

3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates for the H+O₂ Reaction on the CHIPR and DMBE IV Potential Energy Surfaces

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Supplementary Information

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Figure 1 depicts rotationally resolved state-to-state reaction probability at a specific final vibrational state ($v' = 0$) of OH diatom for the title reaction starting from the initial rovibrational state $v = 0, j = 1$ of the O₂ diatom at four different collision energies, *viz.*, $E_c = 0.5$ eV, 1.0 eV, 1.5 eV and 2.0 eV. One can clearly see that the reaction probabilities are very small at $E_c = 0.5$ eV, which essentially is the signature of existence of the threshold value for opening of the product channel. Moreover, as the collision energy increases, the state-to-state reaction probabilities also gradually increases, which is consistent with the feature of the total reaction probability profile [see Fig. 1 of the main text]. The general feature of the profiles is that all of them start with some moderate value, goes through some maxima and then gradually diminishes at higher j 's. Also, it is quite evident that the reaction probabilities are well converged within the collision energies of our consideration. As expected, the convergence profiles of reaction probabilities becomes gradually right shifted with the increase of collision energy indicating the requirement of more j 's at higher collision energy. On the other hand, the convergence profiles of rotationally resolved reaction probabilities at $v' = 1$ are shown in Figure 2, where the trends of the profiles at those four collision energies are similar to that of Figure 1, except the fact that the profiles converges faster with respect to j '. Moreover, the magnitudes of the reaction probabilities at most of the collision energies are lesser as compared to the $v' = 0$ case.

On the other hand, Figure 3 displays the rotationally summed vibrationally resolved reaction probabilities at four different collision energies, $E_c = 0.5$ eV, 1.0 eV, 1.5 eV and 2.0 eV for the title reaction starting from the

initial rovibrational state $v = 0, j = 1$ of the O_2 diatom. Here, in all the energies, the profiles generally starts with a higher value and then gradually diminishes as v' increases. Moreover, as the collision energy increase, the v' required for convergence also increases. One can clearly see that the profiles are well converged within the range of v' ($= 0 - 10$) considered in our calculation.

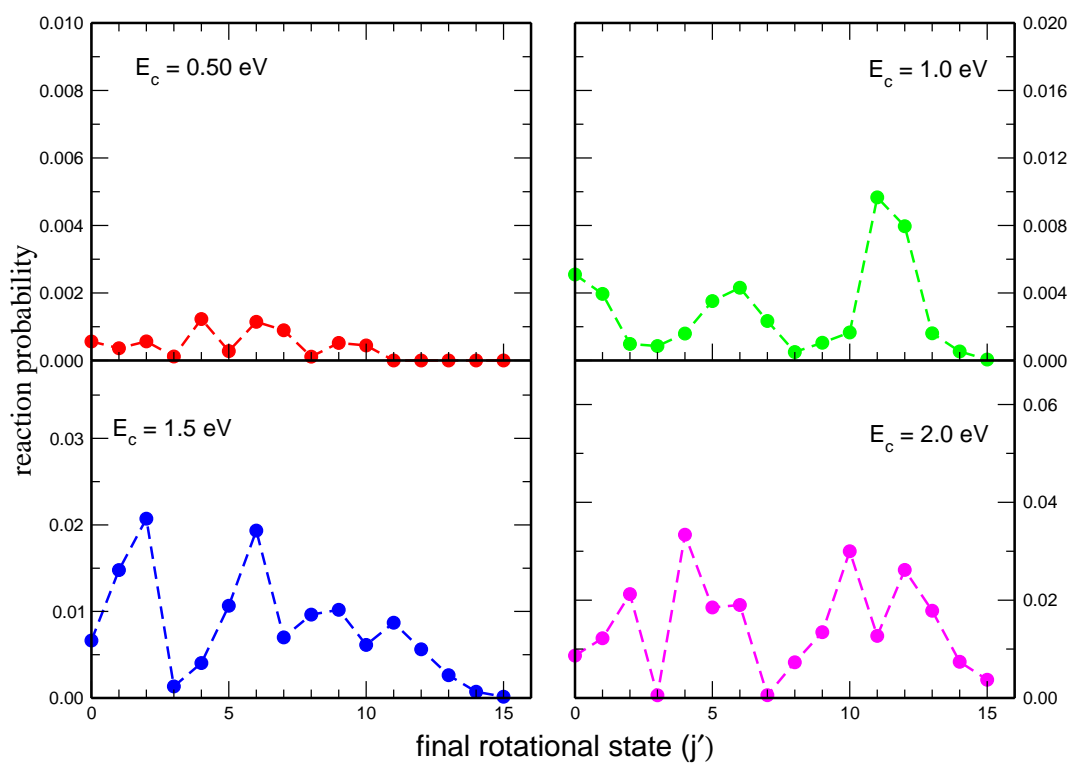
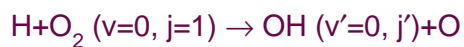


Figure 1: Rotationally resolved state-to-state reaction probability for $\text{H} + \text{O}_2 (v=0, j=1) \rightarrow \text{OH} (v' = 0) + \text{O}$ reaction as a function of various final rotational states, *viz.*, $j' = 0 - 15$ at four different collision energies (0.5 eV, 1.0 eV, 1.5 eV and 2.0 eV).

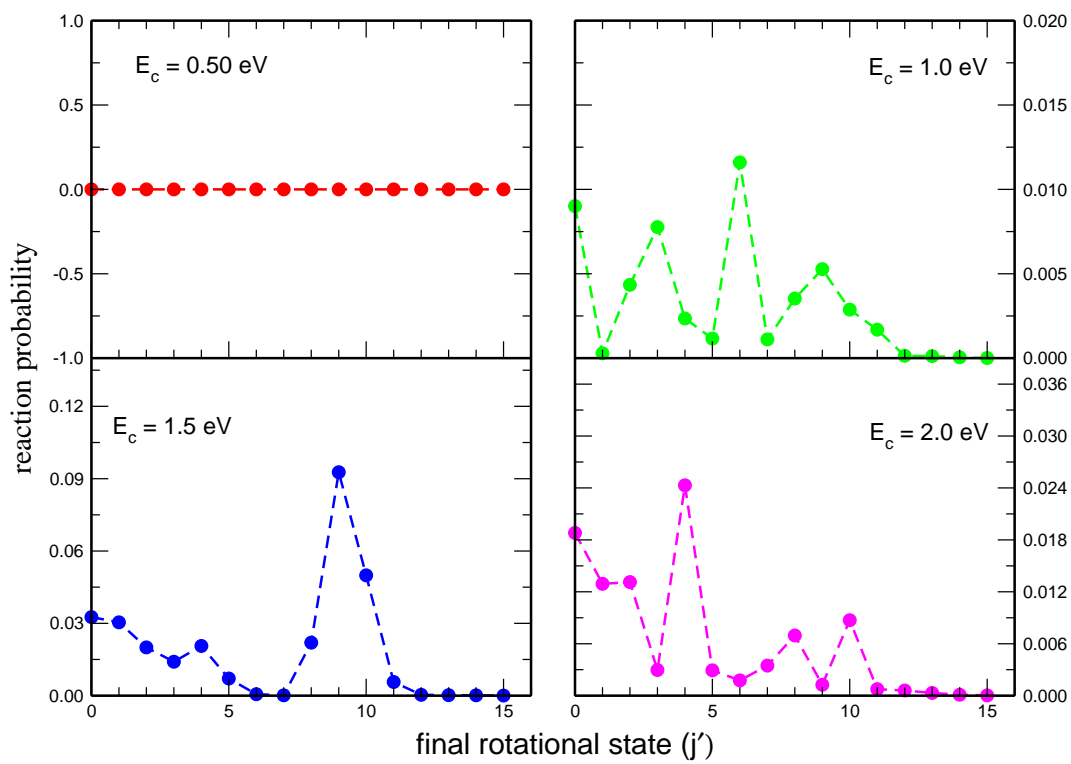
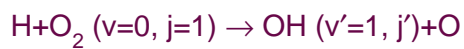


