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**ANALYTICAL REPRESENTATION OF ELECTRON IMPACT
EXCITATION CROSS SECTIONS OF VIBRATIONALLY
EXCITED H₂ AND D₂ MOLECULES**

R. Celiberto

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Centro di Studio per la Chimica dei Plasmi del Consiglio Nazionale delle Ricerche,
Bari, Italy

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International Atomic Energy Agency, Vienna, Austria

February 1995

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ABSTRACT

The excitation cross sections for electron-impact induced $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ and $X^1\Sigma_g^+ \rightarrow C^1\Pi_u^+$ electronic transitions for vibrationally excited H_2 and D_2 molecules have been recalculated within the impact-parameter method (in the energy range from threshold to 200 eV) with explicit summation over the final vibrational states and assuming their rotational degeneracy. The total excitation cross sections from each individual initial vibrational state are represented by analytical expressions containing a finite number of fitting parameters. The analytic fits represent the calculated data with an accuracy better than 0.1%.

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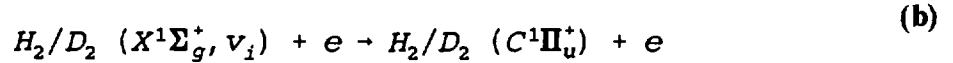
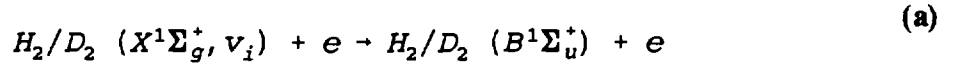
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I. INTRODUCTION

Modeling and diagnostics of various H₂ and D₂ plasmas require large sets of electron-molecule cross section data as input in the numerical treatment of the associated coupled-level kinetics¹. In particular, the knowledge of the electron-impact cross sections for the processes involving vibrationally excited molecules is of fundamental importance for understanding the plasma edge kinetics in fusion devices^{2,3}.

Extensive calculations of electron-impact collision processes for vibrationally excited H₂/D₂ molecule have been performed in the last years by using different theoretical methods^{1,2}. In view of their use as input data in the computer codes for plasma chemistry and plasma physics applications, it is useful to represent these data in analytical form by using suitable parametrizations of the calculated cross sections.

In this paper we give analytic expressions for the electron-molecule cross sections for the following excitation processes:



where the initial vibrational quantum number v_i covers the range 0-14 for hydrogen and 0-20 for deuterium. The analytical expressions have been chosen on general physics (theoretical) grounds and the free parameters in these expressions were determined by performing a non-linear fit of the cross sections calculated by using the impact-parameter method. In Section II we discuss briefly the computational procedure for obtaining the cross sections of processes (a) and (b), while in Section III we provide the analytic expressions and details on the numerical fits.

II. EXCITATION CROSS SECTIONS

The total cross sections for the processes (a) and (b) have been previously calculated in Ref. 4 for the range of collision energies from ~ 10 to 100 eV by using the impact-parameter approximation and considering the vibrational levels in the final electronic state of the molecule

as degenerate. In the present paper we have recalculated the cross sections for the same transitions by using the impact-parameter method in the formulation given in Ref. 5, i.e. explicitly summing over all the individual final vibrational states and assuming that the final rotational levels are degenerate. Moreover, we have extended the range of collision energies down to the threshold and up 200 eV using an energy step of 1 eV. The cross sections for $X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ and $X^1\Sigma_g^+ \rightarrow C^1\Pi_u$ electronic excitation transitions for e-H₂(v₁) and e-D₂(v₁) colliding systems, summed over the final state vibrational levels, are given in figures 1a-b and 2a-b, respectively.

III. ANALYTICAL EXPRESSIONS

The total cross sections for the processes (a) and (b) have been fitted by using the following analytical expression (E_{\min} and \bar{E} are defined below):

$X^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$ transition:

for $E_{\min} \leq E \leq \bar{E}$:

$$\sigma_{v_1}(E) = c_1 x \exp(-c_2 x) + c_4 x^{c_5}, \quad x = E - C_3 \quad (1)$$

for $E \geq \bar{E} + 1$ eV:

$$\sigma_{v_1}(E) = \frac{c_6}{x} \left(\frac{x-1}{x+1} \right)^{c_{10}} \left[c_7 + c_8 \left(1 - \frac{1}{2x} \right) \ln(c_9 + \sqrt{x-1}) \right], \quad x = E/\Delta E \quad (2)$$

