

Supplementary Information

***Ab Initio* Kinetics of Pyrene + OH Reaction: A Revisited Study**

Tam V.-T. Mai^{1,3,*}, Loc T. Nguyen^{2,3}, and Lam K. Huynh^{2,3,*}

¹ University of Science, Ho Chi Minh City, Vietnam.

² International University, Ho Chi Minh City, Vietnam.

³ Vietnam National University, Ho Chi Minh City, Vietnam.

* Corresponding authors. Email address: mvttam@hcmus.edu.vn (TVTM) & hklam@hcmiu.edu.vn (LKH) Tel: (84-8) 2211.4046 (Ext. 3233) Fax: (84-8) 3724.4271

Contents

Table S1: Optimized geometries, rotational constants (GHz), electronic energies at 0 K (E_{elec}^{0K}), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at ROCBS-QB3//M06-2X/aug-cc-pVTZ level of theory for the title reaction.....	4
Table S2: Calculated total rate constants, k_{tot} , of the Pyrene + OH $\rightarrow$ products over the range of temperature 200 – 2000 K at different pressures, e.g., $P = 7.6 - 76000$ Torr, including the HIR treatments, Eckart quantum tunneling effects. Units are in $\text{cm}^3/\text{molecule/s}$. $k_{tot}(T, P)$ values at different pressures are fitted as the double modified Arrhenius formats based on the ROCBS-QB3//M06-2X PES.....	24
Table S3: The calculated Eckart tunneling factor via tight transition state channels over the wide temperature range of 200 – 2000 K based on the ROCBS-QB3//M06-2X PES.	25
Table S4: Individual and total rate constants for Pyrene + OH $\rightarrow$ Products ($\text{cm}^3/\text{molecule/s}$) at different pressures (7.6, 76, 760, 7600 and 76000 Torr) based on the ROCBS-QB3//M06-2X PES. (“Unc.” stands for the uncertainty). Units are in $\text{cm}^3/\text{molecule/s}$	26
Table S5: Calculated branching ratios for each species of Pyrene + OH $\rightarrow$ products reactions at $P = 760$ Torr based on the ROCBS-QB3//M06-2X PES.....	33
Table S6: Acute and chronic toxicity classification (mg/L).....	33
Table S7: Rate constants for typical PAHs (Poly Aromatic Hydrocarbons) + OH reactions in gas and condensed phases under ambient conditions.	34
Table S8: Predicted thermochemical data of the adducts and products at 298 K.....	34
Table S9: Relative energies with respect to the isolated reactants for the primary transition states of the reaction between pyrene and OH radicals in the gas phase and in water (SMD model ⁸), calculated at the ROCBS-QB3//M06-2X/aug-cc-pVTZ level.	34
Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the Pyrene + OH reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths and bond angles are in Å and degree ($^\circ$), respectively. ^{a, b} obtained from Huber <i>et al.</i> ¹ , Hoy <i>et al.</i> ⁹ , respectively.	37
Figure S2: Predicted rate coefficients, $k(T, P)$, for the Pyrene + OH $\rightarrow$ I1 as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.	38
Figure S3: Predicted rate coefficients, $k(T, P)$, for the Pyrene + OH $\rightarrow$ I2 as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.	38
Figure S4: Predicted rate coefficients, $k(T, P)$, for the Pyrene + OH $\rightarrow$ I3 as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.	39
Figure S5: Calculated overall rate coefficients, $k_{tot}(T, P)$, for the Pyrene + OH $\rightarrow$ Products as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.....	39

Figure S6: Calculated overall rate constant, k_{tot} , for the Pyrene + OH $\rightarrow$ products reaction at $P = 760$ Torr as a function of temperature with (solid line) and without (dashed line) HIR treatment, based on the ROCBS-QB3//M06-2X PES.	40
Figure S7: Hindrance potentials for the species involved in the Pyrene + OH reaction, calculated at M06-2X/cc-pVDZ level of theory.	47

Table S1: Optimized geometries, rotational constants (GHz), electronic energies at 0 K (E_{elec}^{0K}), zero-point energy (ZPE) corrections and harmonic wavenumbers of the species involved with the lowest-energy conformer of a given species, calculated at ROCBS-QB3//M06-2X/aug-cc-pVTZ level of theory for the title reaction.

