Dynamics of the O + H_2^+ → OH^+ + H, OH + H^+ proton and hydrogen atom transfer reactions on the two lowest potential energy surfaces

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Supplementary Information

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Table S1. Cross sections

Property	v_0=0									v_0=1									
	j_0=0			j_0=2			j_0=4			j_0=0			j_0=2			j_0=4			
E_{col}	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**GROUND PES**
σ (E_{col})/ Å^2	181.3	60.8	41.4	182.6	62.1	41.3	181.3	60.0	39.8	167.9	58.6	39.7	175.3	60.2	40.2	175.1	58.2	38.8	
b_{max} / Å	7.81	4.86	4.01	7.73	4.93	4.11	7.73	4.93	4.08	7.84	4.89	4.05	7.74	4.98	4.15	7.74	4.96	4.09	
Probability	0.95	0.82	0.82	0.97	0.81	0.78	0.97	0.79	0.76	0.87	0.78	0.77	0.93	0.77	0.74	0.93	0.75	0.74	
E_{col}	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**EXCITED PES**
σ (E_{col})/ Å^2	57.9	35.6	27.8	56.3	35.1	27.9	56.2	34.5	27.5	54.9	34.2	27.8	53.8	34.1	27.7	53.9	33.5	27.1	
b_{max} / Å	4.44	3.60	3.34	4.32	3.61	3.37	4.32	3.52	3.33	4.48	3.65	3.39	4.34	3.67	3.42	4.34	3.58	3.38	
Probability	0.94	0.87	0.80	0.96	0.86	0.78	0.96	0.92	0.79	0.87	0.82	0.77	0.91	0.81	0.75	0.91	0.83	0.75	

Table S2. Average energy fractions

Property	v_0=0									v_0=1									
	j_0=0			j_0=2			j_0=4			j_0=0			j_0=2			j_0=4			
E_{col}	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**GROUND PES**
$\langle f'_T \rangle$	0.23	0.25	0.26	0.21	0.25	0.25	0.21	0.23	0.24	0.21	0.22	0.23	0.20	0.22	0.22	0.19	0.21	0.21	
$\langle f'_V \rangle$	0.52	0.50	0.50	0.53	0.50	0.50	0.54	0.52	0.51	0.56	0.55	0.56	0.56	0.54	0.55	0.58	0.55	0.55	
$\langle f'_R \rangle$	0.25	0.25	0.24	0.26	0.25	0.25	0.25	0.25	0.25	0.23	0.22	0.21	0.24	0.24	0.23	0.23	0.24	0.24	
E_{col}	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**0.05**	**0.25**	**0.50**	**EXCITED PES**
$\langle f'_T \rangle$	0.30	0.30	0.34	0.29	0.30	0.32	0.29	0.30	0.30	0.28	0.30	0.32	0.28	0.30	0.31	0.29	0.29	0.30	
$\langle f'_V \rangle$	0.41	0.41	0.38	0.42	0.40	0.38	0.42	0.40	0.39	0.44	0.42	0.40	0.44	0.40	0.40	0.43	0.41	0.40	
$\langle f'_R \rangle$	0.29	0.29	0.28	0.29	0.30	0.30	0.29	0.30	0.31	0.28	0.28	0.28	0.28	0.30	0.29	0.28	0.30	0.30	

Table S3. Average properties of the J, l' and j' vectors for H_2^+(v=0, j=0)

Ground PES ($1^2A''$)

E_{col}/eV	0.05	0.15	0.30	0.50
<cos(***Jl***')>	0.267	0.382	0.413	0.444
$\left\langle \frac{l'}{J} \right\rangle$	0.729	0.591	0.566	0.516
<cos(***Jj***')>	0.770	0.838	0.857	0.886
$\left\langle \frac{j'}{J} \right\rangle$	1.093	0.994	0.969	0.955
<cos(***l'j'***)>	$-1.0\ 10^{-2}$	$-8.6\ 10^{-3}$	$4.2\ 10^{-4}$	$-6.2\ 10^{-3}$
$\left\langle \frac{l'}{j'} \right\rangle$	0.850	0.717	0.711	0.633

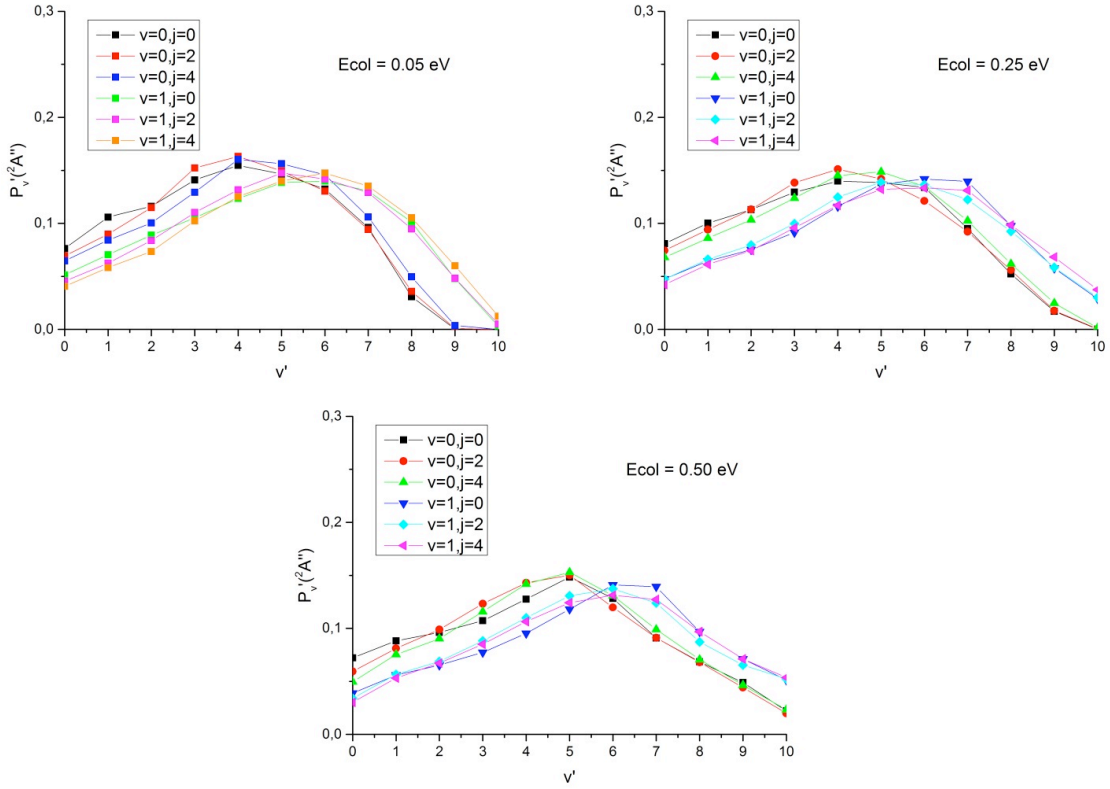
Excited PES ($1^2A'$)

