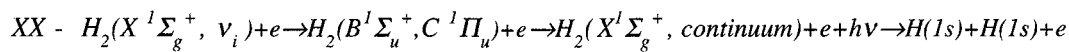
## GRAPH XIX. Excitation-Radiative Decay Vibrational Excitation Cross Sections

See page 171 for Explanation of Graphs

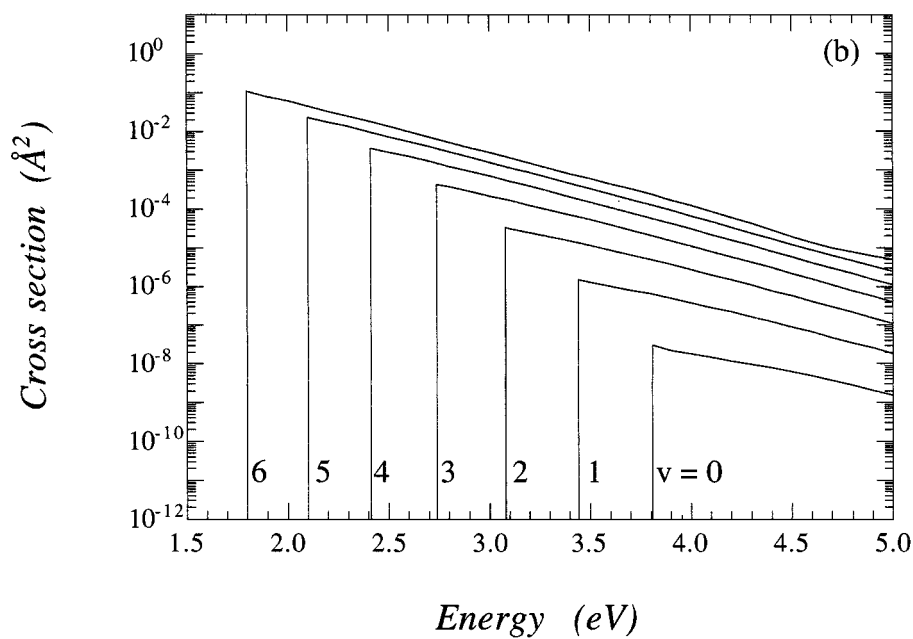
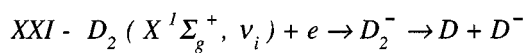
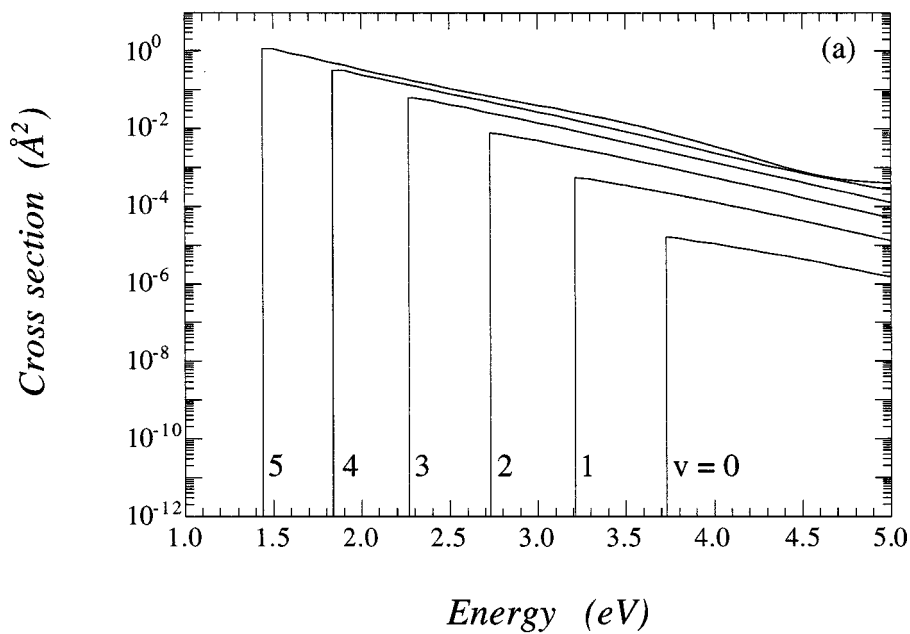
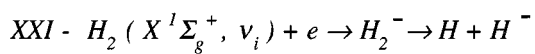