Species		Cartesian coordinate (Å)			Rotational constants (GHz)	E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
OH (C _{∞v})	8	0.000000000	0.000000000	0.107999000	564.211029	-75.658449	0.008530	3744.2022 (3737.8) ¹		
	1	0.000000000	0.000000000	-0.863995000						
H₂O (C _{2v})	8	0.000000000	0.000000000	0.116332000	834.47311	-76.358585	0.021565	1615.7190	3873.1681	3977.2474
	1	0.000000000	0.762680000	-0.465326000	431.04032			(1595.0; 3657.0 ² ; 3756.0 ¹)		
	1	0.000000000	-0.762680000	-0.465326000	284.22579					
H (D _{∞h})	1	0.000000000	0.000000000	0.000000000	/	-0.499818	0.00000	/		
Pyrene (D _{2h})	6	-3.502874000	-0.000002000	-0.000359000	1.01981	-614.826446	0.208788	97.0871	150.7791	212.3695
	6	-2.815009000	-1.203713000	-0.000300000	0.56183			248.4122	264.1171	359.8351
	6	-1.420433000	-1.226118000	-0.000158000	0.36226			403.7692	411.8452	462.1547
	6	-0.711665000	0.000000000	-0.000074000				503.4755	507.5624	507.7590
	6	-1.420436000	1.226119000	-0.000136000				521.6902	540.4595	550.5724
	6	-2.815007000	1.203712000	-0.000279000				598.1032	606.1750	702.7824
	6	-0.674544000	-2.454332000	-0.000094000				705.7646	738.5760	750.1584
	6	0.711665000	-0.000001000	0.000073000				769.7580	802.6044	815.7197
	6	1.420433000	-1.226118000	0.000135000				828.6324	838.0845	881.1923
	6	0.674544000	-2.454332000	0.000045000				886.2507	933.7761	945.8811
	6	2.815009000	-1.203712000	0.000279000				989.1339	1006.1840	1011.9949
	1	3.356926000	-2.140856000	0.000326000				1012.3742	1019.0518	1023.4086
	6	3.502874000	-0.000002000	0.000362000				1101.6688	1121.9798	1129.2367
	6	2.815007000	1.203713000	0.000303000				1148.8776	1169.2363	1199.7969
	6	1.420436000	1.226119000	0.000159000				1206.7084	1240.5895	1266.2087
	6	0.674543000	2.454333000	0.000092000				1271.2446	1274.1620	1328.0758
	6	-0.674543000	2.454333000	-0.000048000				1364.0931	1404.4183	1436.3783
	1	-1.225027000	3.386623000	-0.000099000				1452.5050	1469.9832	1475.6176
	1	1.225026000	3.386623000	0.000159000				1504.1874	1550.7371	1552.9770
	1	-1.225027000	-3.386621000	-0.000161000				1624.1495	1662.0100	1666.4049
	1	-4.584300000	0.000000000	-0.000468000				1679.6430	1710.3196	3190.7722
	1	-3.356926000	-2.140856000	-0.000364000				3190.8345	3194.1937	3194.4154
	1	-3.356929000	2.140853000	-0.000327000				3200.7066	3200.9700	3208.6128
	1	1.225027000	-3.386621000	0.000093000				3208.8518	3219.5282	3219.7104
	1	4.584300000	0.000001000	0.000474000						
	1	3.356930000	2.140853000	0.000369000						

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\text{ K}}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)			
RC (C ₁)	6	3.186237000	0.576247000	-0.563946000	0.82821	-690.491609	0.219165	9.3281	25.2124	93.5711	
	6	2.661681000	-0.708942000	-0.613681000	0.44067			103.6399	124.1892	159.8379	
	6	1.289135000	-0.922770000	-0.462178000	0.31966			215.0746	253.5799	265.0524	
	6	0.437407000	0.189136000	-0.252547000				360.1753	404.0856	410.9468	
	6	0.980592000	1.497220000	-0.203745000				415.7934	462.6942	504.7992	
	6	2.357303000	1.667779000	-0.361923000				507.9904	508.0933	523.2997	
	6	0.714019000	-2.238269000	-0.493890000				545.0269	550.4839	598.9102	
	6	-0.962945000	-0.007596000	-0.088278000				606.7335	705.1286	707.4530	
	6	-1.503711000	-1.315435000	-0.131928000				742.6845	749.8171	777.3889	
	6	-0.613262000	-2.424165000	-0.338351000				807.3635	815.9585	837.5018	
	6	-2.878550000	-1.486104000	0.030019000				838.7126	884.5230	887.0348	
	1	-3.292718000	-2.485769000	-0.002799000				940.5018	952.0565	989.6473	
	6	-3.708087000	-0.393589000	0.231288000				1010.4469	1016.6265	1019.4713	
	6	-3.184159000	0.889268000	0.276249000				1023.4248	1024.4694	1101.9453	
	6	-1.815010000	1.103895000	0.119306000				1122.7405	1130.3683	1150.8901	
	6	-1.236239000	2.418315000	0.161604000				1171.9942	1200.5106	1208.7331	
	6	0.091377000	2.605397000	0.009143000				1240.7877	1267.3549	1272.7789	
	1	0.514688000	3.601287000	0.043342000				1274.0971	1328.7767	1365.0558	
	1	-1.895681000	3.262225000	0.320548000				1403.7040	1437.8711	1454.5699	
	1	1.376817000	-3.081305000	-0.640456000				1471.3628	1476.4322	1505.7954	
	1	4.251977000	0.721881000	-0.671597000				1549.2943	1551.6612	1621.6999	
	1	3.314222000	-1.558255000	-0.766457000				1661.4146	1662.8200	1679.1464	
	1	2.772321000	2.666697000	-0.320847000				1709.1440	3189.8332	3192.2396	
	1	-1.035380000	-3.420864000	-0.362910000				3193.3615	3197.6888	3199.8087	
	1	-4.771945000	-0.543277000	0.354617000				3206.3257	3207.6724	3210.4007	
	1	-3.836120000	1.738866000	0.434666000				3218.5230	3224.0834	3762.5896	
	8	3.163388000	-1.133493000	1.959705000							
	1	2.399978000	-0.535878000	2.031392000							
II (C ₁)	6	-3.271165000	1.050701000	-0.076402000	0.74056	-690.531532	0.222926	47.5001	105.9806	156.9856	
	6	-2.864773000	-0.284459000	-0.173126000	0.52513			199.7445	234.0033	275.3210	
	6	-1.528126000	-0.619072000	-0.180433000	0.31267			307.8961	345.0220	361.1495	
	6	-0.553010000	0.395752000	-0.081206000				383.1767	421.5307	444.4165	
	6	-0.962997000	1.745775000	0.012273000				489.8331	495.3225	506.4917	
	6	-2.332928000	2.051247000	0.011292000				532.1284	558.7580	570.8726	
	6	-1.137705000	-2.077134000	-0.297769000				586.7399	618.8366	667.8188	
	6	0.846645000	0.083656000	-0.061838000				687.2148	726.4150	741.5111	
	6	1.274570000	-1.283206000	-0.121882000				771.9135	791.5636	801.1762	
	6	0.331525000	-2.304917000	-0.219026000				807.2723	833.0141	867.1580	