E_{col}/eV	0.05	0.15	0.30	0.50
<cos(***Jl'***)>	0.218	0.219	0.268	0.373
$\left\langle \frac{l'}{J} \right\rangle$	0.982	0.696	0.574	0.487
<cos(***Jj'***)>	0.658	0.802	0.868	0.894
$\left\langle \frac{j'}{J} \right\rangle$	1.241	1.110	1.065	0.994
<cos(***l'j'***)>	$-3.5\ 10^{-3}$	$-5.7\ 10^{-3}$	$-2.6\ 10^{-3}$	$-8.0\ 10^{-3}$
$\left\langle \frac{l'}{j'} \right\rangle$	1.183	0.810	0.608	0.535

Figure S1

Product vibrational distributions

Ground PES ($1^2A''$)



Excited PES ($1^2A'$)

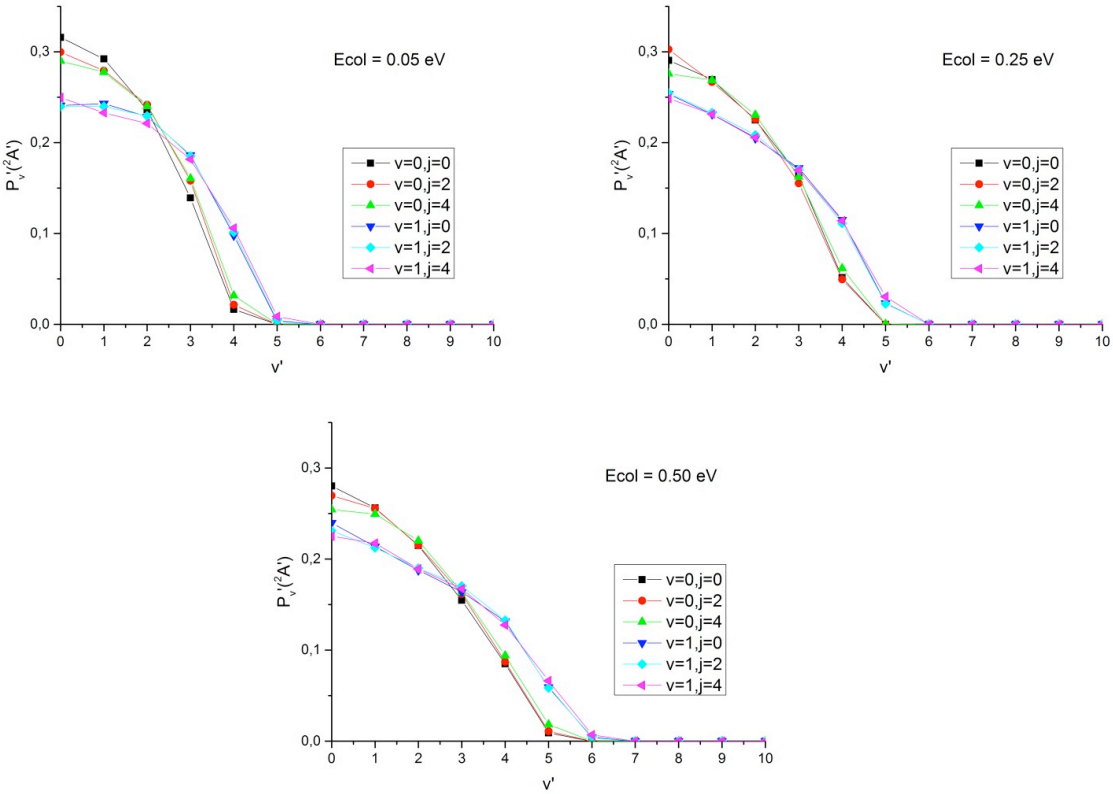
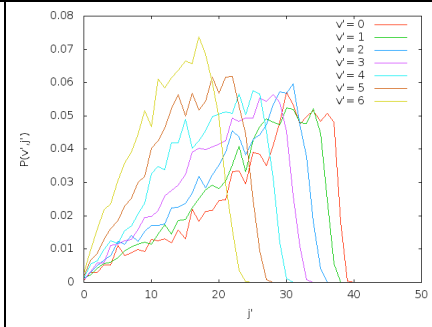
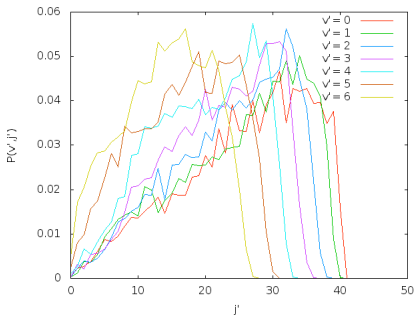