Figure 2: Same as Fig. 1, but for $v' = 1$.

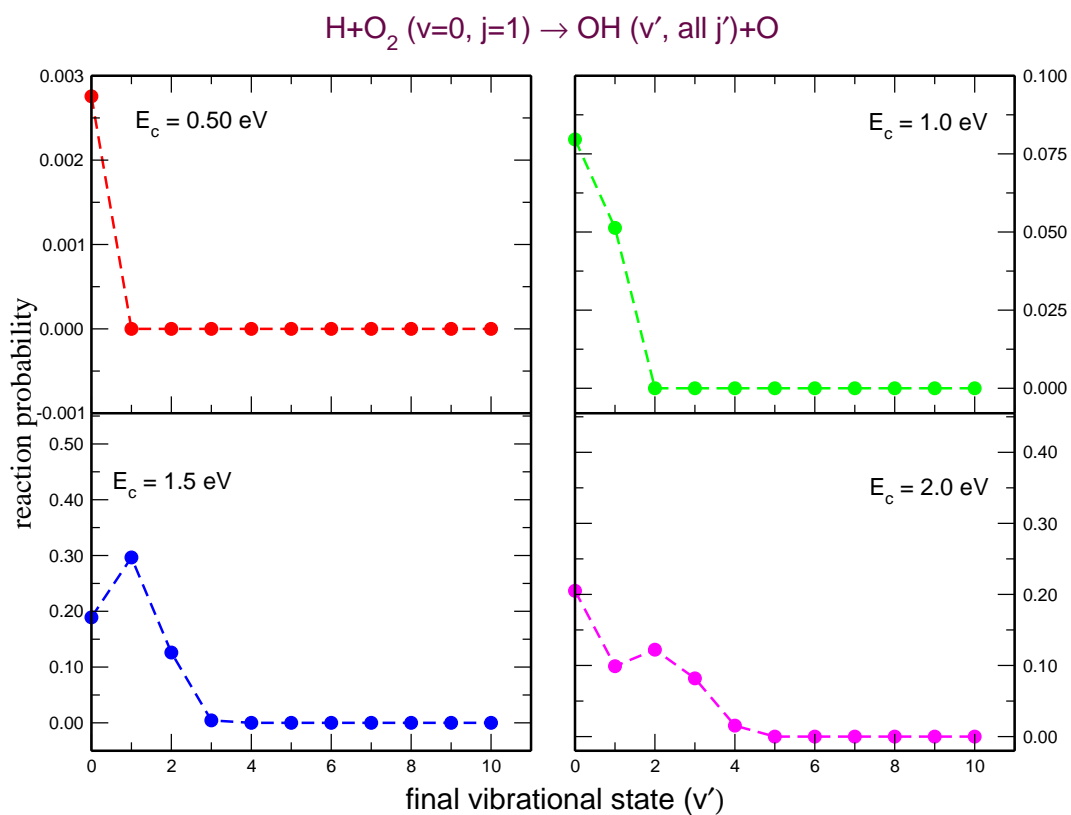


Figure 3: State-to-state reaction probability for $\text{H} + \text{O}_2 (v=0, j=1) \rightarrow \text{OH} (v', j') + \text{O}$ reaction at various final vibrational states, *viz.*, $v' = 0 - 10$.

Table 1: Data for initialization, projection, and absorbing potential discussed in the text: H +O₂ ($v = 0, j = 1; J = 0$)

Grid size:		
N_ρ		256
N_θ		64
N_ϕ		128
$(\rho_{min}, \rho_{max})/\text{\AA}$		(1.0, 12.0)
Translational wave packet:		
$R_0/\text{\AA}$		6.50 (~ 7.55) ^a
$\sigma/\text{\AA}$		0.21
k_0 (\AA^{-1})		29.00772
Initial state:		
E_{vj} (eV)		0.097909
Propagation:		
Δt (10^{-16} s)		0.50
Magnitude of the five last Lanczos vectors ^b		$10^{-8} - 10^{-7}$
Absorbing potential:		
V_{opt}/eV		0.163
ρ_I (\AA)		10.5
Range of the absorbing potential (\AA)		10.5 - 12.0
Projection:		
R^* (\AA)		3.5 (~ 4.45) ^a
vib. states		$v' = 0, \dots, 10$
rot. states		$j' = 0, \dots, 15$
Rotational Constants of O...OH Complex:		
	CHIPR PES	DMBE IV PES
A^\ddagger (cm^{-1})	35.51	44.95
B^\ddagger (cm^{-1})	0.249	0.289
Maximum Value of Total Angular Momentum:		
J_{max}		63

^a The transformed values of various parameters in ρ - space are shown in the parenthesis.

^b All vectors are normalized.