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\text{ K}}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
	6	2.656737000	-1.554899000	-0.075651000				879.0558	919.2368	944.7534
	1	2.985244000	-2.585213000	-0.118832000				959.5315	1006.7780	1012.3950
	6	3.583712000	-0.529175000	0.017570000				1015.0239	1023.3490	1049.8669
	6	3.168409000	0.788785000	0.073902000				1080.1533	1110.3208	1119.1085
	6	1.796281000	1.110482000	0.039989000				1124.5602	1160.3079	1190.1596
	6	1.348218000	2.470313000	0.116884000				1194.0423	1214.8413	1224.8536
	6	0.032097000	2.772023000	0.106216000				1238.2731	1260.2585	1263.8604
	1	-0.298125000	3.801196000	0.169516000				1324.6077	1350.5891	1359.1390
	1	2.092944000	3.252698000	0.189607000				1381.9473	1403.1771	1421.8501
	1	-1.504915000	-2.455047000	-1.258756000				1448.5883	1462.7025	1473.3405
	1	-4.325241000	1.291990000	-0.073973000				1486.6686	1539.9260	1560.1062
	1	-3.602301000	-1.074243000	-0.236463000				1614.6827	1640.7741	1670.9836
	1	-2.638424000	3.087488000	0.082318000				1690.0952	3022.2969	3190.0139
	1	0.659803000	-3.335917000	-0.249132000				3193.5646	3195.4323	3198.7325
	1	4.639310000	-0.762407000	0.046580000				3202.3541	3203.4967	3207.9812
	1	3.892524000	1.589428000	0.148874000				3219.6560	3219.8337	3843.3198
	8	-1.833121000	-2.887374000	0.652883000						
	1	-1.560786000	-2.606207000	1.532443000						
I2 (C ₁)	6	-3.173782000	0.846244000	-0.202522000	0.90814 0.44474 0.30433	-690.539256	0.222995	54.3538	97.0431	175.3307
	6	-2.795770000	-0.601177000	-0.271648000				196.6354	225.7165	271.9783
	6	-1.306054000	-0.834619000	-0.197680000				291.2825	338.0515	384.5652
	6	-0.398765000	0.233590000	-0.103476000				403.7197	415.7415	456.3402
	6	-0.855688000	1.583365000	-0.068676000				480.7754	499.0347	508.3302
	6	-2.277074000	1.834039000	-0.107662000				520.4612	527.3013	566.5193
	6	-0.825699000	-2.147859000	-0.215835000				594.3648	623.5975	684.7170
	6	0.995453000	-0.031127000	-0.032316000				688.8028	712.1545	752.2625
	6	1.465295000	-1.368259000	-0.055461000				776.0055	778.8372	813.7360
	6	0.519934000	-2.417182000	-0.147808000				834.3137	848.3801	859.9149
	6	2.852969000	-1.607793000	0.013424000				884.0541	925.7512	930.4776
	1	3.208782000	-2.629768000	-0.003865000				987.6686	989.7532	1003.6313
	6	3.745927000	-0.557501000	0.100574000				1012.1111	1017.3059	1041.1865
	6	3.292964000	0.755337000	0.123594000				1078.6621	1110.2985	1131.8187
	6	1.922112000	1.043538000	0.059650000				1141.1436	1163.0505	1200.1409
	6	1.424978000	2.372901000	0.083822000				1202.9039	1220.8047	1232.8070
	6	0.074238000	2.622570000	0.023635000				1239.1059	1245.6181	1264.8783
	1	-0.287809000	3.642951000	0.048881000				1324.5697	1340.8630	1365.7230
	1	2.130250000	3.190703000	0.153166000				1386.9540	1402.8952	1405.9243
	1	-1.540643000	-2.958527000	-0.276953000				1438.1231	1456.4714	1479.1369