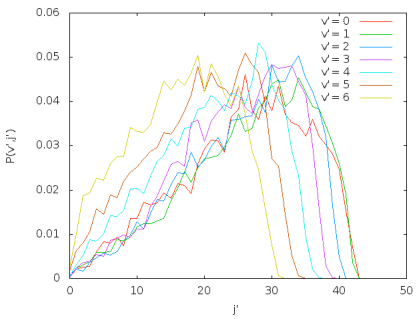
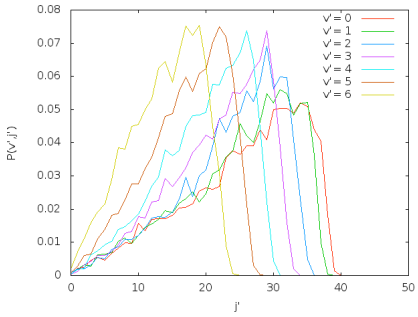
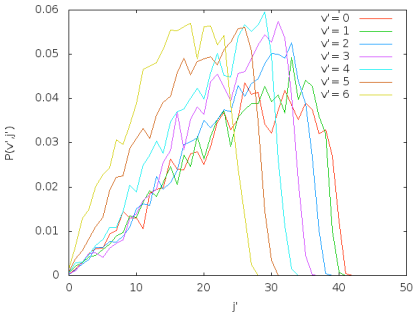
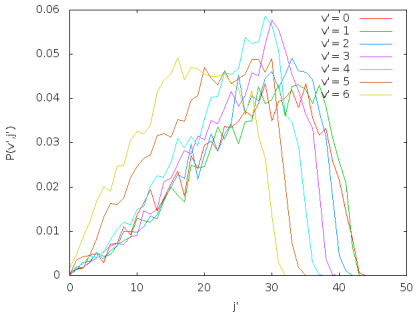
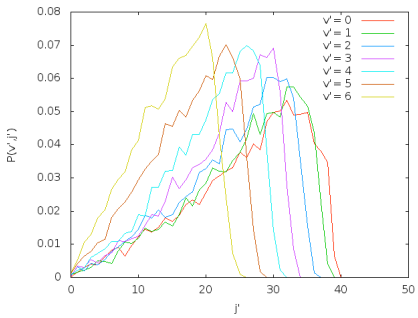
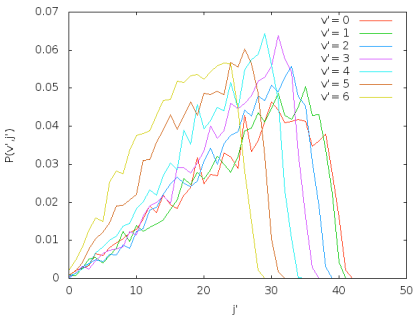
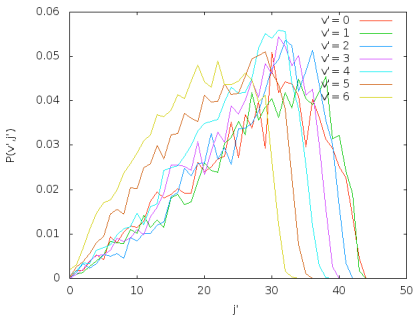
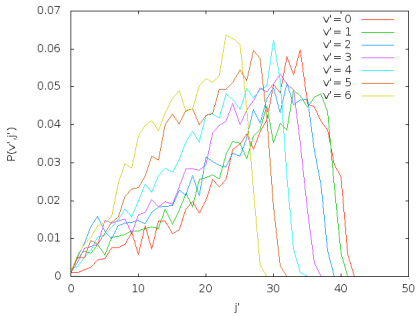
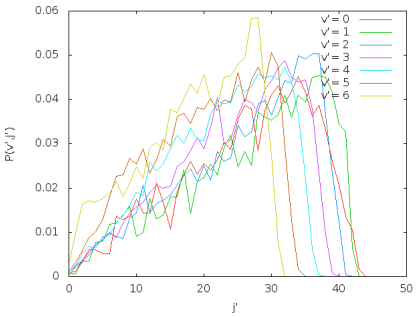
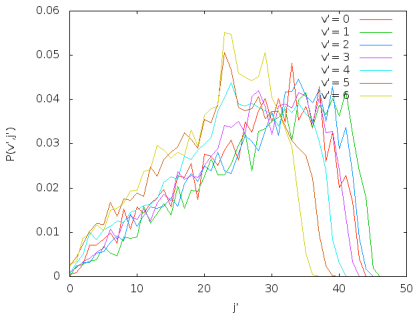


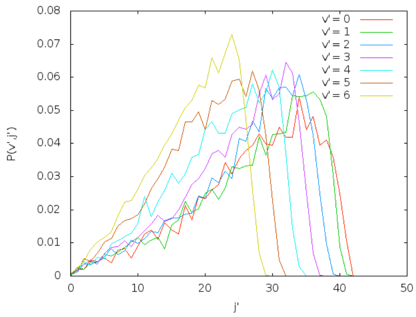
Figure S2

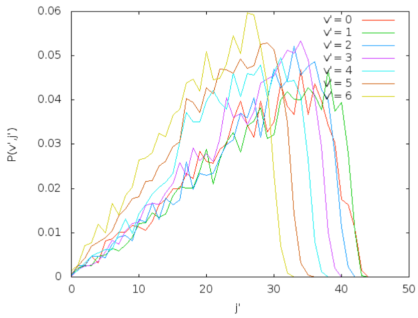
Product rotational distributions

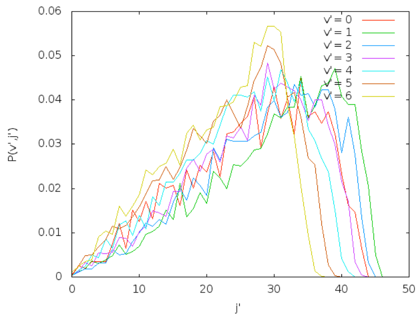
Ground PES ($1^2A''$)