## GRAPH XX. Excitation-Radiative Decay Dissociation Cross Sections

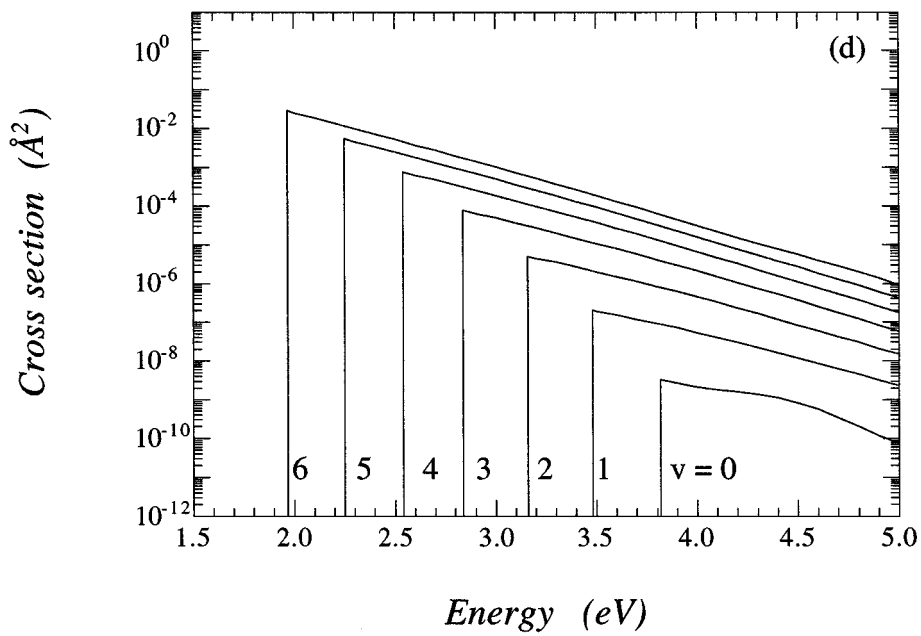
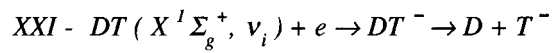
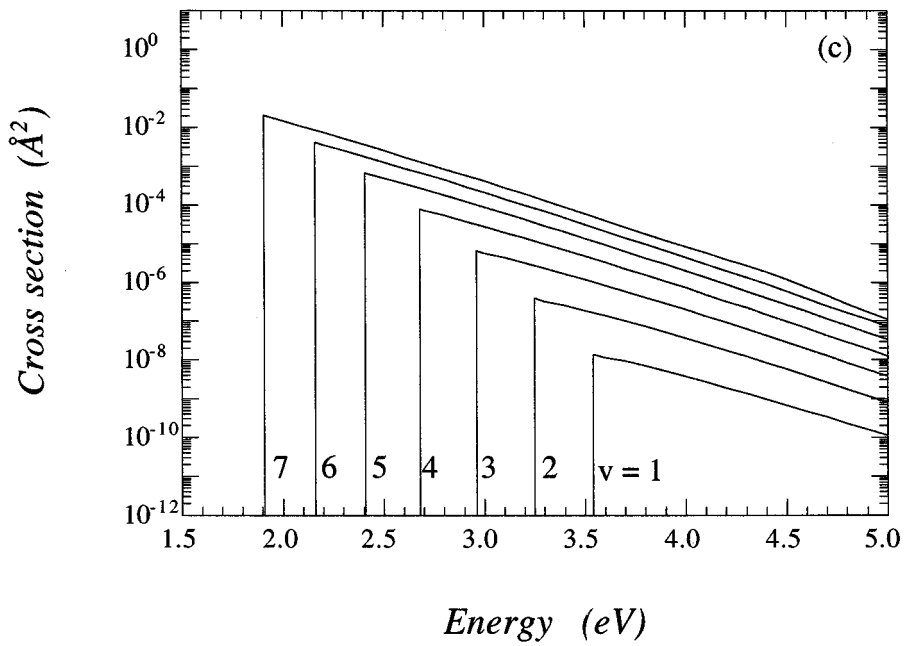
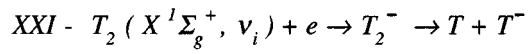
See page 171 for Explanation of Graphs



GRAPH XXI. Dissociative Electron Attachment Cross Sections  
See page 171 for Explanation of Graphs