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\text{ K}}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
	1	-4.235464000	1.056601000	-0.219384000				1514.6285	1547.6797	1569.2543
	1	-3.170548000	-1.021702000	-1.210947000				1608.9260	1624.0318	1630.6552
	1	-2.606607000	2.864812000	-0.051320000				1693.8475	3030.8392	3182.7341
	1	0.874983000	-3.439558000	-0.165439000				3191.6209	3195.1828	3196.1045
	1	4.807435000	-0.757898000	0.151485000				3203.1037	3206.8513	3209.4698
	1	3.997962000	1.573730000	0.192129000				3210.8716	3219.7779	3843.6260
	8	-3.492974000	-1.354516000	0.723374000						
	1	-3.200779000	-1.041617000	1.585571000						
I3 (C _s)	6	-0.287912000	3.254631000	0.000000000	0.97443 0.40515 0.29167	-690.515879	0.222185	55.7326	127.9965	136.0137
	6	-0.234724000	2.431557000	1.242406000				205.8478	213.3838	279.7049
	6	-0.151233000	1.069336000	1.239572000				294.5190	319.9736	375.7525
	6	-0.114460000	0.346565000	0.000000000				382.8717	429.9983	459.8540
	6	-0.151233000	1.069336000	-1.239572000				492.0269	494.7618	505.3356
	6	-0.234724000	2.431557000	-1.242406000				521.6165	530.8189	551.7646
	6	-0.092991000	0.309026000	2.469270000				552.5894	600.4784	676.8923
	6	-0.024522000	-1.062663000	0.000000000				690.1938	721.2145	756.6751
	6	0.022551000	-1.776835000	1.227545000				774.9146	786.1583	806.9114
	6	-0.014423000	-1.033669000	2.461292000				823.3859	829.3856	866.4350
	6	0.106298000	-3.165776000	1.204499000				871.6973	885.2445	930.5548
	1	0.141261000	-3.706550000	2.141682000				943.2542	962.5394	1006.6239
	6	0.146670000	-3.854573000	0.000000000				1010.6568	1015.9225	1018.3397
	6	0.106298000	-3.165776000	-1.204499000				1049.4979	1088.1126	1111.5632
	6	0.022551000	-1.776835000	-1.227545000				1121.6420	1137.3326	1167.1657
	6	-0.014423000	-1.033669000	-2.461292000				1199.1272	1218.5701	1223.3915
	6	-0.092991000	0.309026000	-2.469270000				1249.9820	1255.9807	1268.7042
	1	-0.119068000	0.855637000	-3.403344000				1299.2576	1357.8578	1365.4297
	1	0.024083000	-1.587869000	-3.390652000				1390.0224	1427.7729	1430.7679
	1	-0.119068000	0.855637000	3.403344000				1431.1630	1449.5847	1477.6956
	1	-1.211156000	3.848566000	0.000000000				1480.8023	1548.5979	1602.7929
	1	-0.249123000	2.972746000	2.180688000				1619.5584	1652.7207	1670.7874
	1	-0.249123000	2.972746000	-2.180688000				1682.5683	2996.5614	3190.2198
	1	0.024083000	-1.587869000	3.390652000				3190.4549	3192.9904	3194.1679
	1	0.211682000	-4.933876000	0.000000000				3194.5331	3199.9672	3208.5926
	1	0.141261000	-3.706550000	-2.141682000				3208.8845	3220.6187	3844.3462
	8	0.734526000	4.262449000	0.000000000						
	1	1.584561000	3.810367000	0.000000000						
I4 (C ₁)	6	-3.321680000	0.444237000	-0.525334000	0.86743 0.50486	-690.502025	0.221632	74.6036	129.4833	157.9459
	6	-2.805731000	-0.809586000	-0.401125000				198.5437	240.6073	272.1191