	0.05 eV	0.25 eV	0.50 eV
v=0 j=0			
v=0 j=2			
v=0 j=4			
v=1 j=0			

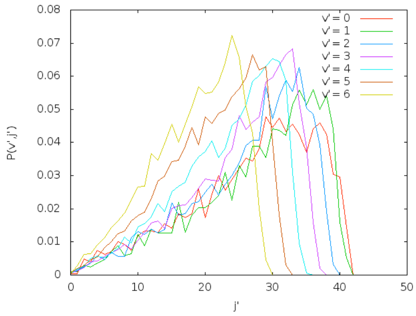
v=1 j=2

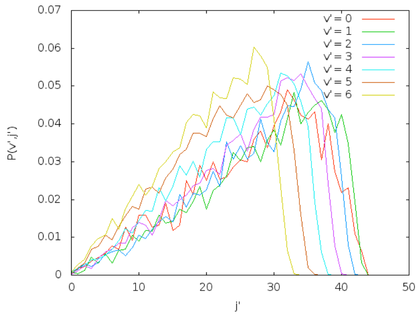

P(v',j')
j'
v' = 0
v' = 1
v' = 2
v' = 3
v' = 4
v' = 5
v' = 6


P(v',j')
j'
v' = 0
v' = 1
v' = 2
v' = 3
v' = 4
v' = 5
v' = 6


P(v',j')
j'
v' = 0
v' = 1
v' = 2
v' = 3
v' = 4
v' = 5
v' = 6

v=1 j=4


P(v',j')
j'
v' = 0
v' = 1
v' = 2
v' = 3
v' = 4
v' = 5
v' = 6


P(v',j')
j'
v' = 0
v' = 1
v' = 2
v' = 3
v' = 4
v' = 5
v' = 6

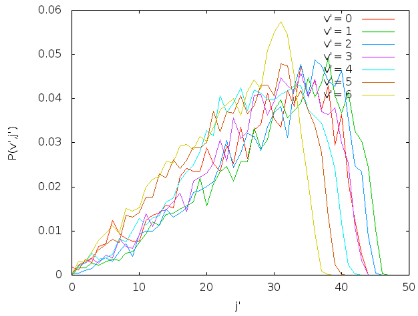
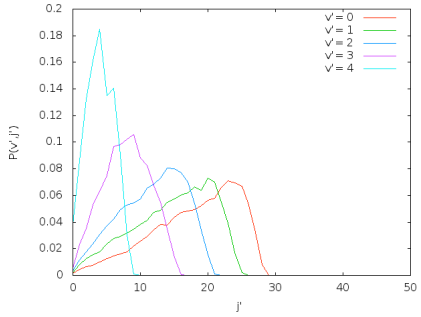
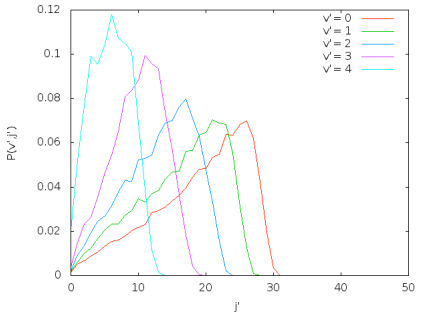
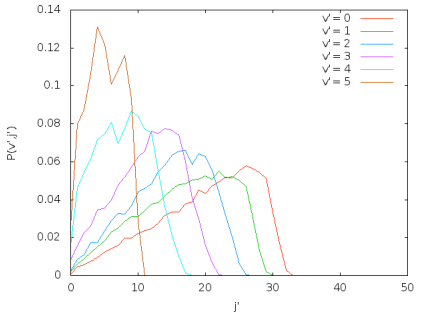
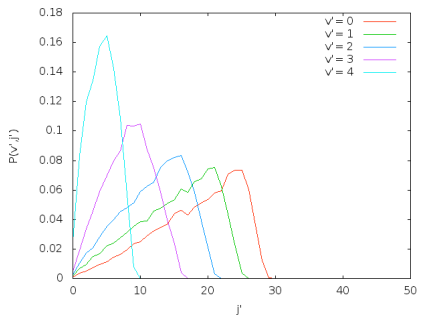
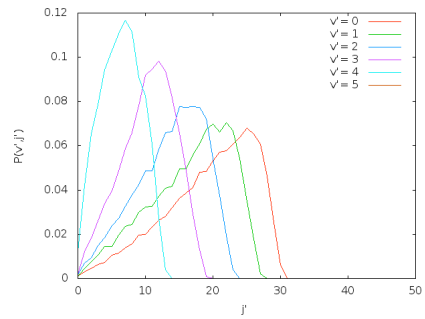
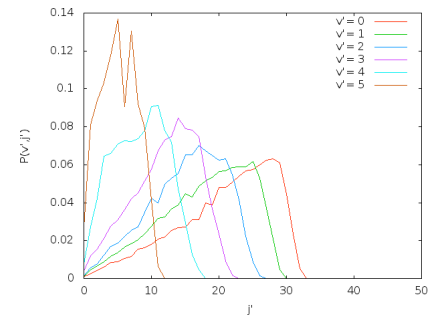
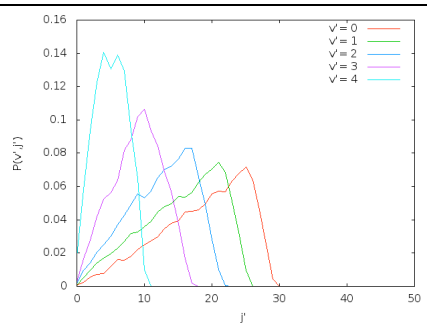
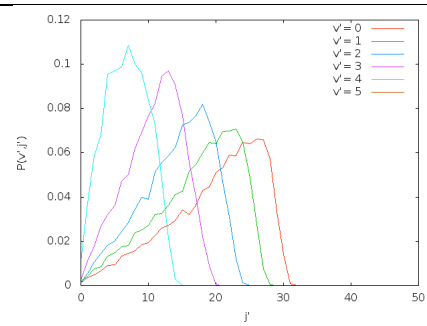
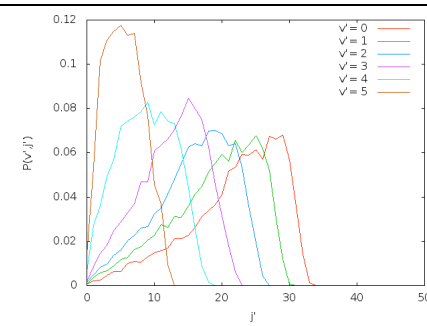
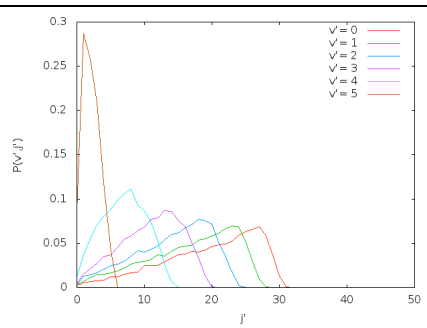
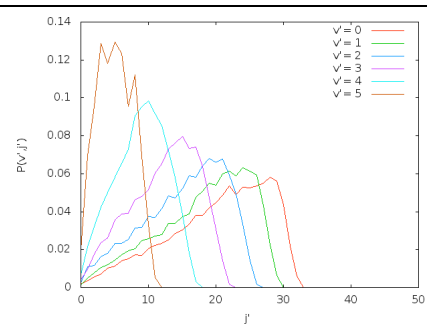
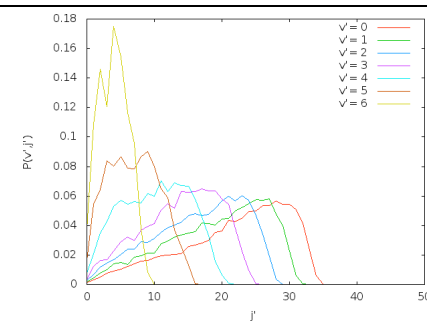