Table 2: Total Reaction probability for $v = 0, j=1$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.220627	0.003421
0.243345	0.002732
0.266063	0.002769
0.288781	0.002850
0.311499	0.002517
0.334217	0.002356
0.356935	0.002504
0.379652	0.002607
0.402370	0.002655
0.425088	0.002335
0.447806	0.002538
0.470524	0.002937
0.493242	0.002807
0.515960	0.002798
0.538678	0.003246
0.561396	0.003260
0.584114	0.004379
0.606831	0.004339
0.629549	0.006088
0.652267	0.004494
0.674985	0.017951
0.697703	0.009258
0.720421	0.025010
0.743139	0.021053
0.765857	0.037028
0.788575	0.032204
0.811293	0.039335
0.834011	0.040992
0.856728	0.053218
0.879446	0.066097
0.902164	0.112607
0.924882	0.090403
0.947600	0.087908
0.970318	0.095481
0.993036	0.150086
1.015754	0.110880
1.038472	0.187544
1.061190	0.141219
1.083907	0.178613
1.106625	0.111308
1.129343	0.144310
1.152061	0.167947
1.174779	0.149420
1.197497	0.207480
1.220215	0.189779
1.242933	0.178050
1.265651	0.221402
1.288369	0.256467
1.311087	0.224742
1.333804	0.300127
1.356522	0.231329
1.379240	0.314394
1.401958	0.216867
1.424676	0.248595
1.447394	0.474079
1.470112	0.413832

Table 3: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.492830	0.525428
1.515548	0.422228
1.538266	0.589298
1.560983	0.431309
1.583701	0.478639
1.606419	0.654052
1.629137	0.595277
1.651855	0.518751
1.674573	0.564686
1.697291	0.713160
1.720009	0.479785
1.742727	0.563699
1.765445	0.521046
1.788163	0.551727
1.810880	0.506807
1.833598	0.659730
1.856316	0.578885
1.879034	0.391747
1.901752	0.536330
1.924470	0.486824
1.947188	0.533286
1.969906	0.579722
1.992624	0.674487
2.015342	0.529813
2.038059	0.557522
2.060777	0.633528
2.083495	0.563234
2.106213	0.625224
2.128931	0.507851
2.151649	0.556557
2.174367	0.622278
2.197085	0.390074
2.219803	0.420233
2.242521	0.529038
2.265239	0.581084
2.287956	0.546999
2.310674	0.663748
2.333392	0.561514
2.356110	0.536913
2.378828	0.616523
2.401546	0.574050
2.424264	0.496524
2.446982	0.668281
2.469700	0.444631
2.492418	0.461760
2.515135	0.569897

Table 4: Total Reaction probability for $v = 0, j=3$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.224917	0.005380
0.250159	0.004602
0.275401	0.004885
0.300643	0.004952
0.325885	0.004480
0.351127	0.004295
0.376369	0.004094
0.401611	0.004803
0.426854	0.005011
0.452096	0.004907
0.477338	0.004100
0.502580	0.005485
0.527822	0.006289
0.553064	0.009885
0.578306	0.010073
0.603548	0.009635
0.628790	0.014902
0.654033	0.023740
0.679275	0.027995
0.704517	0.037417
0.729759	0.034745
0.755001	0.037173
0.780243	0.141791
0.805485	0.110836
0.830727	0.110866
0.855970	0.137720
0.881212	0.224619
0.906454	0.254730
0.931696	0.305317
0.956938	0.196339
0.982180	0.344382
1.007422	0.235179
1.032664	0.238182
1.057906	0.330669
1.083149	0.293236
1.108391	0.281391
1.133633	0.413137
1.158875	0.290966
1.184117	0.299269
1.209359	0.286683
1.234601	0.303439
1.259843	0.311126
1.285085	0.358701
1.310328	0.421693
1.335570	0.413239
1.360812	0.502012
1.386054	0.379359
1.411296	0.535818
1.436538	0.581942
1.461780	0.520137
1.487022	0.504256

Table 5: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.512265	0.610502
1.537507	0.588251
1.562749	0.543885
1.587991	0.525135
1.613233	0.640513
1.638475	0.572324
1.663717	0.505374
1.688959	0.467029
1.714201	0.588213
1.739444	0.674327
1.764686	0.495004
1.789928	0.529519
1.815170	0.547480
1.840412	0.569609
1.865654	0.491385
1.890896	0.452366
1.916138	0.626578
1.941381	0.630174
1.966623	0.595183
1.991865	0.635300
2.017107	0.553093
2.042349	0.431248
2.067591	0.593736
2.092833	0.567303
2.118075	0.446837
2.143317	0.524595
2.168560	0.578799
2.193802	0.506684
2.219044	0.561004
2.244286	0.620867
2.269528	0.641567
2.294770	0.657940
2.320012	0.636043
2.345254	0.450395
2.370496	0.611707
2.395739	0.509784
2.420981	0.576434
2.446223	0.496902
2.471465	0.484001
2.496707	0.504464

Table 6: Total Reaction probability for $v = 0, j=5$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.228094	0.003790
0.253336	0.002932
0.278578	0.002302
0.303820	0.002153
0.329062	0.002425
0.354304	0.003125
0.379547	0.002561
0.404789	0.002292
0.430031	0.002175
0.455273	0.002782
0.480515	0.003697
0.505757	0.004322
0.530999	0.003379
0.556241	0.008636
0.581483	0.005630
0.606726	0.011876
0.631968	0.012925
0.657210	0.011285
0.682452	0.036049
0.707694	0.056880
0.732936	0.040097
0.758178	0.057163
0.783420	0.164594
0.808662	0.117967
0.833905	0.100239
0.859147	0.148588
0.884389	0.200845
0.909631	0.213335
0.934873	0.250530
0.960115	0.301105
0.985357	0.360892
1.010599	0.316824
1.035842	0.292361
1.061084	0.367923
1.086326	0.197399
1.111568	0.247272
1.136810	0.418993
1.162052	0.246986
1.187294	0.253475
1.212536	0.187912
1.237778	0.301336
1.263021	0.376667
1.288263	0.306798
1.313505	0.437486
1.338747	0.522178
1.363989	0.400851
1.389231	0.344052
1.414473	0.391821
1.439715	0.408819
1.464958	0.418497
1.490200	0.529230

Table 7: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.515442	0.530049
1.540684	0.487142
1.565926	0.563504
1.591168	0.648602
1.616410	0.502908
1.641652	0.568023
1.666894	0.524843
1.692137	0.511415
1.717379	0.590392
1.742621	0.486760
1.767863	0.469515
1.793105	0.577594
1.818347	0.505570
1.843589	0.398083
1.868831	0.630875
1.894073	0.619600
1.919316	0.614237
1.944558	0.538844
1.969800	0.431511
1.995042	0.522727
2.020284	0.613494
2.045526	0.537484
2.070768	0.601203
2.096010	0.669721
2.121253	0.555113
2.146495	0.595664
2.171737	0.557277
2.196979	0.740813
2.222221	0.470775
2.247463	0.496791
2.272705	0.541005
2.297947	0.680766
2.323189	0.598753
2.348432	0.711364
2.373674	0.600533
2.398916	0.495306
2.424158	0.524109
2.449400	0.567219
2.474642	0.603702
2.499884	0.451579