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
	6	-1.435014000	-1.028512000	0.165474000	0.34401			296.8711	303.6370	368.2218
	6	-0.555275000	0.185157000	-0.006321000				391.8230	425.5916	459.1797
	6	-1.127896000	1.454021000	-0.065193000				471.9728	495.9497	510.6140
	6	-2.529295000	1.580043000	-0.281672000				514.9078	544.0214	553.4223
	6	-0.774123000	-2.286340000	-0.320365000				567.4692	594.4735	663.8856
	6	0.845704000	0.038578000	-0.012358000				682.6611	708.4956	731.4896
	6	1.430879000	-1.250004000	-0.169219000				739.9324	783.5754	799.1938
	6	0.549717000	-2.386267000	-0.408840000				806.5333	819.6819	825.4323
	6	2.800382000	-1.369498000	-0.177090000				865.2951	876.9903	945.8338
	1	3.247277000	-2.346573000	-0.311357000				946.8552	986.5451	988.2718
	6	3.625346000	-0.239794000	-0.030671000				998.8341	1006.0732	1014.1472
	6	3.076367000	1.011850000	0.077033000				1018.1265	1078.2592	1089.7315
	6	1.676502000	1.182641000	0.066911000				1101.0245	1126.4718	1146.3600
	6	1.067689000	2.467556000	0.107755000				1164.9058	1184.1056	1202.7858
	6	-0.281208000	2.599685000	0.016027000				1224.9239	1246.0384	1264.2798
	1	-0.736740000	3.581820000	-0.003039000				1283.2043	1322.6801	1341.3630
	1	1.702606000	3.341402000	0.179951000				1383.5090	1417.1641	1425.5966
	1	-1.417502000	-3.138460000	-0.499192000				1432.7626	1438.4805	1469.4810
	1	-4.354655000	0.575523000	-0.818313000				1503.7823	1547.3276	1576.8799
	1	-3.413366000	-1.688062000	-0.575038000				1627.0369	1660.5922	1666.2200
	1	-2.963043000	2.568904000	-0.341321000				1729.0981	3186.2428	3190.3590
	1	1.012056000	-3.326778000	-0.682799000				3193.6064	3195.5337	3199.8250
	1	4.699752000	-0.361821000	-0.027897000				3205.7341	3206.8679	3208.0668
	1	3.710059000	1.885937000	0.156508000				3218.0558	3219.8564	3827.5915
	8	-1.608093000	-1.268260000	1.594099000						
	1	-2.075879000	-0.508426000	1.959630000						
I5 (C ₁)	6	3.404414000	-0.000006000	-0.466963000	0.89091 0.52012 0.35963	-690.496581	0.221264	89.5024	126.1507	177.1052
	6	2.720611000	1.219438000	-0.375380000				215.3420	235.8082	251.4914
	6	1.370964000	1.262260000	-0.112783000				297.2427	314.4619	365.4264
	6	0.672651000	0.000002000	0.330001000				390.4254	400.1912	448.1646
	6	1.370965000	-1.262258000	-0.112775000				462.0676	500.9004	505.3179
	6	2.720633000	-1.219433000	-0.375360000				527.6896	531.6594	561.2677
	6	0.611303000	2.470780000	-0.122264000				575.1903	585.5579	691.9955
	6	-0.801366000	-0.000001000	0.027854000				693.1598	713.2080	744.7801
	6	-1.487575000	1.214718000	-0.056359000				759.9631	782.9380	794.6344
	6	-0.738156000	2.457517000	-0.060063000				813.2059	816.7018	832.9139
	6	-2.877142000	1.201114000	-0.189845000				870.3569	922.3414	939.8684
	1	-3.411225000	2.140617000	-0.254146000				946.2084	967.7281	973.2571