P(v',j')
j'
v' = 0
v' = 1
v' = 2
v' = 3
v' = 4
v' = 5
v' = 6

Figure S2 (cont.)

Product rotational distributions

Excited PES ($1^2A'$)

	0.05 eV	0.25 eV	0.50 eV
v=0 j=0			
v=0 j=2			
v=0 j=4			
v=1 j=0			

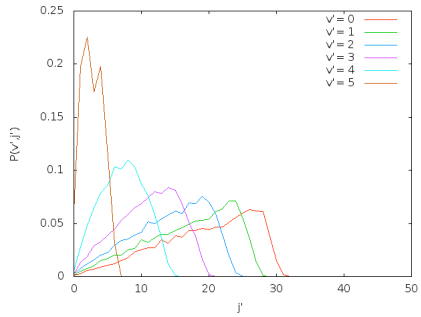
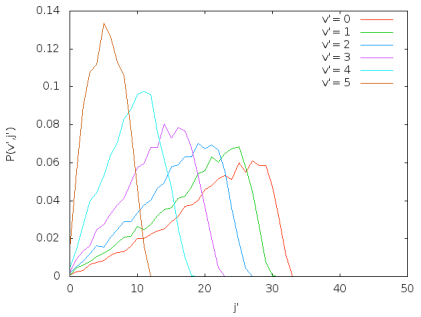
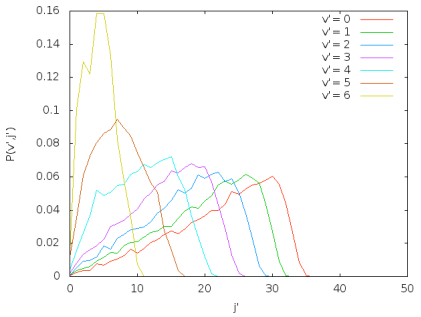
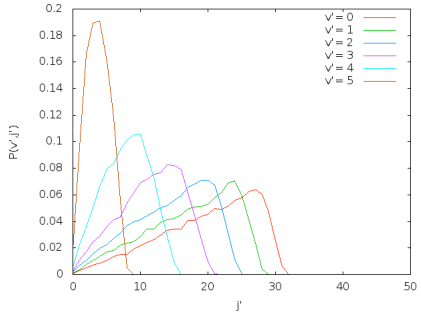
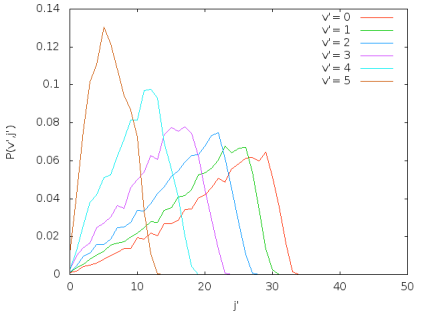
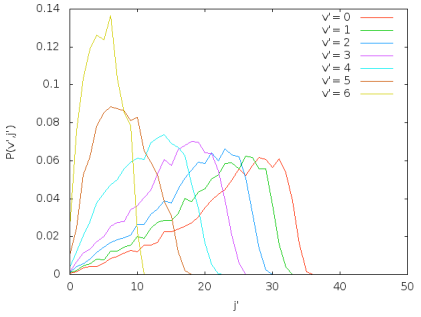
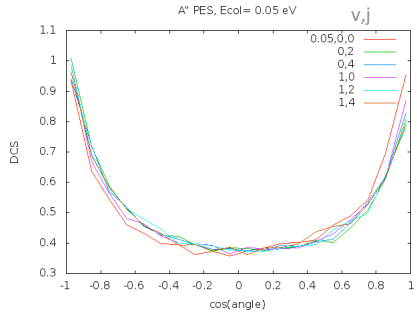
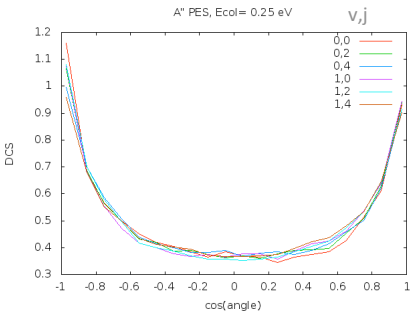
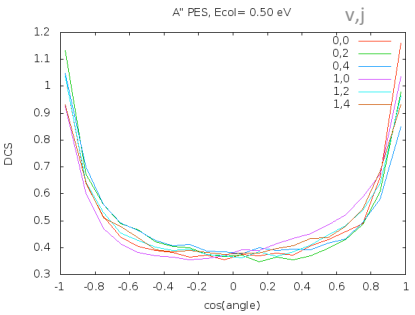
v=1 j=2	 v' = 0 v' = 1 v' = 2 v' = 3 v' = 4 v' = 5 P(v', j') j'	 v' = 0 v' = 1 v' = 2 v' = 3 v' = 4 v' = 5 P(v', j') j'	 v' = 0 v' = 1 v' = 2 v' = 3 v' = 4 v' = 5 v' = 6 P(v', j') j'
v=1 j=4	 v' = 0 v' = 1 v' = 2 v' = 3 v' = 4 v' = 5 P(v', j') j'	 v' = 0 v' = 1 v' = 2 v' = 3 v' = 4 v' = 5 P(v', j') j'	 v' = 0 v' = 1 v' = 2 v' = 3 v' = 4 v' = 5 v' = 6 P(v', j') j'