Table 8: Total Reaction probability for $v = 1, j=1$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.316706	0.017320
0.338162	0.014881
0.359618	0.015105
0.381074	0.014143
0.402529	0.013265
0.423985	0.013504
0.445441	0.012949
0.466897	0.012819
0.488353	0.013939
0.509808	0.017152
0.531264	0.014043
0.552720	0.013574
0.574176	0.033418
0.595632	0.042719
0.617087	0.026312
0.638543	0.068848
0.659999	0.050396
0.681455	0.101401
0.702911	0.172984
0.724366	0.243900
0.745822	0.265687
0.767278	0.243667
0.788734	0.240882
0.810190	0.442402
0.831645	0.236360
0.853101	0.387592
0.874557	0.534876
0.896013	0.348095
0.917469	0.201091
0.938924	0.343571
0.960380	0.402742
0.981836	0.539095
1.003292	0.528119
1.024748	0.680352
1.046203	0.444041
1.067659	0.513068
1.089115	0.266533
1.110571	0.276144
1.132027	0.486536
1.153482	0.471960
1.174938	0.533228
1.196394	0.554749
1.217850	0.624691
1.239306	0.375180
1.260761	0.663738
1.282217	0.443983
1.303673	0.265853
1.325129	0.426325
1.346585	0.414125
1.368040	0.518078
1.389496	0.650475
1.410952	0.607639
1.432408	0.658986
1.453864	0.727415
1.475319	0.504273
1.496775	0.486092

Table 9: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.518231	0.468822
1.539687	0.692962
1.561142	0.694113
1.582598	0.647882
1.604054	0.651129
1.625510	0.625289
1.646966	0.714803
1.668421	0.572401
1.689877	0.653365
1.711333	0.592316
1.732789	0.683297
1.754245	0.572970
1.775700	0.664451
1.797156	0.630649
1.818612	0.443971
1.840068	0.537203
1.861524	0.534281
1.882979	0.614065
1.904435	0.486471
1.925891	0.681830
1.947347	0.519187
1.968803	0.612366
1.990258	0.576474
2.011714	0.604310
2.033170	0.643995
2.054626	0.583664
2.076082	0.518791
2.097537	0.655612
2.118993	0.686101
2.140449	0.626362
2.161905	0.631626
2.183361	0.669624
2.204816	0.646999
2.226272	0.480681
2.247728	0.562771
2.269184	0.527432
2.290640	0.584615
2.312095	0.596868
2.333551	0.586137
2.355007	0.580798
2.376463	0.546499
2.397919	0.433714
2.419374	0.440896
2.440830	0.641944
2.462286	0.681623
2.483742	0.576572
2.505198	0.588478

Table 10: Total Reaction probability for $v = 1, j=3$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.314032	0.013110
0.335488	0.010729
0.356944	0.010702
0.378400	0.010286
0.399856	0.010265
0.421311	0.011394
0.442767	0.014160
0.464223	0.011896
0.485679	0.014369
0.507135	0.016271
0.528590	0.019915
0.550046	0.023182
0.571502	0.025375
0.592958	0.068632
0.614414	0.076469
0.635869	0.129866
0.657325	0.125433
0.678781	0.105020
0.700237	0.102805
0.721693	0.239506
0.743148	0.233460
0.764604	0.174995
0.786060	0.338036
0.807516	0.416916
0.828972	0.526600
0.850427	0.401831
0.871883	0.593744
0.893339	0.399431
0.914795	0.251893
0.936251	0.394391
0.957706	0.288407
0.979162	0.733375
1.000618	0.696021
1.022074	0.604027
1.043530	0.381073
1.064985	0.518137
1.086441	0.524381
1.107897	0.226508
1.129353	0.444270
1.150809	0.439214
1.172264	0.520969
1.193720	0.652227
1.215176	0.644802
1.236632	0.509394
1.258087	0.536717
1.279543	0.397392
1.300999	0.356888
1.322455	0.424331
1.343911	0.477449
1.365366	0.479981
1.386822	0.640628
1.408278	0.575943
1.429734	0.683464
1.451190	0.722093
1.472645	0.643901
1.494101	0.654120

Table 11: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.515557	0.592225
1.537013	0.581106
1.558469	0.503629
1.579924	0.701478
1.601380	0.734262
1.622836	0.617154
1.644292	0.642017
1.665748	0.725097
1.687203	0.619983
1.708659	0.595005
1.730115	0.676373
1.751571	0.592672
1.773027	0.740266
1.794482	0.793557
1.815938	0.467207
1.837394	0.739449
1.858850	0.535662
1.880306	0.528983
1.901761	0.568009
1.923217	0.541456
1.944673	0.759007
1.966129	0.765194
1.987585	0.587281
2.009040	0.708082
2.030496	0.535093
2.051952	0.499310
2.073408	0.641366
2.094864	0.607005
2.116319	0.491410
2.137775	0.605102
2.159231	0.629301
2.180687	0.615302
2.202143	0.592927
2.223598	0.549147
2.245054	0.665107
2.266510	0.601420
2.287966	0.659043
2.309422	0.670799
2.330877	0.596863
2.352333	0.565162
2.373789	0.689166
2.395245	0.692957
2.416701	0.596904
2.438156	0.546699
2.459612	0.654300
2.481068	0.606368
2.502524	0.625463

Table 12: Total Reaction probability for $v = 1, j=5$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.317170	0.010296
0.338626	0.008525
0.360082	0.008291
0.381538	0.008235
0.402994	0.008153
0.424449	0.008596
0.445905	0.009897
0.467361	0.009609
0.488817	0.009994
0.510273	0.016402
0.531728	0.012387
0.553184	0.024078
0.574640	0.023666
0.596096	0.070462
0.617552	0.073240
0.639007	0.150818
0.660463	0.152976
0.681919	0.119207
0.703375	0.146270
0.724831	0.330727
0.746286	0.258940
0.767742	0.158630
0.789198	0.430695
0.810654	0.504014
0.832110	0.586092
0.853565	0.474657
0.875021	0.682410
0.896477	0.458224
0.917933	0.289563
0.939389	0.422455
0.960844	0.307177
0.982300	0.747118
1.003756	0.656708
1.025212	0.688776
1.046668	0.466834
1.068123	0.568896
1.089579	0.621454
1.111035	0.287999
1.132491	0.405251
1.153947	0.419117
1.175402	0.501972
1.196858	0.676309
1.218314	0.644963
1.239770	0.611625
1.261226	0.491638
1.282681	0.457566
1.304137	0.302324
1.325593	0.427293
1.347049	0.408662
1.368505	0.470688
1.389960	0.668395
1.411416	0.589323
1.432872	0.792711
1.454328	0.640206
1.475784	0.675982
1.497239	0.565682