$X^1\Sigma_g^+ \rightarrow C^1\Pi_u$ transition:

for $E_{\min} \leq E \leq \bar{E}$:

$$\sigma_{v_1}(E) = c_1 x \exp(-c_2 x) + c_4 x^{c_5} + c_6 x \exp(-c_7 x), \quad x = E - C_3 \quad (3)$$

for $E \geq \bar{E} + 1$ eV:

$$\sigma_{v_1}(E) = \frac{c_8}{x^{c_{13}}} \left(\frac{x-1}{x+1} \right)^{c_{12}} \left[c_9 + c_{10} \left(1 - \frac{1}{2x} \right) \ln(c_{11} + \sqrt{x-1}) \right], \quad x = E/\Delta E \quad (4)$$

where the collision energy E is expressed in electronvolts and the cross section $\sigma_{v_1}(E)$ in \AA^2 . The expression (1) and (3) have been used near to the threshold in order to properly interpolate

the small maximum arising in the cross sections for low incident energies. The parameter E_{\min} is very close to the threshold energy so that the cross section for $E \leq E_{\min}$ is assumed to be zero. Far from the threshold ($E > \bar{E} + 1$ eV) we used the expression (2) and (4), where x is defined in terms of transition energy ΔE given as a difference between the first vibrational eigenvalue ($v_f = 0$) of the upper (B or C) electronic state and the v_i -th energy eigenvalue belonging to the ground electronic state of the molecule. The parameter \bar{E} defines the two ranges of energy (near and far from the threshold). It depends on the vibrational quantum number v_i .

The cross sections from the regions $E \leq \bar{E}$ and $E \geq \bar{E} + 1$ were linked by a linear interpolation over the range $\bar{E} < E < \bar{E} + 1$.

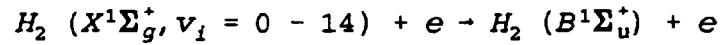
The transition energy, the parameter \bar{E} , the threshold energy E_{\min} , and the rms deviation for $X \rightarrow B$ and $X \rightarrow C$ transitions in hydrogen are given in Tables I and II, respectively, while the corresponding fitting coefficients c_i appearing in the expressions (1) - (4) are given in Tables III and IV. The corresponding quantities for deuterium are given in Tables V to VIII.

REFERENCES

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- 2) M. Capitelli, R. Celiberto, "The Dependence of Electron Impact Excitation and Ionization Cross Sections of H₂ and D₂ Molecules on Vibrational Quantum Number", in *Atomic and Molecular Processes in Fusion Edges Plasmas* (R. Janev, ed.), Plenum (New York), 1995, (in press).
- 3) R.K. Janev, *Comments At. Mol Phys.* 26, 83 (1991)
- 4) R. Celiberto and T.N. Rescigno, *Phys Rev A* 47, 1939 (1993).
- 5) M.J. Redmon, B.C. Garret, L.T. Redmon and C.W. Mc Curdy, *Phys. Rev. A* 32, 3354 (1985).

CAPTIONS

Figure 1a. Total cross sections as a function of collision energy for the process:



The cross sections increase from $v_i = 0$ through $v_i = 10$ (full lines) and follow the opposite trend for $v_i > 10$ (dashed lines).

Figure 1b. Total cross sections as a function of collision energy for the process:

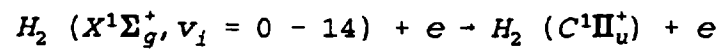


Figure 2a. Same as in Figure 1a, but for the process:

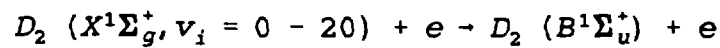


Figure 2b. Same as in Figure 1b, but for the process:

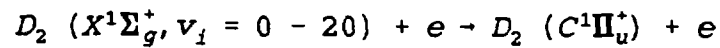
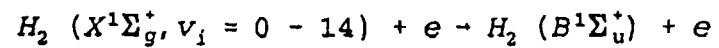


Figure 1a. Total cross sections as a function of collision energy for the process:



The cross sections increase from $v_i = 0$ through $v_i = 10$ (full lines) and follow the opposite trend for $v_i > 10$ (dashed lines).