Figure S3

Angular distributions (kk')

Ground PES ($1^2A''$)

0.05 eV	0.25 eV	0.50 eV
		

Excited PES ($1^2A'$)

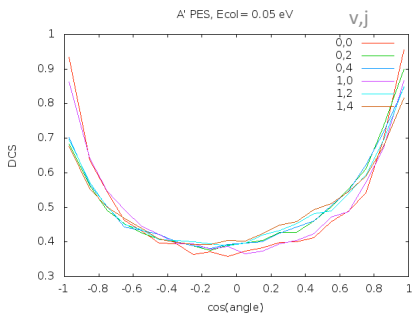
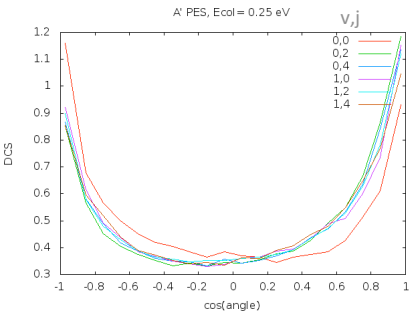
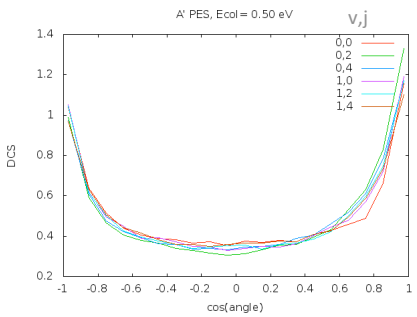
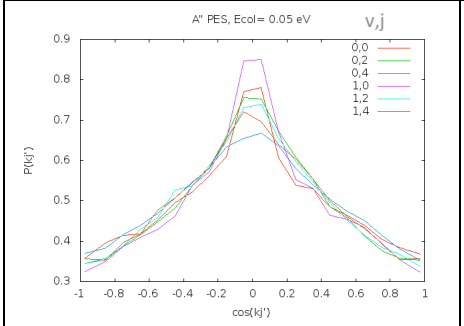
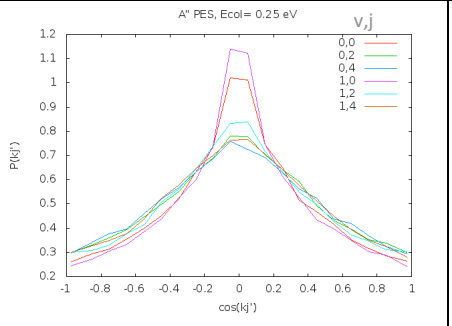
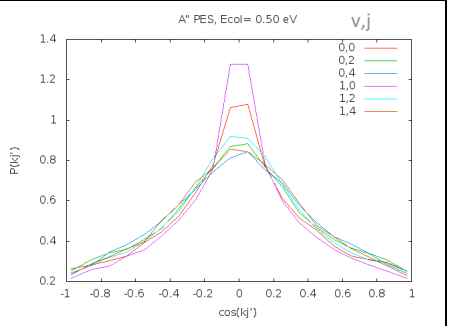
0.05 eV	0.25 eV	0.50 eV
		

Figure S4

Angular distributions (kj')

Ground PES ($1^2A''$)

0.05 eV	0.25 eV	0.50 eV
		

Excited PES ($1^2A'$)