GRAPH XXI. Dissociative Electron Attachment Cross Sections  
See page 171 for Explanation of Graphs





GRAPH XXI. Dissociative Electron Attachment Cross Sections  
See page 171 for Explanation of Graphs

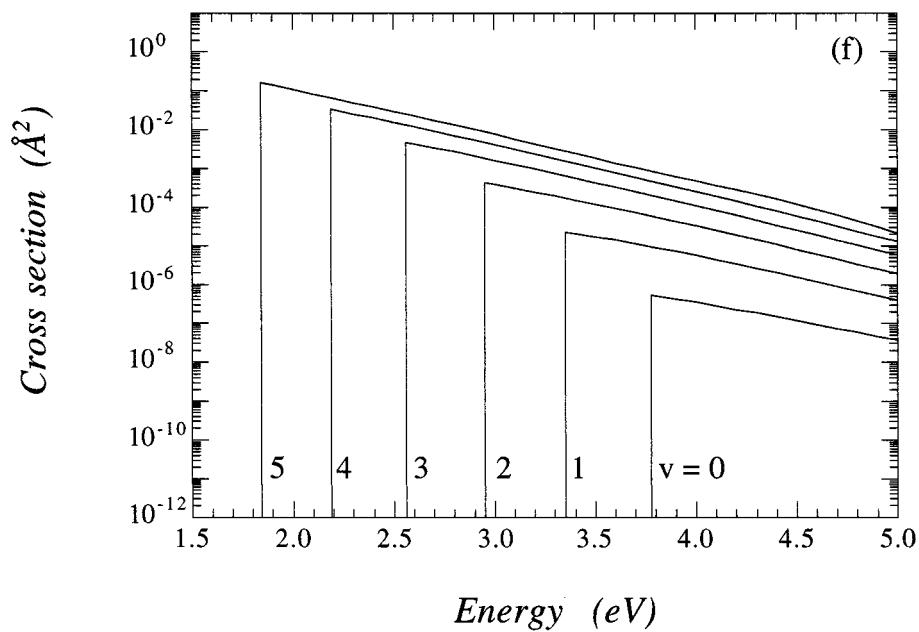
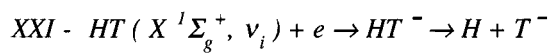
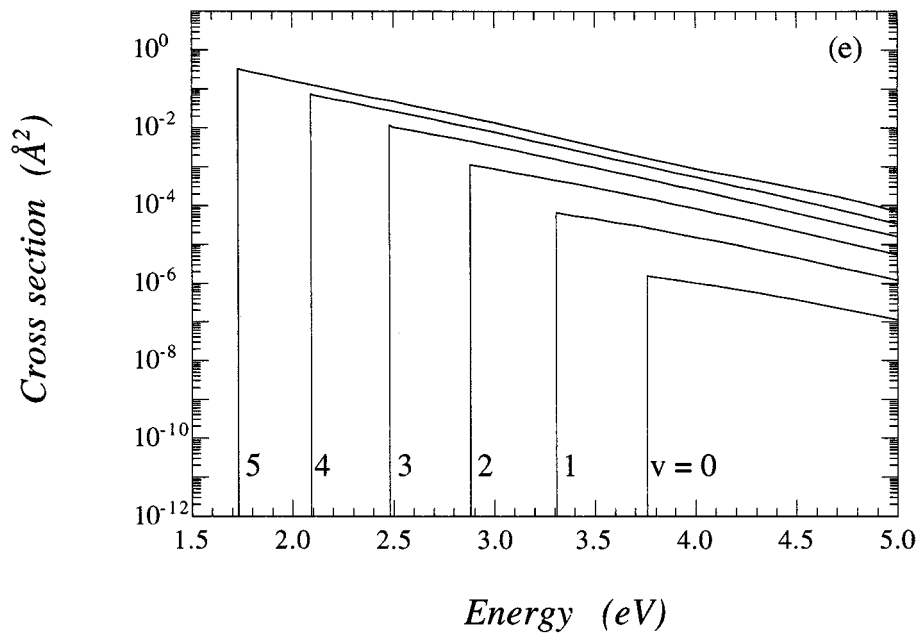
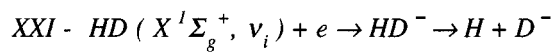