Table 13: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.518695	0.683983
1.540151	0.755005
1.561607	0.678319
1.583063	0.669768
1.604518	0.648980
1.625974	0.529544
1.647430	0.619036
1.668886	0.779572
1.690342	0.558066
1.711797	0.609086
1.733253	0.677687
1.754709	0.542270
1.776165	0.665039
1.797621	0.568071
1.819076	0.573350
1.840532	0.470636
1.861988	0.479203
1.883444	0.656437
1.904900	0.425213
1.926355	0.644380
1.947811	0.670624
1.969267	0.657847
1.990723	0.484846
2.012179	0.603508
2.033634	0.751466
2.055090	0.575830
2.076546	0.565329
2.098002	0.567323
2.119458	0.666589
2.140913	0.568529
2.162369	0.794135
2.183825	0.637908
2.205281	0.693264
2.226737	0.589644
2.248192	0.675059
2.269648	0.565352
2.291104	0.727963
2.312560	0.567603
2.334016	0.620557
2.355471	0.632653
2.376927	0.662130
2.398383	0.619769
2.419839	0.536658
2.441295	0.620023
2.462750	0.677650
2.484206	0.587941
2.505662	0.559120

Table 14: Total Reaction probability for $v = 2, j=1$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.029659	0.006301
0.054271	0.005133
0.078882	0.004796
0.103493	0.004656
0.128104	0.006578
0.152715	0.006289
0.177326	0.007192
0.201937	0.009207
0.226548	0.013872
0.251159	0.022253
0.275770	0.075264
0.300381	0.115132
0.324992	0.092947
0.349603	0.158443
0.374214	0.232026
0.398825	0.206235
0.423436	0.251192
0.448048	0.336983
0.472659	0.244851
0.497270	0.400487
0.521881	0.589493
0.546492	0.351811
0.571103	0.546304
0.595714	0.328771
0.620325	0.315042
0.644936	0.522593
0.669547	0.394276
0.694158	0.569020
0.718769	0.607668
0.743380	0.530963
0.767991	0.513318
0.792602	0.544052
0.817214	0.240603
0.841825	0.518578
0.866436	0.606395
0.891047	0.521224
0.915658	0.808657
0.940269	0.693044
0.964880	0.556956
0.989491	0.458303
1.014102	0.342333
1.038713	0.463169
1.063324	0.573250
1.087935	0.525672
1.112546	0.567242
1.137157	0.654282
1.161768	0.667442
1.186379	0.494515
1.210991	0.608660
1.235602	0.523111
1.260213	0.403838
1.284824	0.584618
1.309435	0.580970
1.334046	0.618147
1.358657	0.661174
1.383268	0.557205

Table 15: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.407879	0.662400
1.432490	0.615822
1.457101	0.665487
1.481712	0.695122
1.506323	0.666939
1.530934	0.561452
1.555545	0.662212
1.580156	0.572088
1.604768	0.586000
1.629379	0.566172
1.653990	0.676990
1.678601	0.782065
1.703212	0.665314
1.727823	0.665217
1.752434	0.712132
1.777045	0.660082
1.801656	0.623077
1.826267	0.690449
1.850878	0.436108
1.875489	0.641924
1.900100	0.558038
1.924711	0.503145
1.949322	0.520210
1.973933	0.719535
1.998545	0.533140
2.023156	0.612718
2.047767	0.594376
2.072378	0.658158
2.096989	0.622276
2.121600	0.558819
2.146211	0.605246
2.170822	0.693398
2.195433	0.605870
2.220044	0.527155
2.244655	0.611564
2.269266	0.460494
2.293877	0.641967
2.318488	0.635703
2.343099	0.640133
2.367710	0.825259
2.392322	0.595017
2.416933	0.725555
2.441544	0.606385
2.466155	0.640796
2.490766	0.671225
2.515377	0.539457

Table 16: Total Reaction probability for $v = 2$, $j=3$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.025242	0.009233
0.049853	0.008848
0.074464	0.008009
0.099075	0.006578
0.123686	0.007220
0.148297	0.007028
0.172908	0.011520
0.197520	0.025062
0.222131	0.032619
0.246742	0.052906
0.271353	0.080911
0.295964	0.101255
0.320575	0.386521
0.345186	0.373086
0.369797	0.200271
0.394408	0.471287
0.419019	0.272357
0.443630	0.390648
0.468241	0.345432
0.492852	0.507984
0.517463	0.684833
0.542074	0.408824
0.566686	0.632233
0.591297	0.462418
0.615908	0.302612
0.640519	0.393893
0.665130	0.363871
0.689741	0.603073
0.714352	0.530048
0.738963	0.469032
0.763574	0.439304
0.788185	0.573802
0.812796	0.317421
0.837407	0.465857
0.862018	0.519222
0.886629	0.651103
0.911240	0.679857
0.935851	0.731849
0.960463	0.551841
0.985074	0.410934
1.009685	0.414420
1.034296	0.448359
1.058907	0.495356
1.083518	0.461402
1.108129	0.621101
1.132740	0.645010
1.157351	0.628893
1.181962	0.727452
1.206573	0.508578
1.231184	0.550647
1.255795	0.517323
1.280406	0.581256
1.305017	0.609616
1.329628	0.631775
1.354240	0.691525

Table 17: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.378851	0.611887
1.403462	0.658162
1.428073	0.649928
1.452684	0.593725
1.477295	0.628095
1.501906	0.777667
1.526517	0.611575
1.551128	0.570343
1.575739	0.570168
1.600350	0.682957
1.624961	0.475972
1.649572	0.692354
1.674183	0.795418
1.698794	0.668967
1.723405	0.628616
1.748017	0.647990
1.772628	0.539296
1.797239	0.562995
1.821850	0.597282
1.846461	0.455389
1.871072	0.590309
1.895683	0.654551
1.920294	0.624601
1.944905	0.677475
1.969516	0.590548
1.994127	0.654150
2.018738	0.527716
2.043349	0.644694
2.067960	0.529752
2.092571	0.580663
2.117182	0.643981
2.141794	0.554271
2.166405	0.649776
2.191016	0.658598
2.215627	0.495337
2.240238	0.569081
2.264849	0.647837
2.289460	0.493395
2.314071	0.477695
2.338682	0.515288
2.363293	0.733014
2.387904	0.544314
2.412515	0.561313
2.437126	0.617869
2.461737	0.523461
2.486348	0.603458
2.510960	0.680351