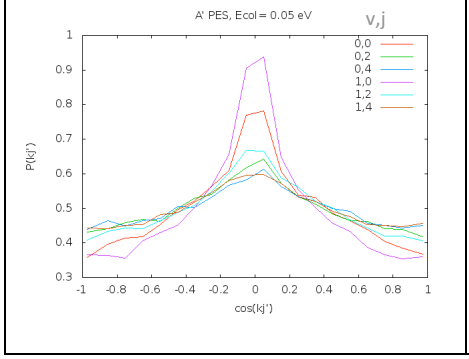
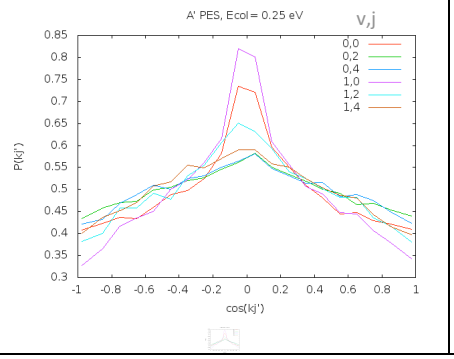
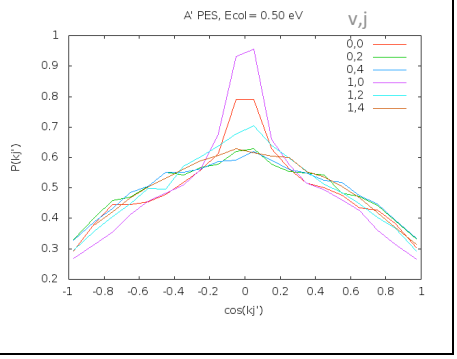
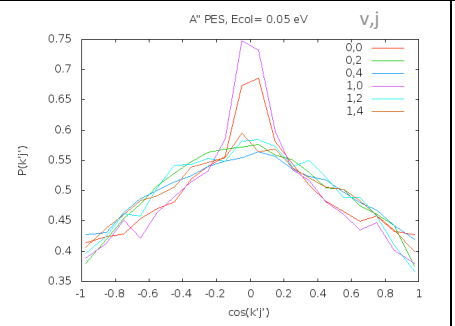
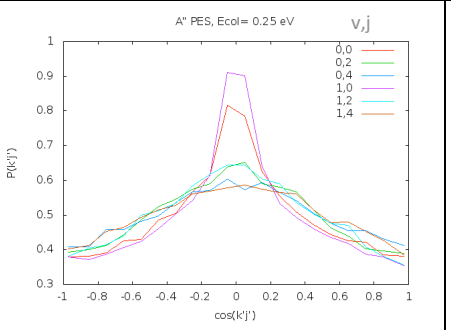
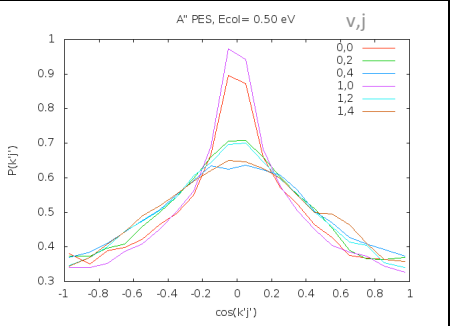
0.05 eV	0.25 eV	0.50 eV
		

Figure S5

Angular distributions (k'j')

Ground PES ($1^2A''$)

0.05 eV	0.25 eV	0.50 eV
		

Excited PES ($1^2A'$)

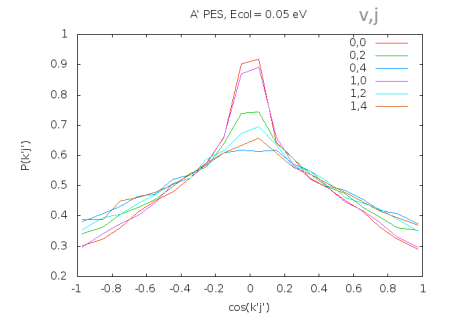
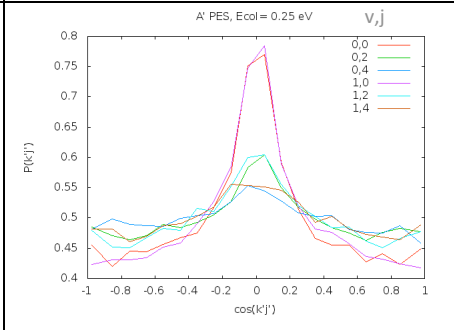
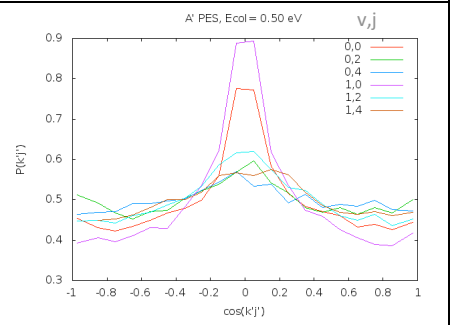
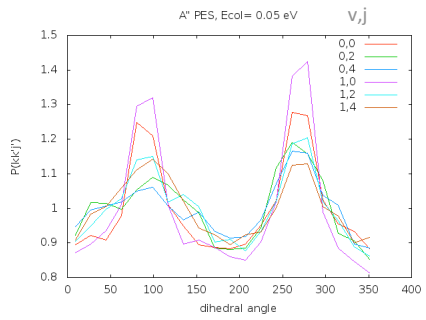
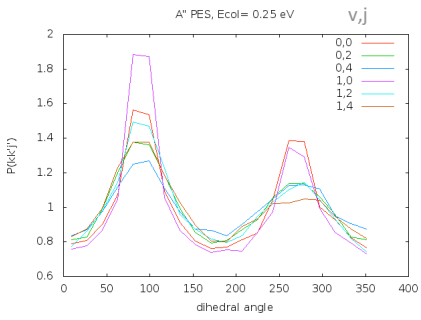
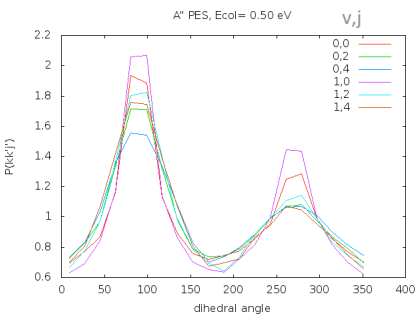
0.05 eV	0.25 eV	0.50 eV
		

Figure S6

Angular distributions (kk'j')

Ground PES ($1^2A''$)