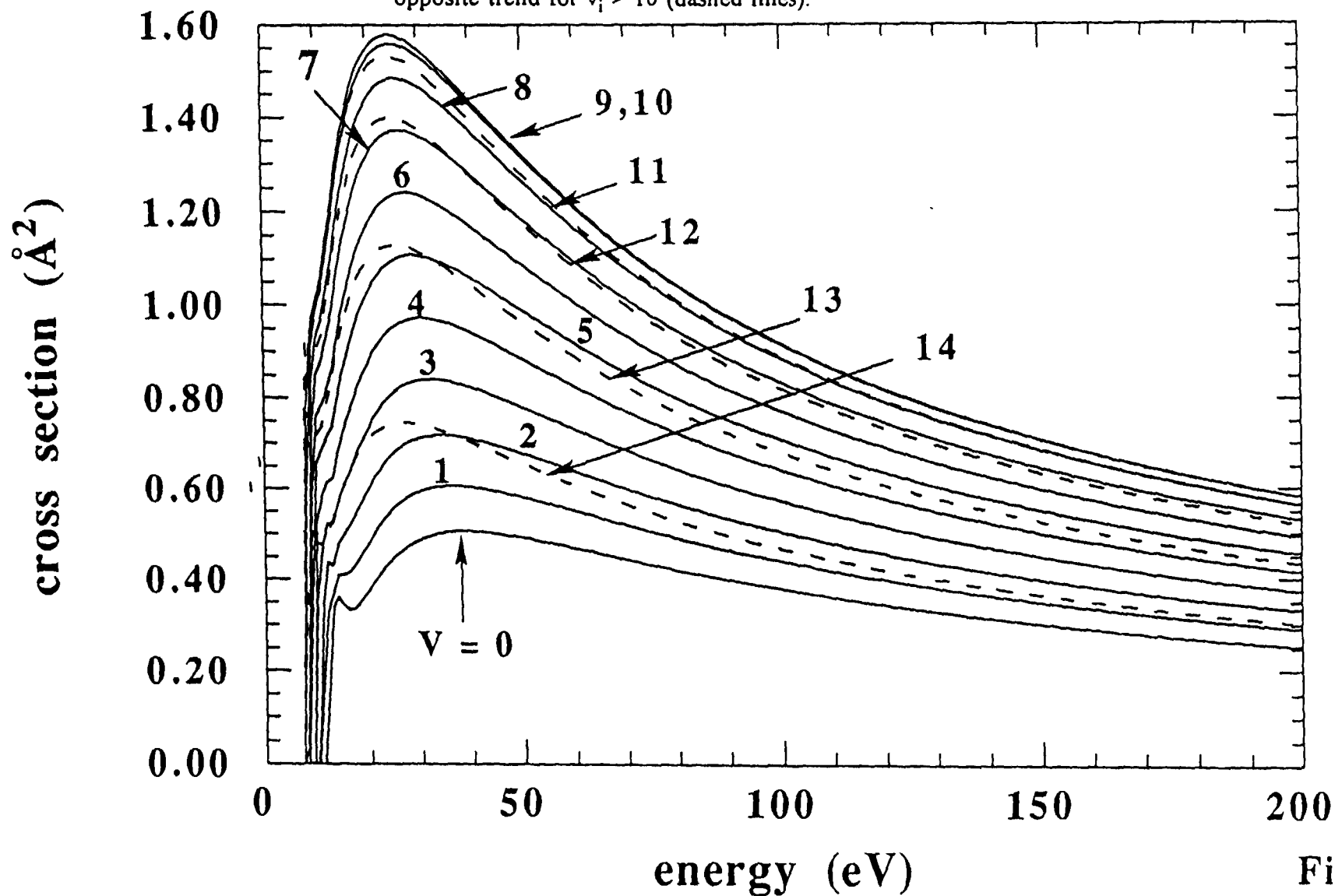


Fig.1a

Figure 1b. Total cross sections as a function of collision energy for the process:

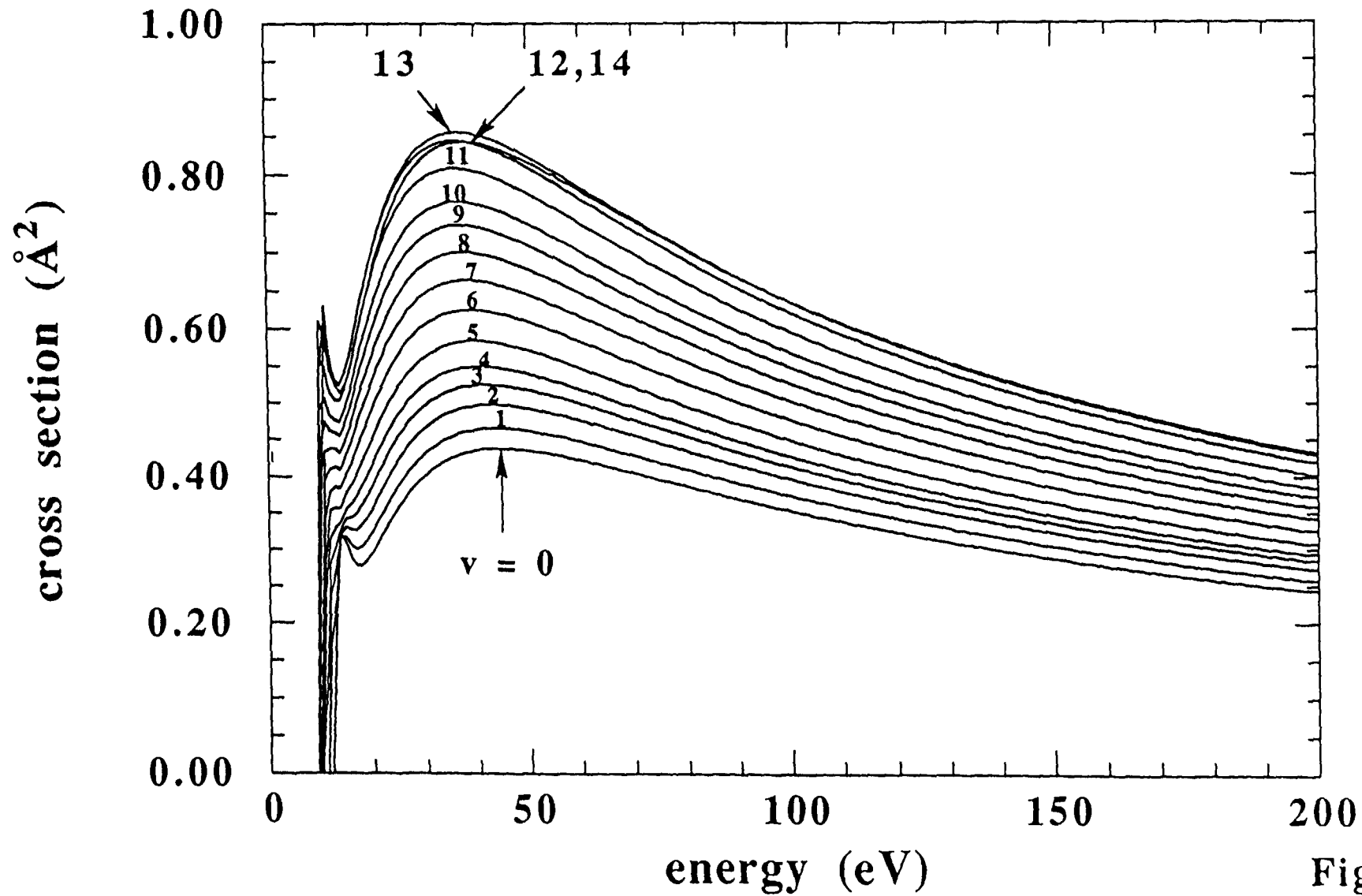
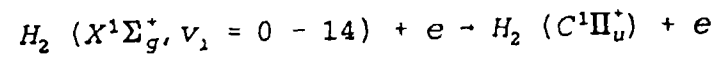