TABLE I. Energy Parameters and Fitting Coefficients for the Process  $H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(B^1\Sigma_u^+) + e$ 

See page 171 for Explanation of Tables

$v_i$	$\Delta E(eV)$	$\bar{E}(eV)$	$E_{min}(eV)$	$rms\ deviation\ \%$
0	11.184	19.0	12.0	0.18
1	10.668	18.0	11.0	0.34
2	10.181	17.0	11.0	0.26
3	9.720	17.0	10.0	0.30
4	9.293	17.0	10.0	0.24
5	8.891	17.0	9.0	0.20
6	8.518	17.0	9.0	0.13
7	8.173	17.0	9.0	0.10
8	7.857	17.0	9.0	0.25
9	7.573	17.0	9.0	0.11
10	7.322	17.0	8.0	0.11
11	7.107	15.0	8.0	0.06
12	6.931	15.0	8.0	0.05
13	6.801	15.0	8.0	0.09
14	6.728	12.0	8.0	0.57

$v_i$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
0	0.42566	0.77443	11.779	0.12348	0.52783
1	0.18587	0.54890	10.657	0.18158	0.41690
2	204.43	8.2291	10.999	0.38253	0.18743
3	0.33555	1.0022	9.4783	0.31928	0.35993
4	0.58584	1.1664	9.1842	0.36943	0.37479
5	-0.17229	0.26616	8.9927	0.78985	0.16288
6	0.81749	1.1943	8.5233	0.47785	0.38492
7	0.92882	1.3186	8.4091	0.56917	0.35835
8	0.99807(-1)	0.18517(-3)	-0.62248	-0.13667(-2)	1.9877
9	0.77975	1.2227	7.6998	0.64647	0.35969
10	1.0400	1.3663	7.4995	0.65988	0.35626
11	1.1981	1.2854	7.3894	0.59678	0.39410
12	1.5766	1.3453	7.1073	0.51796	0.40905
13	1.4026	1.2931	7.1190	0.39449	0.42743
14	-60.135	19.035	7.9949	0.51074	-0.45264(-1)
$v_i$	$c_6$	$c_7$	$c_8$	$c_9$	$c_{10}$
0	1.3204	-0.41817	2.4241	1.5734	0.65554
1	1.4717	-0.13197	2.4646	1.3141	0.65343
2	1.5461	0.73359	2.4239	0.46240	0.53316
3	1.6301	0.64238	2.7458	0.48972	0.45566
4	1.7350	0.56070	3.0202	0.51226	0.39730
5	1.5320	0.60858	3.9202	0.51458	0.34594
6	1.9010	0.44166	3.5723	0.53076	0.30894
7	2.0227	0.40399	3.7513	0.53283	0.29153
8	2.1438	0.29802	3.9108	0.55645	0.27578
9	2.1457	0.22872	4.1795	0.57404	0.27130
10	2.1576	0.38416(-1)	4.3488	0.62831	0.26689
11	2.3242	-0.67696(-1)	4.0416	0.71734	0.33856
12	2.3338	-0.94302	4.1097	1.2971	0.47889
13	2.1836	-0.70133	3.6786	1.1129	0.49914
14	1.7421	-0.70482(-1)	3.0156	0.93408	0.75610

TABLE II. Energy Parameters and Fitting Coefficients for the Process  $H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2(C^1\Pi_u) + e$ 

See page 171 for Explanation of Tables

$v_i$	$\Delta E(eV)$	$\bar{E}(eV)$	$E_{min}(eV)$	$rms\ deviation\ \%$
0	12.286	20.0	13.0	0.32
1	11.770	20.0	12.0	0.23
2	11.284	21.0	12.0	0.17
3	10.825	20.0	11.0	0.25
4	10.395	20.0	11.0	0.18
5	9.994	20.0	11.0	0.16
6	9.620	20.0	11.0	0.21
7	9.275	20.0	11.0	0.15
8	8.959	20.0	11.0	0.13
9	8.675	20.0	10.0	0.12
10	8.424	20.0	10.0	0.10
11	8.209	20.0	10.0	0.08
12	8.033	20.0	10.0	0.06
13	7.903	19.0	10.0	0.05
14	7.827	19.0	10.0	0.09