Table 18: Total Reaction probability for $v = 2$, $j=5$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.025242	0.010149
0.049853	0.008521
0.074464	0.006721
0.099075	0.005063
0.123686	0.009172
0.148297	0.010176
0.172908	0.014179
0.197520	0.026947
0.222131	0.030413
0.246742	0.062718
0.271353	0.090802
0.295964	0.101278
0.320575	0.391891
0.345186	0.362493
0.369797	0.195582
0.394408	0.464038
0.419019	0.352204
0.443630	0.415671
0.468241	0.380829
0.492852	0.547422
0.517463	0.687495
0.542074	0.435713
0.566686	0.691288
0.591297	0.536357
0.615908	0.288888
0.640519	0.441404
0.665130	0.359757
0.689741	0.626093
0.714352	0.608960
0.738963	0.496971
0.763574	0.444226
0.788185	0.560545
0.812796	0.294848
0.837407	0.468448
0.862018	0.590250
0.886629	0.678466
0.911240	0.702579
0.935851	0.700958
0.960463	0.582382
0.985074	0.419408
1.009685	0.366604
1.034296	0.434920
1.058907	0.478077
1.083518	0.453434
1.108129	0.694531
1.132740	0.716525
1.157351	0.655052
1.181962	0.767480
1.206573	0.553914
1.231184	0.615615
1.255795	0.495264
1.280406	0.609428
1.305017	0.505647
1.329628	0.604736
1.354240	0.632166

Table 19: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.378851	0.620322
1.403462	0.732539
1.428073	0.676556
1.452684	0.719167
1.477295	0.736316
1.501906	0.593416
1.526517	0.616160
1.551128	0.564249
1.575739	0.671964
1.600350	0.689298
1.624961	0.448890
1.649572	0.580291
1.674183	0.745454
1.698794	0.496408
1.723405	0.568330
1.748017	0.650513
1.772628	0.452168
1.797239	0.691235
1.821850	0.563718
1.846461	0.581173
1.871072	0.574445
1.895683	0.486694
1.920294	0.696322
1.944905	0.460601
1.969516	0.642714
1.994127	0.677196
2.018738	0.731010
2.043349	0.578568
2.067960	0.531503
2.092571	0.571256
2.117182	0.701989
2.141794	0.487686
2.166405	0.652356
2.191016	0.663116
2.215627	0.773383
2.240238	0.596970
2.264849	0.492990
2.289460	0.587937
2.314071	0.476344
2.338682	0.681099
2.363293	0.700509
2.387904	0.576844
2.412515	0.462050
2.437126	0.449745
2.461737	0.573897
2.486348	0.577746
2.510960	0.613779

Table 20: Total Reaction probability for $v = 3, j=1$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.029659	0.000000
0.054271	0.000000
0.078882	0.000000
0.103493	0.016734
0.128104	0.042708
0.152715	0.056708
0.177326	0.045279
0.201937	0.083948
0.226548	0.140353
0.251159	0.146008
0.275770	0.503932
0.300381	0.439410
0.324992	0.272343
0.349603	0.397811
0.374214	0.482892
0.398825	0.404921
0.423436	0.400714
0.448048	0.494535
0.472659	0.294818
0.497270	0.438994
0.521881	0.677218
0.546492	0.370715
0.571103	0.650295
0.595714	0.350219
0.620325	0.297477
0.644936	0.486800
0.669547	0.342148
0.694158	0.523250
0.718769	0.628406
0.743380	0.526543
0.767991	0.410084
0.792602	0.517887
0.817214	0.217148
0.841825	0.467120
0.866436	0.583281
0.891047	0.478466
0.915658	0.781518
0.940269	0.722346
0.964880	0.507964
0.989491	0.430638
1.014102	0.415180
1.038713	0.505441
1.063324	0.525160
1.087935	0.536815
1.112546	0.635156
1.137157	0.583724
1.161768	0.666376
1.186379	0.440596
1.210991	0.683427
1.235602	0.533372
1.260213	0.448968
1.284824	0.604728
1.309435	0.583119
1.334046	0.582403
1.358657	0.695954
1.383268	0.456723

Table 21: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.407879	0.475161
1.432490	0.624345
1.457101	0.545565
1.481712	0.559808
1.506323	0.655922
1.530934	0.425538
1.555545	0.543586
1.580156	0.502863
1.604768	0.498102
1.629379	0.421924
1.653990	0.588035
1.678601	0.495194
1.703212	0.493266
1.727823	0.454277
1.752434	0.623769
1.777045	0.597990
1.801656	0.543390
1.826267	0.600799
1.850878	0.671791
1.875489	0.551313
1.900100	0.664460
1.924711	0.577531
1.949322	0.596229
1.973933	0.523395
1.998545	0.567382
2.023156	0.634357
2.047767	0.510926
2.072378	0.518909
2.096989	0.586758
2.121600	0.538811
2.146211	0.603873
2.170822	0.571878
2.195433	0.663665
2.220044	0.732454
2.244655	0.566013
2.269266	0.512284
2.293877	0.545792
2.318488	0.630000
2.343099	0.490266
2.367710	0.529863
2.392322	0.594107
2.416933	0.566515
2.441544	0.670501
2.466155	0.493660
2.490766	0.436928
2.515377	0.612940

Table 22: Total Reaction probability for $v = 3, j=3$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.025242	0.000000
0.049853	0.000000
0.074464	0.010061
0.099075	0.019465
0.123686	0.072820
0.148297	0.092663
0.172908	0.099413
0.197520	0.248046
0.222131	0.170458
0.246742	0.194396
0.271353	0.312815
0.295964	0.277960
0.320575	0.641914
0.345186	0.572253
0.369797	0.265249
0.394408	0.612335
0.419019	0.344865
0.443630	0.385226
0.468241	0.358717
0.492852	0.524263
0.517463	0.662305
0.542074	0.383661
0.566686	0.620412
0.591297	0.442332
0.615908	0.283946
0.640519	0.398397
0.665130	0.348345
0.689741	0.608035
0.714352	0.521023
0.738963	0.439167
0.763574	0.445895
0.788185	0.565894
0.812796	0.291980
0.837407	0.470169
0.862018	0.530896
0.886629	0.679478
0.911240	0.648384
0.935851	0.716387
0.960463	0.591576
0.985074	0.438778
1.009685	0.449054
1.034296	0.506955
1.058907	0.487699
1.083518	0.460952
1.108129	0.626563
1.132740	0.629116
1.157351	0.608488
1.181962	0.662909
1.206573	0.549740
1.231184	0.606391
1.255795	0.533432
1.280406	0.700331
1.305017	0.511881
1.329628	0.656217
1.354240	0.743006

Table 23: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.378851	0.527494
1.403462	0.600740
1.428073	0.504389
1.452684	0.600292
1.477295	0.580282
1.501906	0.607027
1.526517	0.471103
1.551128	0.375623
1.575739	0.456684
1.600350	0.592295
1.624961	0.326355
1.649572	0.606038
1.674183	0.508906
1.698794	0.658058
1.723405	0.616868
1.748017	0.613271
1.772628	0.509496
1.797239	0.553627
1.821850	0.595623
1.846461	0.472297
1.871072	0.742538
1.895683	0.683721
1.920294	0.459594
1.944905	0.631928
1.969516	0.521427
1.994127	0.577412
2.018738	0.583730
2.043349	0.748410
2.067960	0.635507
2.092571	0.605663
2.117182	0.670222
2.141794	0.660874
2.166405	0.646011
2.191016	0.576654
2.215627	0.560105
2.240238	0.610423
2.264849	0.707760
2.289460	0.629617
2.314071	0.491617
2.338682	0.423853
2.363293	0.652824
2.387904	0.626896
2.412515	0.611007
2.437126	0.497248
2.461737	0.483922
2.486348	0.564898
2.510960	0.599143