Fig.1b

Figure 2a. Same as in Figure 1a, but for the process:

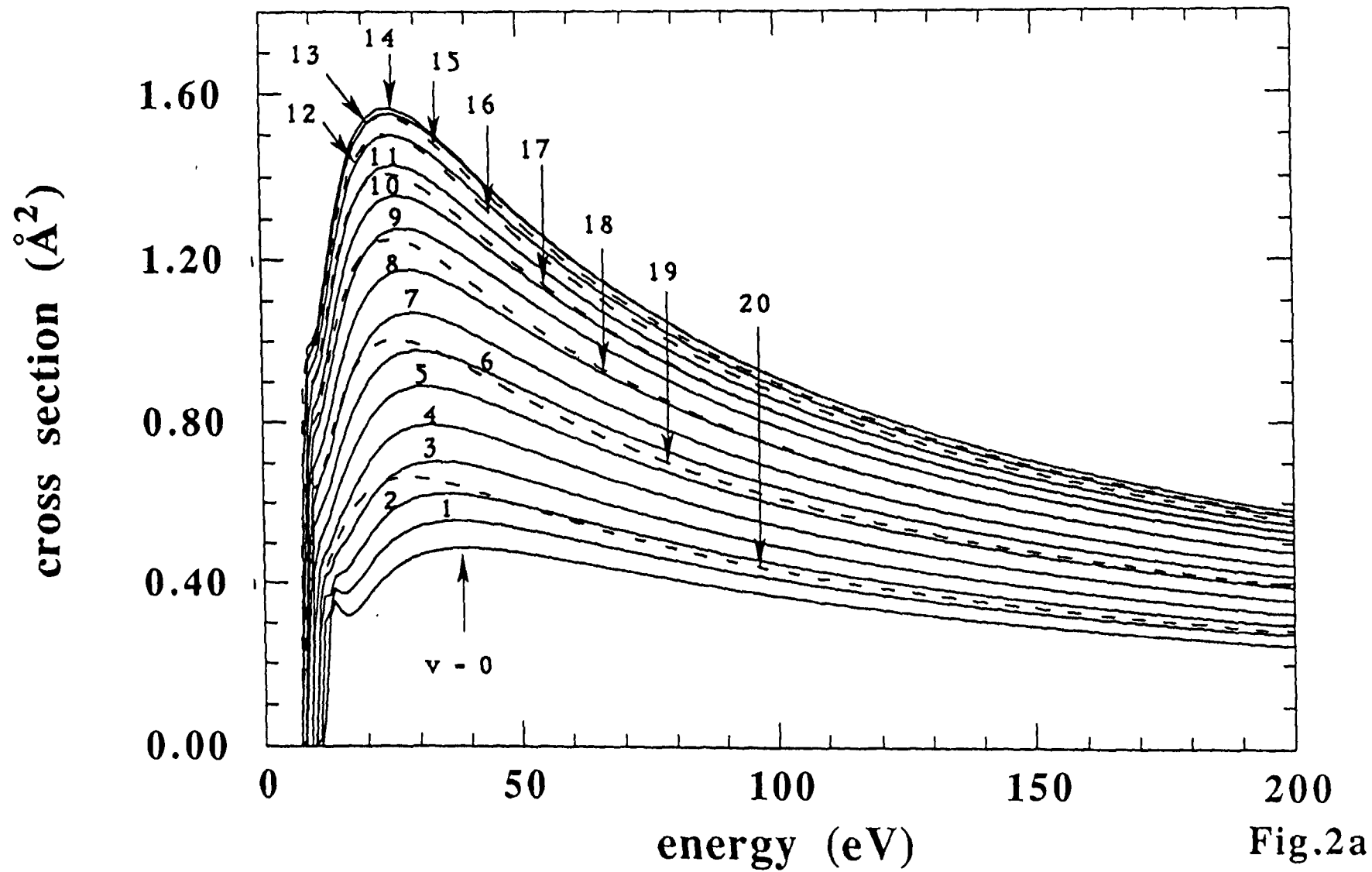
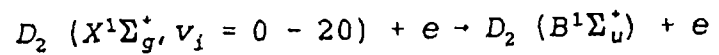