$v_i$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$c_6$	$c_7$
0	-21.104	7.5183	12.982	0.33278	-0.12174	0.15650(-4)	-0.82171
1	-5.6133	1.8255	11.060	1.0203	-1.0879	0.26640(-1)	0.38005(-2)
2	-5.1597	1.2903	9.9600	2.8643	-1.5687	0.28243(-1)	0.11213(-2)
3	1039.7	5325.6	11.000	0.28241	0.12567	0.20179(-6)	-1.0019
4	0.94696(-1)	1.2590	10.741	0.27962	0.15267	0.39886(-4)	-0.44900
5	0.29713	1.2037	10.573	0.25451	0.24534	0.60266(-6)	-0.79353
6	-15.175	11.648	10.596	0.36577	-0.80066(-1)	0.15964(-1)	-0.23501(-1)
7	0.44044	0.76833	9.4456	0.16712	0.68358	-0.23623(-1)	-0.20746(-1)
8	0.50732	0.73511	9.2031	0.14399	0.74461	-0.16500(-1)	-0.44010(-1)
9	0.58310	0.70071	8.7542	0.13343	0.84653	-0.24827(-1)	-0.40838(-1)
10	0.64865	0.70313	8.5216	0.12030	0.79792	-0.75871(-2)	-0.81168(-1)
11	0.75869	0.71280	8.3024	0.12198	0.78819	-0.49496(-2)	-0.99475(-1)
12	0.87782	0.76076	8.4109	0.14269	0.71022	-0.25767(-2)	-0.12122
13	-0.26847	0.20917	9.9543	0.84057	0.13306	-0.23326(-2)	-0.16704
14	0.72749	1.2724	10.000	0.41301	0.34294(-1)	0.12402(-1)	-0.62748(-1)
$v_i$	$c_8$	$c_9$	$c_{10}$	$c_{11}$	$c_{12}$	$c_{13}$	
0	1.2634	0.53604	1.7887	0.91350	0.84579	0.97791	
1	0.89589	0.99339	2.6247	0.78349	0.87587	0.97108	
2	1.3223	0.71412	1.9027	0.83987	0.91615	0.96520	
3	1.3474	0.66045	1.9566	1.0497	0.97251	0.95727	
4	1.3594	0.64618	1.9662	1.2854	1.0338	0.94678	
5	0.67008	1.4074	4.0764	1.4930	1.0948	0.93639	
6	1.3629	0.75903	2.0443	1.7497	1.1600	0.92431	
7	1.3735	0.80852	2.0533	2.0464	1.2200	0.91235	
8	1.4009	0.82039	2.0331	2.3989	1.2751	0.90089	
9	1.0210	-0.14058	1.1700	50.529	1.2422	0.76367	
10	1.5907	-0.17221	2.4144	3.2491	1.2642	0.90686	
11	1.8729	-1.0566	2.8283	3.0753	1.1474	0.93537	
12	2.0642	-1.4724	3.0355	2.9882	1.0945	0.94792	
13	1.9755	-1.5326	3.0406	3.5696	1.2178	0.93072	
14	1.8940	-1.7711	3.2045	3.8388	1.2842	0.92496	

TABLE III. Energy Parameters and Fitting Coefficients for the Process  $D_2(X^1\Sigma_g^+, v_i) + e \rightarrow D_2(B^1\Sigma_u^+) + e$ 

See page 171 for Explanation of Tables

$v_i$	$\Delta E(eV)$	$\bar{E}(eV)$	$E_{min}(eV)$	rms deviation %
0	11.232	20.0	12.0	0.18
1	10.858	20.0	11.0	0.62
2	10.502	17.0	11.0	0.40
3	10.160	17.0	11.0	0.26
4	9.832	17.0	10.0	0.53
5	9.519	17.0	10.0	0.17
6	9.219	17.0	10.0	0.15
7	8.935	17.0	9.0	0.14
8	8.664	17.0	9.0	0.11
9	8.407	17.0	9.0	0.10
10	8.165	17.0	9.0	0.10
11	7.938	17.0	9.0	0.10
12	7.725	17.0	9.0	0.09
13	7.529	17.0	8.0	0.10
14	7.349	17.0	8.0	0.11
15	7.187	17.0	8.0	0.12
16	7.043	12.0	8.0	0.14
17	6.921	12.0	8.0	0.16
18	6.820	12.0	8.0	0.20
19	6.745	12.0	8.0	0.29
20	6.696	12.0	8.0	0.65