Table 24: Total Reaction probability for $v = 3$, $j=5$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.025242	0.000000
0.049853	0.000000
0.074464	0.015904
0.099075	0.019432
0.123686	0.119641
0.148297	0.159210
0.172908	0.138300
0.197520	0.327981
0.222131	0.237139
0.246742	0.279042
0.271353	0.338175
0.295964	0.351585
0.320575	0.692757
0.345186	0.580865
0.369797	0.264168
0.394408	0.637870
0.419019	0.382510
0.443630	0.473573
0.468241	0.431389
0.492852	0.556413
0.517463	0.677832
0.542074	0.398822
0.566686	0.685301
0.591297	0.529094
0.615908	0.289022
0.640519	0.435276
0.665130	0.347672
0.689741	0.611275
0.714352	0.588327
0.738963	0.456979
0.763574	0.403790
0.788185	0.559621
0.812796	0.290519
0.837407	0.486770
0.862018	0.593513
0.886629	0.685557
0.911240	0.693683
0.935851	0.705648
0.960463	0.650219
0.985074	0.400888
1.009685	0.379601
1.034296	0.508147
1.058907	0.585957
1.083518	0.548664
1.108129	0.721930
1.132740	0.637926
1.157351	0.665922
1.181962	0.710476
1.206573	0.565489
1.231184	0.639437
1.255795	0.530168
1.280406	0.625679
1.305017	0.561040
1.329628	0.546717
1.354240	0.705061

Table 25: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.378851	0.651722
1.403462	0.691872
1.428073	0.618460
1.452684	0.678911
1.477295	0.567022
1.501906	0.529378
1.526517	0.608440
1.551128	0.513464
1.575739	0.387099
1.600350	0.503282
1.624961	0.521865
1.649572	0.527904
1.674183	0.670877
1.698794	0.374661
1.723405	0.518460
1.748017	0.560239
1.772628	0.546253
1.797239	0.612355
1.821850	0.411558
1.846461	0.572072
1.871072	0.594115
1.895683	0.578978
1.920294	0.736031
1.944905	0.519420
1.969516	0.558548
1.994127	0.576437
2.018738	0.509836
2.043349	0.600902
2.067960	0.547429
2.092571	0.666762
2.117182	0.566533
2.141794	0.534702
2.166405	0.642688
2.191016	0.550307
2.215627	0.605035
2.240238	0.529061
2.264849	0.675002
2.289460	0.592231
2.314071	0.473698
2.338682	0.468148
2.363293	0.607127
2.387904	0.591607
2.412515	0.587496
2.437126	0.595958
2.461737	0.581310
2.486348	0.469747
2.510960	0.473563

Table 26: Total Reaction probability for $v = 4$, $j=1$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.029659	0.000000
0.054271	0.000000
0.078882	0.005277
0.103493	0.009817
0.128104	0.045507
0.152715	0.046083
0.177326	0.075483
0.201937	0.084770
0.226548	0.162317
0.251159	0.179280
0.275770	0.448243
0.300381	0.485137
0.324992	0.293822
0.349603	0.470691
0.374214	0.442278
0.398825	0.441951
0.423436	0.389662
0.448048	0.481018
0.472659	0.330553
0.497270	0.463112
0.521881	0.639319
0.546492	0.379775
0.571103	0.665601
0.595714	0.381172
0.620325	0.327431
0.644936	0.534445
0.669547	0.379654
0.694158	0.526602
0.718769	0.665943
0.743380	0.513774
0.767991	0.419327
0.792602	0.547655
0.817214	0.313560
0.841825	0.487395
0.866436	0.587191
0.891047	0.434323
0.915658	0.782190
0.940269	0.703752
0.964880	0.499310
0.989491	0.503087
1.014102	0.589410
1.038713	0.586464
1.063324	0.458381
1.087935	0.600592
1.112546	0.642511
1.137157	0.493662
1.161768	0.544657
1.186379	0.471465
1.210991	0.436089
1.235602	0.389547
1.260213	0.337614
1.284824	0.500884
1.309435	0.500764
1.334046	0.470240
1.358657	0.437492

Table 27: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.383268	0.589582
1.407879	0.502684
1.432490	0.642816
1.457101	0.586724
1.481712	0.569025
1.506323	0.625766
1.530934	0.472676
1.555545	0.480907
1.580156	0.459857
1.604768	0.564993
1.629379	0.462186
1.653990	0.696395
1.678601	0.605938
1.703212	0.538794
1.727823	0.519305
1.752434	0.715317
1.777045	0.658510
1.801656	0.604744
1.826267	0.749064
1.850878	0.462626
1.875489	0.694573
1.900100	0.673934
1.924711	0.424982
1.949322	0.572464
1.973933	0.498244
1.998545	0.641238
2.023156	0.591600
2.047767	0.572420
2.072378	0.636846
2.096989	0.447230
2.121600	0.521868
2.146211	0.483259
2.170822	0.648193
2.195433	0.598142
2.220044	0.595299
2.244655	0.546795
2.269266	0.569691
2.293877	0.604426
2.318488	0.602414
2.343099	0.601298
2.367710	0.579865
2.392322	0.432171
2.416933	0.652623
2.441544	0.528005
2.466155	0.669645
2.490766	0.621323
2.515377	0.648774

Table 28: Total Reaction probability for $v = 4$, $j=3$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.025242	0.000000
0.049853	0.000000
0.074464	0.000000
0.099075	0.000000
0.123686	0.165989
0.148297	0.151195
0.172908	0.208426
0.197520	0.285752
0.222131	0.205559
0.246742	0.227782
0.271353	0.272404
0.295964	0.334433
0.320575	0.613171
0.345186	0.627671
0.369797	0.239258
0.394408	0.607156
0.419019	0.391079
0.443630	0.370688
0.468241	0.391076
0.492852	0.511397
0.517463	0.644811
0.542074	0.376770
0.566686	0.603110
0.591297	0.437030
0.615908	0.292995
0.640519	0.414160
0.665130	0.369930
0.689741	0.625069
0.714352	0.544261
0.738963	0.456183
0.763574	0.484419
0.788185	0.621525
0.812796	0.337007
0.837407	0.513186
0.862018	0.556523
0.886629	0.692503
0.911240	0.663759
0.935851	0.749151
0.960463	0.658943
0.985074	0.530617
1.009685	0.521257
1.034296	0.652859
1.058907	0.524101
1.083518	0.590104
1.108129	0.604056
1.132740	0.514008
1.157351	0.552964
1.181962	0.492726
1.206573	0.467739
1.231184	0.441555
1.255795	0.341468
1.280406	0.415231
1.305017	0.422005
1.329628	0.471792
1.354240	0.496356