Fig.2a

Figure 2b. Same as in Figure 1b, but for the process:

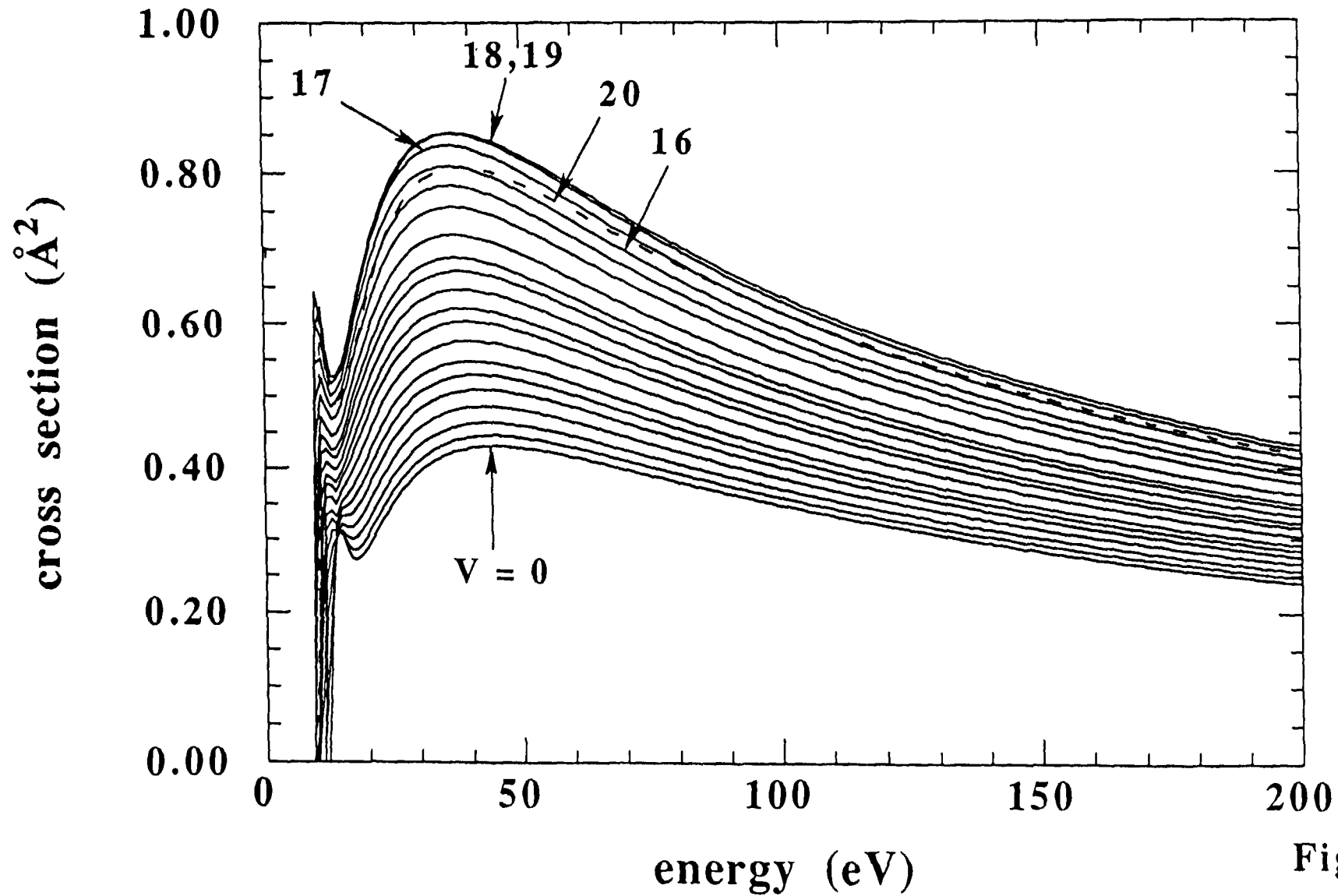
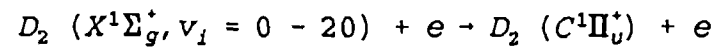
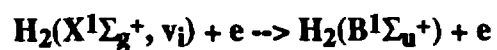


Fig.2b

TABLE I

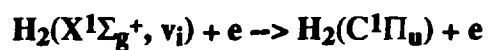
Transition energy ΔE , parameter \bar{E} , threshold energy E_{\min} , and rms deviation as a function of the initial vibrational quantum number v_i , for the process:



v_i	ΔE (eV)	\bar{E} (eV)	E_{\min} (eV)	rms deviation %
0	11.184	19.0	12.0	0.013
1	10.668	18.0	11.0	0.025
2	10.181	17.0	11.0	0.019
3	9.720	17.0	10.0	0.022
4	9.293	17.0	10.0	0.170
5	8.891	17.0	9.0	0.014
6	8.518	17.0	9.0	0.009
7	8.173	17.0	9.0	0.008
8	7.857	17.0	9.0	0.018
9	7.573	17.0	9.0	0.008
10	7.322	17.0	8.0	0.008
11	7.107	15.0	8.0	0.004
12	6.931	15.0	8.0	0.003
13	6.801	15.0	8.0	0.006
14	6.728	12.0	8.0	0.041