$v_i$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$
0	0.42471	0.76300	11.906	0.11262	0.54884
1	0.17721	0.67170	10.999	0.20505	0.32861
2	243.18	9.0523	10.999	0.33873	0.15726
3	33.760	6.7297	10.994	0.37842	0.18106
4	-10543.	1283.2	9.8222	0.40500	0.20033
5	0.40097	1.2569	9.2975	0.35437	0.34032
6	0.54444	1.1953	8.8956	0.36592	0.37665
7	0.53678	1.0710	8.8104	0.39234	0.39768
8	0.66759	1.2311	8.6775	0.46194	0.37088
9	0.83828	1.3704	8.5001	0.52064	0.35862
10	0.98306	1.4197	8.4226	0.56806	0.35291
11	1.1122	1.4878	8.3761	0.62009	0.34236
12	1.4462	1.6945	8.2921	0.67725	0.32690
13	1.2428	1.4429	7.6842	0.64729	0.35649
14	1.3696	1.5038	7.6953	0.66871	0.34893
15	1.5980	1.5373	7.4954	0.64900	0.35537
16	1.3686	0.92554	6.9246	0.33385	0.68554
17	-0.40586	0.30323	7.8413	1.2166	0.14048
18	1.3783	1.1302	7.0212	0.36912	0.52474
19	1.2250	1.2477	7.3473	0.33168	0.45997
20	0.85479	1.3836	7.8065	0.25622	0.34867
$v_i$	$c_6$	$c_7$	$c_8$	$c_9$	$c_{10}$
0	1.3798	-0.57477	2.3389	1.6385	0.60737
1	1.5429	-0.53135	2.3520	1.5352	0.56493
2	1.4439	0.79528	2.2281	0.45151	0.60139
3	1.5138	0.71871	2.4330	0.45596	0.51944
4	1.5889	0.65506	2.6589	0.48388	0.47477
5	1.6425	0.59310	2.9201	0.51277	0.43529
6	1.6879	0.54635	3.1419	0.52071	0.39136
7	1.8102	0.50676	3.2103	0.51510	0.35527
8	1.8759	0.44042	3.4495	0.53940	0.33437
9	1.9416	0.41979	3.6438	0.54478	0.32171
10	1.9902	0.36310	3.8044	0.55190	0.29602
11	2.0394	0.31872	3.9435	0.55279	0.27636
12	2.2200	0.23524	3.8673	0.57247	0.27459
13	2.1998	0.15565	4.1138	0.59573	0.27384
14	2.2974	5.6316(-2)	4.0488	0.62592	0.27591
15	2.3062	-7.7798(-2)	4.0914	0.67479	0.28483
16	2.3426	-0.26682	3.9999	1.1235	0.57471
17	2.0763	-0.23612	4.3338	1.0334	0.57721
18	2.0186	-0.17849	4.0675	0.97688	0.60907
19	2.0036	-0.10929	3.4256	0.94620	0.68477
20	1.6757	-1.7776(-2)	2.9165	0.90989	0.85543

TABLE IV. Energy Parameters and Fitting Coefficients for the Process  $\text{D}_2(X^1\Sigma_g^+, v_i) + e \rightarrow \text{D}_2(C^1\Pi_u) + e$ 

See page 171 for Explanation of Tables

$v_i$	$\Delta E(\text{eV})$	$\bar{E}(\text{eV})$	$E_{\min}(\text{eV})$	rms deviation %
0	12.327	20.0	13.0	0.27
1	11.953	20.0	13.0	0.25
2	11.596	20.0	12.0	0.23
3	11.255	20.0	12.0	0.32
4	10.927	20.0	12.0	0.26
5	10.613	20.0	11.0	0.29
6	10.314	20.0	11.0	0.25
7	10.029	20.0	11.0	0.21
8	9.759	20.0	11.0	0.17
9	9.502	20.0	11.0	0.14
10	9.260	20.0	11.0	0.10
11	9.032	20.0	10.0	0.08
12	8.820	20.0	10.0	0.06
13	8.623	20.0	10.0	0.05
14	8.443	20.0	10.0	0.06
15	8.281	20.0	10.0	0.05
16	8.138	20.0	10.0	0.05
17	8.015	20.0	10.0	0.05
18	7.915	20.0	10.0	0.04
19	7.839	20.0	10.0	0.03
20	7.791	20.0	10.0	0.04