Table 29: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.378851	0.496313
1.403462	0.581766
1.428073	0.509346
1.452684	0.485608
1.477295	0.458025
1.501906	0.629325
1.526517	0.493875
1.551128	0.499682
1.575739	0.550771
1.600350	0.593300
1.624961	0.463518
1.649572	0.623157
1.674183	0.639858
1.698794	0.542931
1.723405	0.644757
1.748017	0.688571
1.772628	0.558576
1.797239	0.473290
1.821850	0.554571
1.846461	0.449958
1.871072	0.766493
1.895683	0.588305
1.920294	0.565998
1.944905	0.656461
1.969516	0.561574
1.994127	0.468449
2.018738	0.501674
2.043349	0.539117
2.067960	0.612144
2.092571	0.548518
2.117182	0.597755
2.141794	0.589993
2.166405	0.639779
2.191016	0.484710
2.215627	0.540604
2.240238	0.545350
2.264849	0.504641
2.289460	0.533318
2.314071	0.405460
2.338682	0.506963
2.363293	0.719229
2.387904	0.617698
2.412515	0.589799
2.437126	0.597853
2.461737	0.479043
2.486348	0.607014
2.510960	0.532313

Table 30: Total Reaction probability for $v = 4$, $j=5$ (CHIPR PES)

Energy (eV)	Reaction Probability
0.025242	0.000000
0.049853	0.000000
0.074464	0.014843
0.099075	0.041552
0.123686	0.188140
0.148297	0.162011
0.172908	0.186240
0.197520	0.299356
0.222131	0.281521
0.246742	0.287231
0.271353	0.319337
0.295964	0.432967
0.320575	0.667008
0.345186	0.648692
0.369797	0.261747
0.394408	0.642526
0.419019	0.400010
0.443630	0.460587
0.468241	0.453018
0.492852	0.564021
0.517463	0.678509
0.542074	0.399836
0.566686	0.686574
0.591297	0.527150
0.615908	0.312238
0.640519	0.455605
0.665130	0.393227
0.689741	0.618615
0.714352	0.623430
0.738963	0.434491
0.763574	0.427084
0.788185	0.583986
0.812796	0.328465
0.837407	0.568000
0.862018	0.642576
0.886629	0.731123
0.911240	0.702920
0.935851	0.704662
0.960463	0.735127
0.985074	0.456433
1.009685	0.436316
1.034296	0.673492
1.058907	0.686357
1.083518	0.690169
1.108129	0.749566
1.132740	0.572071
1.157351	0.681665
1.181962	0.458537
1.206573	0.555009
1.231184	0.601860
1.255795	0.502840
1.280406	0.636383
1.305017	0.535597
1.329628	0.570966
1.354240	0.516405

Table 31: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.378851	0.581958
1.403462	0.747457
1.428073	0.669560
1.452684	0.488207
1.477295	0.498752
1.501906	0.684491
1.526517	0.457618
1.551128	0.532921
1.575739	0.456683
1.600350	0.514612
1.624961	0.473065
1.649572	0.652532
1.674183	0.739556
1.698794	0.709792
1.723405	0.504727
1.748017	0.686166
1.772628	0.597831
1.797239	0.546947
1.821850	0.682769
1.846461	0.678054
1.871072	0.614177
1.895683	0.514882
1.920294	0.514413
1.944905	0.645303
1.969516	0.568576
1.994127	0.615619
2.018738	0.410239
2.043349	0.406997
2.067960	0.715163
2.092571	0.663220
2.117182	0.558815
2.141794	0.635245
2.166405	0.654151
2.191016	0.562704
2.215627	0.390961
2.240238	0.510773
2.264849	0.493200
2.289460	0.606100
2.314071	0.390019
2.338682	0.453014
2.363293	0.599733
2.387904	0.509592
2.412515	0.582272
2.437126	0.490806
2.461737	0.551810
2.486348	0.613805
2.510960	0.458374

Table 32: Total Reaction probability for $v = 0, j=1$ (DMBE IV PES)

Energy (eV)	Reaction Probability
0.671381	0.005886
0.691574	0.011710
0.711768	0.016678
0.731962	0.010497
0.752156	0.017753
0.772349	0.039393
0.792543	0.015352
0.812737	0.045988
0.832930	0.023505
0.853124	0.028745
0.873318	0.037969
0.893511	0.068876
0.913705	0.023260
0.933899	0.130503
0.954092	0.056154
0.974286	0.051652
0.994480	0.133247
1.014674	0.108026
1.034867	0.118612
1.055061	0.184888
1.075255	0.220180
1.095448	0.232943
1.115642	0.212161
1.135836	0.178799
1.156029	0.317986
1.176223	0.107199
1.196417	0.133465
1.216610	0.288854
1.236804	0.337072
1.256998	0.279702
1.277192	0.285435
1.297385	0.397646
1.317579	0.202168
1.337773	0.290201
1.357966	0.302402
1.378160	0.307027
1.398354	0.295962
1.418547	0.202370
1.438741	0.303247
1.458935	0.266750
1.479128	0.443629
1.499322	0.533839
1.519516	0.415502

Table 33: ... Continued from Previous Page

Energy (eV)	Reaction Probability
1.539710	0.264631
1.559903	0.369040
1.580097	0.417063
1.600291	0.497435
1.620484	0.597264
1.640678	0.474676
1.660872	0.494467
1.681065	0.493433
1.701259	0.267761
1.721453	0.398170
1.741646	0.473990
1.761840	0.322487
1.782034	0.430520
1.802228	0.337693
1.822421	0.505640
1.842615	0.336434
1.862809	0.307861
1.883002	0.335967
1.903196	0.384101
1.923390	0.244238
1.943583	0.358137
1.963777	0.421987
1.983971	0.319937
2.004164	0.375250
2.024358	0.324583
2.044552	0.300246
2.064746	0.313858
2.084939	0.336483
2.105133	0.307592
2.125327	0.341064
2.145520	0.391199
2.165714	0.262278
2.185908	0.352288
2.206101	0.317520
2.226295	0.399392
2.246489	0.476546
2.266682	0.417061
2.286876	0.308690
2.307070	0.266337
2.327264	0.274649
2.347457	0.269510
2.367651	0.290360
2.387845	0.349763
2.408038	0.223641
2.428232	0.243753
2.448426	0.360958
2.468619	0.284062
2.488813	0.320387
2.509007	0.232940