TABLE II

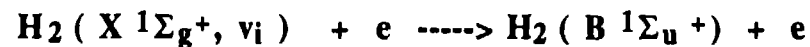
Transition energy ΔE , parameter \bar{E} , threshold energy E_{\min} , and rms deviation as a function of the initial vibrational quantum number v_i , for the process:



v_i	ΔE (eV)	\bar{E} (eV)	E_{\min} (eV)	rms deviation %
0	12.286	20.0	13.0	0.024
1	11.770	20.0	12.0	0.017
2	11.284	21.0	12.0	0.012
3	10.825	20.0	11.0	0.018
4	10.395	20.0	11.0	0.013
5	9.994	20.0	11.0	0.012
6	9.620	20.0	11.0	0.085
7	9.275	20.0	11.0	0.011
8	8.959	20.0	11.0	0.010
9	8.675	20.0	10.0	0.008
10	8.424	20.0	10.0	0.007
11	8.209	20.0	10.0	0.006
12	8.033	20.0	10.0	0.004
13	7.903	19.0	10.0	0.004
14	7.827	19.0	10.0	0.006

Table III

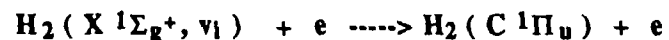
Fitting coefficients for the process:



v_i	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	c_{10}
0	.42566	.77443	11.779	.12348	.52783	1.3204	-.41817	2.4241	1.5734	.65554
1	.18587	.54890	10.657	.18158	.41690	1.4717	-.13197	2.4646	1.3141	.65343
2	204.43	8.2291	10.999	.38253	.18743	1.5461	.73359	2.4239	.46240	.53316
3	.33555	1.0022	9.4783	.31928	.35993	1.6301	.64238	2.7458	.48972	.45566
4	.58584	1.1664	9.1842	.36943	.37479	1.7350	.56070	3.0202	.51226	.39730
5	-.17229	.26616	8.9927	.78985	.16288	1.5320	.60858	3.9202	.51458	.34594
6	.81749	1.1943	8.5233	.47785	.38492	1.9010	.44166	3.5723	.53076	.30894
7	.92882	1.3186	8.4091	.56917	.35835	2.0227	.40399	3.7513	.53283	.29153
8	.99807(-1)	.18517(-3)	-.62248	-.13667(-2)	1.9877	2.1438	.29802	3.9108	.55645	.27578
9	.77975	1.2227	7.6998	.64647	.35969	2.1457	.22872	4.1795	.57404	.27130
10	1.0400	1.3663	7.4995	.65988	.35626	2.1576	.38416(-1)	4.3488	.62831	.26689
11	1.1981	1.2854	7.3894	.59678	.39410	2.3242	-.67696(-1)	4.0416	.71734	.33856
12	1.5766	1.3453	7.1073	.51796	.40905	2.3338	-.94302	4.1097	1.2971	.47889
13	1.4026	1.2931	7.1190	.39449	.42743	2.1836	-.70133	3.6786	1.1129	.49914
14	-60.135	19.035	7.9949	.51074	-.45264(-1)	1.7421	-.70482(-1)	3.0156	.93408	.75610

Table IV

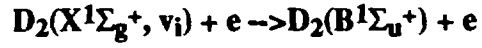
Fitting coefficients for the process:



v_j	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}
0	-21.104	7.5183	12.982	.33278	-.12174	.15650(-4)	-.82171	1.2634	.53604	1.7887	.91350	.84579	.97791
1	-5.6133	1.8255	11.060	1.0203	-1.0879	.26640(-1)	.38005(-2)	.89589	.99339	2.6247	.78349	.87587	.97108
2	-5.1597	1.2903	9.9600	2.8643	-1.5687	.28243(-1)	.11213(-2)	1.3223	.71412	1.9027	.83987	.91615	.96520
3	1039.7	5325.6	11.000	.28241	.12567	.20179(-6)	-1.0019	1.3474	.66045	1.9566	1.0497	.97251	.95727
4	.94696(-1)	1.2590	10.741	.27962	.15267	.39886(-4)	-.44900	1.3594	.64618	1.9662	1.2854	1.0338	.94678
5	.29713	1.2037	10.573	.25451	.24534	.60266(-6)	-.79353	.67008	1.4074	4.0764	1.4930	1.0948	.93639
6	-15.175	11.648	10.596	.36577	-.80066(-1)	.15964(-1)	-.23501(-1)	13.629	.75903	2.0443	1.7497	1.1600	.92431
7	.44044	.76833	9.4456	.16712	.68358	-.23623(-1)	-.20746(-1)	1.3735	.80852	2.0533	2.0464	1.2200	.91235
8	.50732	.73511	9.2031	.14399	.74461	-.16500(-1)	-.44010(-1)	1.4009	.82039	2.0331	2.3989	1.2751	.90089
9	.58310	.70071	8.7542	.13343	.84653	-.24827(-1)	-.40838(-1)	1.0210	-.14058	1.1700	50.529	1.2422	.76367
10	.64865	.70313	8.5216	.12030	.79792	-.75871(-2)	-.81168(-1)	1.5907	-.17221	2.4144	3.2491	1.2642	.90686
11	.75869	.71280	8.3024	.12198	.78819	-.49496(-2)	-.99475(-1)	1.8729	-1.0566	2.8283	3.0753	1.1474	.93537
12	.87782	.76076	8.4109	.14269	.71022	-.25767(-2)	-.12122	2.0642	-1.4724	3.0355	2.9882	1.0945	.94792
13	-.26847	.20917	9.9543	.84057	.13306	-.23326(-2)	-.16704	1.9755	-1.5326	3.0406	3.5696	1.2178	.93072
14	.72749	1.2724	10.000	.41301	.34294(-1)	.12402(-1)	-.62748(-1)	1.8940	-1.7711	3.2045	3.8388	1.2842	.92496