$v_i$	$c_1$	$c_2$	$c_3$	$c_4$	$c_5$	$c_6$	$c_7$
0	0.32639	0.98564	12.817	0.19363	0.18025	0.25607(-4)	-0.56546
1	4.3447	0.65602	7.4652	-1825.1	-4.7057	3.4344(-2)	2.7978(-2)
2	-7.4553	1.2273	9.5075	5.4510	-1.8500	0.21207(-1)	-0.12975(-1)
3	524.62	638.95	12.000	0.29288	0.57725(-1)	0.76303(-6)	-0.99153
4	100.58	8.8569	11.999	0.29807	0.80959(-1)	0.10850(-5)	-0.96085
5	0.17350	1.1783	10.902	0.25746	0.17812	0.16319(-6)	-0.99180
6	0.27941	1.2051	10.724	0.24469	0.22886	0.11475(-7)	-1.2139
7	0.35423	1.1407	10.507	0.23660	0.27326	0.19264(-9)	-1.5644
8	0.40370	1.1069	10.425	0.23384	0.30543	0.40505(-13)	-2.3673
9	0.50801	0.99073	10.060	0.25611	0.68138	-0.81247(-1)	0.92718(-2)
10	0.53662	0.94008	9.8618	0.21754	0.65296	-0.47436(-1)	0.13532(-2)
11	0.55693	0.82815	9.5201	0.17889	0.74806	-0.40187(-1)	-0.16679(-1)
12	0.61671	0.86110	9.3999	0.26340	0.82752	-0.11991	-0.23322(-2)
13	0.64980	0.82813	9.2531	0.25073	0.84678	-0.11294	-0.57026(-2)
14	0.67586	0.74353	8.9355	0.20008	0.91095	-0.87950(-1)	-0.17009(-1)
15	0.73189	0.75758	8.8193	0.16804	0.86057	-0.46903(-1)	-0.26117(-1)
16	0.79759	0.74311	8.5821	0.15762	0.88434	-0.42977(-1)	-0.30501(-1)
17	0.88718	0.72416	8.3442	0.20028	0.95517	-0.97381(-1)	-0.18481(-1)
18	0.96757	0.72012	8.2266	0.16123	0.94599	-0.60737(-1)	-0.25980(-1)
19	0.96791	0.90174	9.0830	0.21247	0.49236	-0.14901(-6)	-0.74653
20	-143.72	3.5354	8.3620	1.2827	-0.14777	-0.32881	0.23099
$v_i$	$c_8$	$c_9$	$c_{10}$	$c_{11}$	$c_{12}$	$c_{13}$	
0	1.2547	0.54778	1.7732	0.88913	0.84823	0.97858	
1	1.2703	0.65898	1.7781	0.78635	0.86937	0.97313	
2	1.2931	0.69227	1.8095	0.78909	0.89254	0.96880	
3	1.3176	0.69682	1.8613	0.84577	0.92152	0.96454	
4	1.3312	0.67057	1.9273	0.98267	0.96132	0.95927	
5	1.3468	0.64895	1.9499	1.1488	1.0052	0.95260	
6	1.3286	0.67380	2.0010	1.2956	1.0487	0.94532	
7	0.51095	1.8672	5.3254	1.4387	1.0958	0.93779	
8	1.3746	0.73665	2.0108	1.5942	1.1394	0.93013	
9	1.2309	0.86404	2.2290	1.7724	1.1805	0.92167	
10	1.3675	0.81862	2.0266	1.9546	1.2207	0.91417	
11	1.3285	0.87650	2.0844	2.2070	1.2639	0.90508	
12	1.3892	0.78664	2.0069	2.5215	1.2922	0.89801	
13	1.0079	-0.15960	1.1456	54.339	1.2477	0.76269	
14	1.5417	0.43687(-1)	2.3172	3.2442	1.2917	0.90106	
15	1.7121	-0.70998	2.6827	3.2087	1.2107	0.92216	
16	1.9018	-1.1833	2.8861	3.0755	1.1376	0.93849	
17	2.0525	-1.4619	3.0292	2.9730	1.0994	0.94813	
18	2.0383	-1.7444	3.3018	2.9469	1.0944	0.95232	
19	2.1991	-1.7929	3.1864	3.0034	1.1227	0.95215	
20	2.1810	-1.7566	3.0518	3.2085	1.2238	0.94339	