0.05 eV	0.25 eV	0.50 eV
		

Excited PES ($1^2A'$)

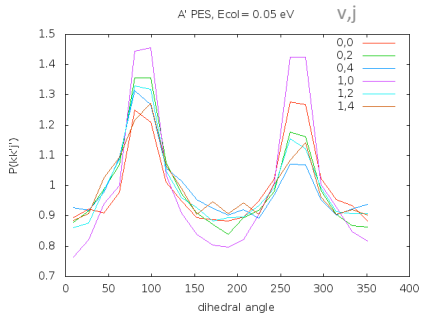
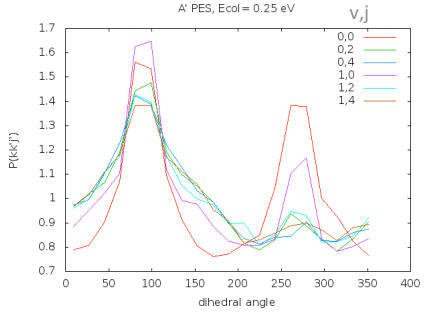
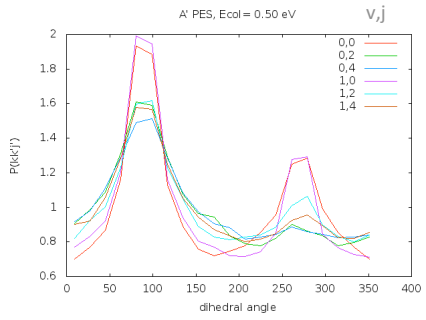
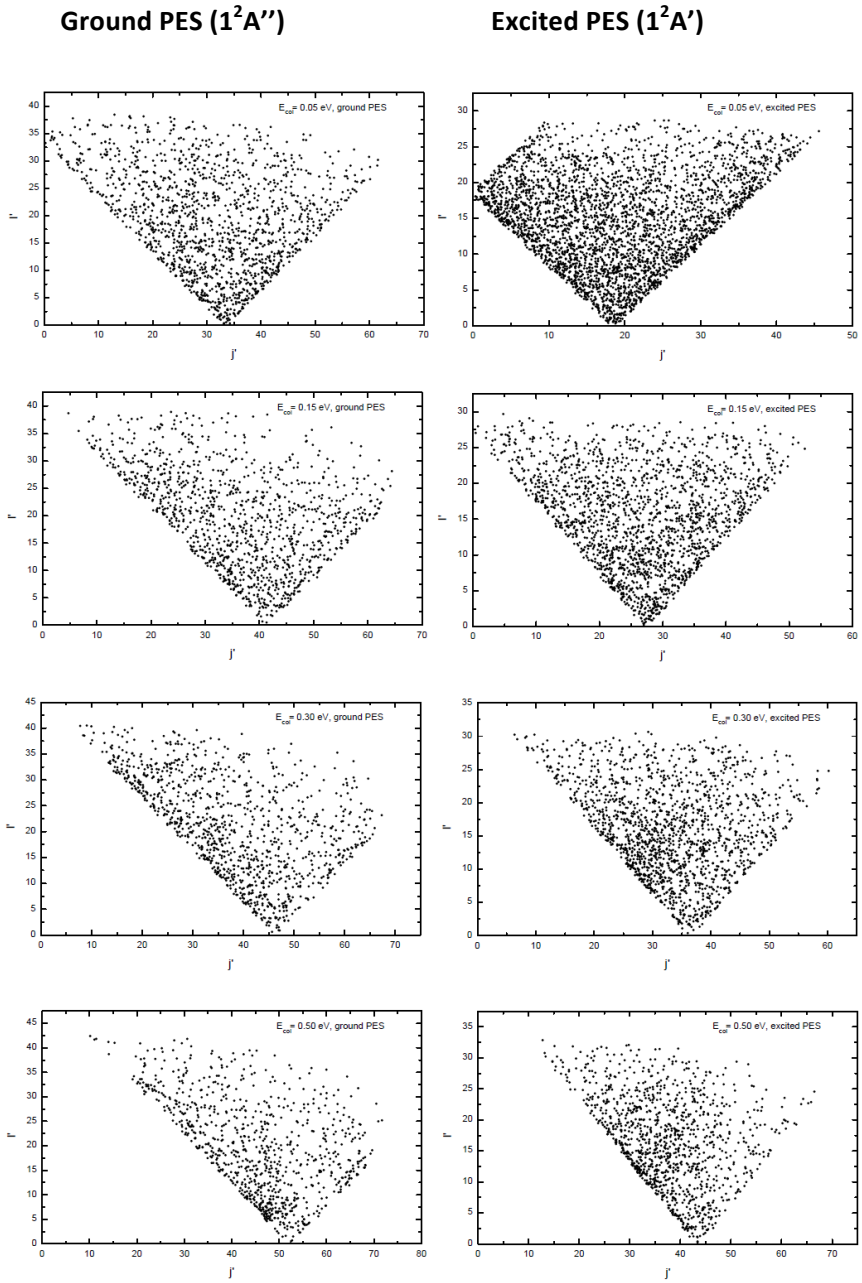
0.05 eV	0.25 eV	0.50 eV
		

Figure S7

Allowed vector modules of the couple (l', j') for the average J value* and H_2^+(*v*=0, *j*=0)



*The average *J* values for E_{col} = 0.05, 0.15, 0.30 and 0.50 eV are the following (units of ħ): 33.3, 41.2, 45.6 and 51.5, respectively (ground PES) and 18.4, 27.4, 35.7 and 43.3, respectively (excited PES).

Movie 1

Time evolution of an example of direct reactive trajectory (mpg file, 65 kB).

Movie 2

As movie 1 but for a non-direct reactive trajectory (mpg file, 163 kB).

Movie 3

As movie 1 but for a collision-complex forming reactive trajectory (mpg file, 163 kB).