TABLE V

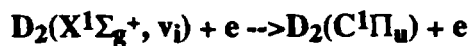
Transition energy ΔE , parameter \bar{E} , threshold energy E_{\min} , and rms deviation as a function of the initial vibrational quantum number v_i , for the process:



v_i	ΔE (eV)	\bar{E} (eV)	E_{\min} (eV)	rms deviation %
0	11.232	20.0	12.0	0.013
1	10.858	20.0	11.0	0.045
2	10.502	17.0	11.0	0.029
3	10.160	17.0	11.0	0.016
4	9.832	17.0	10.0	0.036
5	8.519	17.0	10.0	0.012
6	8.219	17.0	10.0	0.011
7	8.935	17.0	9.0	0.010
8	8.664	17.0	9.0	0.008
9	8.407	17.0	9.0	0.007
10	8.165	17.0	9.0	0.007
11	7.938	17.0	9.0	0.007
12	7.725	17.0	9.0	0.005
13	7.529	17.0	8.0	0.007
14	7.349	17.0	8.0	0.008
15	7.187	17.0	8.0	0.009
16	7.043	12.0	8.0	0.010
17	6.921	12.0	8.0	0.011
18	6.820	12.0	8.0	0.014
19	6.745	12.0	8.0	0.021
20	6.696	12.0	8.0	0.046

TABLE VI

Transition energy ΔE , parameter \bar{E} , threshold energy E_{\min} , and rms deviation as a function of the initial vibrational quantum number v_i , for the process:



v_i	ΔE (eV)	\bar{E} (eV)	E_{\min} (eV)	rms deviation %
0	12.327	20.0	13.0	0.020
1	11.953	20.0	13.0	0.018
2	11.596	20.0	12.0	0.017
3	11.255	20.0	12.0	0.023
4	10.927	20.0	12.0	0.019
5	10.613	20.0	11.0	0.021
6	10.314	20.0	11.0	0.018
7	10.029	20.0	11.0	0.015
8	9.759	20.0	11.0	0.012
9	9.502	20.0	11.0	0.010
10	9.260	20.0	11.0	0.007
11	9.032	20.0	10.0	0.006
12	8.820	20.0	10.0	0.004
13	8.623	20.0	10.0	0.004
14	8.443	20.0	10.0	0.004
15	8.281	20.0	10.0	0.004
16	8.138	20.0	10.0	0.003
17	8.015	20.0	10.0	0.003
18	7.915	20.0	10.0	0.003
19	7.839	20.0	10.0	0.003
20	7.791	20.0	10.0	0.003

Table VII

Fitting coefficients for the process: $D_2(X^1 \Sigma_g^+, v_i) + e \rightarrow D_2(B^1 \Sigma_u^+) + e$