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	6	-3.566051000	-0.000008000	-0.246419000			996.8966	997.3568	1000.3788
	6	-2.877139000	-1.201126000	-0.189841000			1018.1376	1031.0450	1068.9150
	6	-1.487570000	-1.214725000	-0.056356000			1110.7847	1115.1408	1164.4075
	6	-0.738148000	-2.457516000	-0.060063000			1169.7079	1199.5635	1209.9857
	6	0.611320000	-2.470770000	-0.122267000			1238.8640	1250.7387	1262.3717
	1	1.145186000	-3.408144000	-0.219258000			1279.2024	1280.3490	1336.0202
	1	-1.296369000	-3.384581000	-0.084732000			1338.5498	1394.6279	1396.8329
	1	1.145170000	3.408155000	-0.219241000			1439.4707	1467.0571	1483.0366
	1	4.463880000	0.000003000	-0.681273000			1509.7462	1545.5817	1604.3330
	1	3.251881000	2.145516000	-0.556786000			1611.4197	1614.9461	1664.3437
	1	3.251902000	-2.145516000	-0.556739000			1670.7003	3186.8407	3187.0399
	1	-1.296385000	3.384577000	-0.084726000			3190.9711	3192.9809	3194.5930
	1	-4.642737000	-0.000009000	-0.346707000			3198.9594	3207.1744	3207.4543
	1	-3.411218000	-2.140633000	-0.254138000			3219.2297	3219.5341	3824.3489
	8	0.712464000	0.000004000	1.792575000					
	1	1.641923000	0.000073000	2.050434000					
TS1 (C _i)	6	3.412481000	-0.609344000	-0.198314000	-690.492037	0.219933	-373.8968	72.6946	88.3226
	6	2.847702000	0.649685000	-0.360748000			105.9600	154.7064	189.7927
	6	1.468324000	0.813340000	-0.333033000			228.8051	253.7254	271.5115
	6	0.638513000	-0.314710000	-0.135742000			358.3373	395.3283	412.1982
	6	1.217881000	-1.593892000	0.035457000			460.9073	501.7154	503.9280
	6	2.608995000	-1.718432000	-0.000819000			507.0184	509.2992	549.4353
	6	0.854233000	2.113555000	-0.477825000			556.2937	593.7022	604.6896
	6	-0.779646000	-0.167706000	-0.110941000			691.0343	703.3590	731.5798
	6	-1.365986000	1.110463000	-0.301176000			745.4296	756.2808	784.1192
	6	-0.512242000	2.236656000	-0.515241000			805.1161	815.6945	837.2753
	6	-2.756574000	1.231744000	-0.280278000			849.0507	880.8013	890.3372
	1	-3.201684000	2.207812000	-0.424369000			942.4587	953.2192	986.9004
	6	-3.559593000	0.119376000	-0.076660000			996.6178	1013.4709	1017.5043
	6	-2.992307000	-1.130873000	0.107848000			1022.7680	1024.1627	1102.1045
	6	-1.604368000	-1.297006000	0.092486000			1123.0143	1127.5917	1151.4279
	6	-0.987414000	-2.581567000	0.271600000			1164.5169	1199.6871	1207.7524
	6	0.354431000	-2.722492000	0.241908000			1236.8107	1264.9414	1269.1381
	1	0.808463000	-3.696340000	0.374671000			1271.3831	1332.1234	1363.9720
	1	-1.628214000	-3.439878000	0.428731000			1397.2675	1434.5629	1441.8626
	1	1.483122000	2.948480000	-0.746959000			1470.1138	1477.3155	1499.7919
	1	4.487667000	-0.721733000	-0.221478000			1532.3865	1549.9741	1600.7365
	1	3.478290000	1.518314000	-0.498558000			1648.7326	1658.4501	1666.1718

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	1	3.052919000	-2.697170000	0.129597000				1698.7849	3191.2684	3195.3114
	1	-0.960269000	3.208441000	-0.671141000				3196.1868	3201.9196	3204.4796
	1	-4.635175000	0.228959000	-0.061977000				3209.0116	3212.7310	3221.0899
	1	-3.622914000	-1.996698000	0.265006000				3221.4971	3234.1420	3795.7409
	8	0.906435000	2.924060000	1.469966000						
	1	0.419733000	2.214545000	1.915610000						
TS2 (C ₁)	6	-3.176879000	0.652442000	-0.467541000	0.86696	-690.491653	0.219725	-419.9208	68.3838	78.6963
	6	-2.685877000	-0.664173000	-0.465434000	0.44665			114.7600	160.5670	172.7230
	6	-1.297841000	-0.894949000	-0.368139000	0.31522			214.5553	247.9512	269.2986
	6	-0.425585000	0.203278000	-0.194330000				359.8864	400.4265	412.0788
	6	-0.943019000	1.522621000	-0.155995000				461.7636	492.5155	506.9009
	6	-2.325995000	1.720191000	-0.299155000				507.6905	520.0142	544.5853
	6	-0.753083000	-2.215221000	-0.407837000				550.4269	588.5052	606.6074
	6	0.973803000	-0.015620000	-0.065160000				702.3197	705.3160	707.0107
	6	1.490479000	-1.332644000	-0.111896000				737.2553	750.7213	784.3667
	6	0.577764000	-2.424788000	-0.287344000				815.6838	816.1703	838.4637
	6	2.867358000	-1.525884000	0.016759000				843.5313	878.6054	885.9115
	1	3.262896000	-2.532996000	-0.018255000				938.6596	950.0782	989.7303
	6	3.720736000	-0.447026000	0.187608000				1004.0804	1012.5909	1017.4455
	6	3.219924000	0.845183000	0.233126000				1021.2545	1024.1946	1093.4825
	6	1.850209000	1.082487000	0.108601000				1118.5479	1133.4105	1152.4450
	6	1.296305000	2.404783000	0.148678000				1170.0690	1199.5165	1207.7139
	6	-0.034260000	2.613614000	0.021382000				1235.0834	1255.6100	1264.2156
	1	-0.437896000	3.617714000	0.051077000				1272.3227	1333.1400	1363.6378
	1	1.972587000	3.239655000	0.282472000				1406.1990	1438.6892	1444.7587
	1	-1.436655000	-3.046256000	-0.521433000				1467.1772	1471.8732	1510.8980
	1	-4.240267000	0.813932000	-0.572362000				1531.2456	1545.7922	1601.4360
	1	-3.336295000	-1.483206000	-0.731810000				1644.9309	1650.1975	1665.9624
	1	-2.715410000	2.729920000	-0.277612000				1689.1351	3191.3424	3194.6818
	1	0.980306000	-3.429441000	-0.315249000				3195.4791	3199.3865	3201.0487
	1	4.784517000	-0.614241000	0.285555000				3208.7619	3214.3310	3220.7869
	1	3.890272000	1.684846000	0.365671000				3222.0209	3235.0462	3795.8898
	8	-3.263309000	-1.201041000	1.516145000						
	1	-2.741808000	-0.517345000	1.962849000						
TS3 (C ₁)	6	-3.181211000	0.000003000	-0.456288000	0.92365	-690.487705	0.219864	-470.7517	66.9178	81.9026
	6	-2.466986000	-1.215153000	-0.436540000	0.41753			125.0701	161.8621	178.8574
	6	-1.089710000	-1.231268000	-0.282590000	0.30462			217.7745	258.7942	270.7619
	6	-0.383967000	0.000001000	-0.199812000				361.3913	404.1595	410.5866