v_i	c1	c2	c3	c4	c5	c6	c7	c8	c9	c10
0	.42471	.76300	11.906	.11262	.54884	1.3798	-.57477	2.3389	1.6385	.60737
1	.17721	.67170	10.999	.20505	.32861	1.5429	-.53135	2.3520	1.5352	.56493
2	243.18	9.0523	10.999	.33873	.15726	1.4439	.79528	2.2281	.45151	.60139
3	33.760	6.7297	10.994	.37842	.18106	1.5138	.71871	2.433	.45596	.51944
4	-10543.	1283.2	9.8222	.40500	.20033	1.5889	.65506	2.6589	.48388	.47477
5	.40097	1.2569	9.2975	.35437	.34032	1.6425	.59310	2.9201	.51277	.43529
6	.54444	1.1953	8.8956	.36592	.37665	1.6879	.54635	3.1419	.52071	.39136
7	.53678	1.0710	8.8104	.39234	.39768	1.8102	.50676	3.2103	.51510	.35527
8	.66759	1.2311	8.6775	.46194	.37088	1.8759	.44042	3.4495	.53940	.33437
9	.83828	1.3704	8.5001	.52064	.35862	1.9416	.41979	3.6438	.54478	.32171
10	.98306	1.4197	8.4226	.56806	.35291	1.9902	.36310	3.8044	.55190	.29602
11	1.1122	1.4878	8.3761	.62009	.34236	2.0394	.31872	3.9435	.55279	.27636
12	1.4462	1.6945	8.2921	.67725	.32690	2.2200	.23524	3.8673	.57247	.27459
13	1.2428	1.4429	7.6842	.64729	.35649	2.1998	.15565	4.1138	.59573	.27384
14	1.3696	1.5038	7.6953	.66871	.34893	2.2974	5.6316	4.0488	.62592	.27591
15	1.5980	1.5373	7.4954	.64900	.35537	2.3062	-7.7798	4.0914	.67479	.28483
16	1.3686	.92554	6.9246	.33385	.68554	2.3426	-.26682	3.9999	1.1235	.57471
17	-.40586	.30323	7.8413	1.2166	.14048	2.0763	-.23612	4.3338	1.0334	.57721
18	1.3783	1.1302	7.0212	.36912	.52474	2.0186	-.17849	4.0675	.97688	.60907
19	1.2250	1.2477	7.3473	.33168	.45997	2.0036	-.10929	3.4256	.94620	.68477
20	.85479	1.3836	7.8065	.25622	.34867	1.6757	-1.7776	2.9165	.90989	.85543

Table VIII

Fitting coefficients for the process: $D_2 (X^1 \Sigma_g^+, v_i) + e \rightarrow D_2 (C^1 \Pi_u) + e$

v_i	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}
0	.32639	.98564	12.817	.19363	.18025	.25607(-4)	-.56546	1.2547	.54778	1.7732	.88913	.84823	.97858
1	4.3447	.65602	7.4652	-1825.1	-4.7057	3.4344(-1)	2.7978(-1)	1.2703	.65898	1.7781	.78635	.86937	.97313
2	-7.4553	1.2273	9.5075	5.4510	-1.8500	.21207(-1)	-.12975(-1)	1.2931	.69227	1.8095	.78909	.89254	.96880
3	524.62	638.95	12.000	.29288	.57725(-1)	.76303(-6)	-.99153	1.3176	.69682	1.8613	.84577	.92152	.96454
4	100.58	8.8569	11.999	.29807	.80959(-1)	.10850(-5)	-.96085	1.3312	.67057	1.9273	.982670	.96132	.95927
5	.17350	1.1783	10.902	.25746	.17812	.16319(-6)	-.99180	1.3468	.64895	1.9499	1.1488	1.0052	.95260
6	.27941	1.2051	10.724	.24469	.22886	.11475(-7)	-1.2139	1.3286	.67380	2.0010	1.2956	1.0487	.94532
7	.35423	1.1407	10.507	.23660	.27326	.19264(-9)	-15.644	.51095	1.8672	5.3254	1.4387	1.0958	.93779
8	.40370	1.1069	10.425	.23384	.30543	.40505(-13)	-2.3673	1.3746	.73665	2.0108	1.5942	1.1394	.93013
9	.50801	.99073	10.0601	.25611	.68138	-.81247(-1)	.92718(-2)	1.2309	.86404	2.2290	1.7724	1.1805	.92167
10	.53662	.94008	9.8618	.21754	.65296	-.47436(-1)	.13532(-2)	1.3675	.81862	2.0266	1.9546	1.2207	.91417
11	.55693	.82815	9.5201	.17889	.74806	-.40187(-1)	-.16679(-1)	1.3285	.87650	2.0844	2.2070	1.2639	.90508
12	.61671	.86110	9.3999	.26340	.82752	-.11991	-.23322(-2)	1.3892	.78664	2.0069	2.5215	1.2922	.89801
13	.64980	.82813	9.2531	.25073	.84678	-.11294	-.57026(-2)	1.0079	-.15960	1.1456	54.339	1.2477	.76269
14	.67586	.74353	8.9355	.20008	.91095	-.87950(-1)	-.17009(-1)	1.5417	.43687(-1)	2.3172	3.2442	1.2917	.90106
15	.73189	.75758	8.8193	.16804	.86057	-.46903(-1)	-.26117(-1)	1.7121	-.70998	2.6827	3.2087	1.2107	.92216
16	.79759	.74311	8.5821	.15762	.88434	-.42977(-1)	-.30501(-1)	1.9018	-1.1833	2.8861	3.0755	1.1376	.93849
17	.88718	.71416	8.3442	.20028	.95517	-.97381(-1)	-.18481(-1)	2.0525	-1.4619	.30292	2.9730	1.0994	.94813
18	.96757	.72012	8.2266	.16123	.94599	-.60737(-1)	-.25980(-1)	2.0383	-1.7444	3.3018	2.9469	1.0944	.95232
19	.96791	.90174	9.0830	.21247	.49236	-.14901(-6)	-.74653	2.1991	-1.7929	3.1864	3.0034	1.1227	.95215
20	-143.72	3.5354	8.3620	1.2827	-.14777	-.32881	.23099	2.1810	-1.7566	3.0518	3.2085	1.2238	.94339