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	6	-1.089707000	1.231271000	-0.282589000			460.1571	483.7885	505.1729
	6	-2.466985000	1.215158000	-0.436539000			505.8000	526.0980	536.9258
	6	-0.344927000	-2.460173000	-0.205908000			549.0571	571.5379	604.0690
	6	1.027848000	0.000000000	-0.043982000			701.0384	702.0964	732.0024
	6	1.733431000	-1.227335000	0.032263000			750.0601	785.4977	797.1217
	6	0.994434000	-2.457696000	-0.055149000			825.2417	832.2393	836.0363
	6	3.118564000	-1.204486000	0.186201000			844.3090	884.9249	901.4147
	1	3.657882000	-2.141193000	0.244853000			922.9117	947.6579	986.4383
	6	3.801500000	-0.000003000	0.263059000			1008.2257	1013.7846	1019.3754
	6	3.118567000	1.204482000	0.186202000			1019.9079	1023.7527	1076.5003
	6	1.733433000	1.227333000	0.032264000			1116.4429	1127.3358	1143.0365
	6	0.994439000	2.457695000	-0.055148000			1171.0828	1184.8382	1205.0325
	6	-0.344923000	2.460175000	-0.205907000			1233.8967	1266.8262	1268.3979
	1	-0.891731000	3.392246000	-0.270337000			1273.6998	1317.5569	1366.7592
	1	1.543825000	3.388668000	0.003497000			1404.8005	1434.9120	1447.9004
	1	-0.891737000	-3.392243000	-0.270338000			1462.0758	1468.7581	1498.5131
	1	-4.214848000	0.000005000	-0.764519000			1525.5932	1551.4111	1606.6696
	1	-3.010773000	-2.148315000	-0.498200000			1641.1379	1656.2027	1674.1087
	1	-3.010770000	2.148321000	-0.498200000			1700.6033	3191.3762	3191.4412
	1	1.543819000	-3.388670000	0.003496000			3194.3259	3200.6842	3206.9876
	1	4.876324000	-0.000004000	0.382612000			3208.5370	3209.3149	3209.8292
TS4 (C ₁)	1	3.657886000	2.141187000	0.244854000	-690.483628	0.219631	3219.2336	3238.7104	3800.0657
	8	-3.892049000	-0.000010000	1.412525000					
	1	-3.046275000	0.000049000	1.884849000					
	6	-3.338648000	0.426664000	-0.430360000			-525.0387	79.9791	115.0632
	6	-2.776090000	-0.833956000	-0.402589000			154.3000	163.3819	213.2907
	6	-1.386020000	-1.006773000	-0.146510000			240.2716	249.6793	265.0795
	6	-0.557810000	0.172305000	-0.121363000			358.5738	395.1725	412.6905
	6	-1.151689000	1.446782000	-0.114252000			461.1031	477.3395	504.4165
	6	-2.545758000	1.554653000	-0.259764000			506.5422	509.2829	529.5303
	6	-0.735609000	-2.286844000	-0.385043000			547.5485	584.1289	600.0907
	6	0.851975000	0.040831000	-0.072882000			672.4556	698.3663	722.1938
	6	1.450633000	-1.240198000	-0.181673000			742.9899	765.5721	795.2335
	6	0.599312000	-2.392430000	-0.378843000			813.0633	816.1999	832.1223
	6	2.831990000	-1.343705000	-0.132502000			851.9986	854.0445	880.3487
	1	3.292462000	-2.319739000	-0.217471000			926.8005	946.1609	978.7824
	6	3.627519000	-0.208701000	0.020517000			1003.5481	1010.9720	1014.1498
	6	3.054323000	1.043548000	0.106853000			1016.6996	1020.9257	1099.4393

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	6	1.662762000	1.193734000	0.053297000			1120.3176	1124.6726	1149.0215
	6	1.031715000	2.477791000	0.109193000			1170.2380	1190.2467	1204.7605
	6	-0.311741000	2.600415000	0.016040000			1233.4860	1252.3110	1265.0468
	1	-0.778852000	3.576866000	0.037493000			1270.6922	1329.6086	1356.9380
	1	1.658333000	3.354565000	0.212247000			1385.7994	1431.8679	1450.6972
	1	-1.368658000	-3.154393000	-0.513981000			1463.1694	1468.8428	1488.2597
	1	-4.403310000	0.536163000	-0.582122000			1531.1287	1551.8996	1601.6347
	1	-3.387920000	-1.718451000	-0.516206000			1635.9236	1653.1880	1676.8407
	1	-2.995504000	2.539364000	-0.266043000			1712.0395	3191.9219	3195.2873
	1	1.074749000	-3.354406000	-0.522412000			3196.2773	3196.4804	3202.1467
	1	4.703185000	-0.311983000	0.061905000			3209.4727	3210.2607	3217.4412
	1	3.675228000	1.924065000	0.211351000			3220.3390	3224.6307	3794.3713
	8	-1.646614000	-1.304046000	1.752814000					
	1	-2.137977000	-0.504373000	1.992006000					
TS5 (C ₁)	6	3.423424000	0.000054000	-0.373811000	-690.482945	0.219692	-522.8721	96.9295	126.1298
	6	2.740968000	1.211476000	-0.316010000			158.9923	182.0359	205.5191
	6	1.361905000	1.242802000	-0.165361000			206.4127	250.1785	276.3780
	6	0.652571000	0.000027000	0.036415000			361.2657	400.7372	404.9061
	6	1.361938000	-1.242733000	-0.165332000			455.9452	461.4399	507.2388
	6	2.741013000	-1.211375000	-0.315969000			507.3958	520.0959	543.0191
	6	0.609993000	2.461082000	-0.157822000			543.7908	583.4594	597.3845
	6	-0.792275000	0.000009000	-0.073593000			695.2785	704.4454	710.6060
	6	-1.489097000	1.220754000	-0.097866000			748.2904	772.1773	791.5915
	6	-0.738541000	2.452543000	-0.108679000			808.6114	827.7930	829.6386
	6	-2.883537000	1.202835000	-0.133870000			850.1605	880.0855	901.1557
	1	-3.423468000	2.140922000	-0.151918000			935.2552	947.0269	984.1884
	6	-3.572293000	-0.000027000	-0.147608000			1003.3272	1011.6887	1012.4885
	6	-2.883505000	-1.202872000	-0.133953000			1019.7659	1023.9977	1093.8747
	6	-1.489066000	-1.220755000	-0.097939000			1118.4173	1120.3749	1138.1698
	6	-0.738481000	-2.452524000	-0.108794000			1169.7976	1193.0421	1205.9342
	6	0.610056000	-2.461031000	-0.157864000			1243.1684	1261.9315	1269.2787
	1	1.153165000	-3.396001000	-0.208453000			1278.2037	1315.7208	1336.2464
	1	-1.291323000	-3.383434000	-0.108737000			1369.6722	1433.1010	1438.1093
	1	1.153077000	3.396067000	-0.208393000			1466.2023	1468.3711	1484.4054
	1	4.497917000	0.000072000	-0.496491000			1531.5344	1551.5564	1620.3039
	1	3.282096000	2.144175000	-0.408395000			1638.4630	1651.7916	1671.4468
	1	3.282163000	-2.144063000	-0.408330000			1691.2667	3192.0859	3192.1543
	1	-1.291404000	3.383440000	-0.108538000			3195.1538	3195.2662	3201.3467

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
	1	-4.653323000	-0.000041000	-0.173499000				3201.6502	3209.4925	3209.6820
	1	-3.423411000	-2.140973000	-0.152071000				3218.7425	3220.5592	3790.3311
	8	0.696158000	-0.000096000	1.932610000						
	1	1.654810000	-0.000988000	2.072271000						
TS6 (C ₁)	6	-3.196694000	-1.203520000	-0.055549000	0.74475	-690.473492	0.215275	-1096.1547	86.9926	123.7938
	6	-2.868914000	0.147531000	-0.028155000	0.52766			170.8097	232.7609	253.1319
	6	-1.538200000	0.537581000	0.005134000	0.31026			300.4939	309.8600	321.4163
	6	-0.512083000	-0.433811000	0.004284000				356.2626	389.5489	433.0639
	6	-0.857343000	-1.805709000	-0.007527000				437.6470	495.5490	503.7246
	6	-2.206367000	-2.168091000	-0.038202000				509.1104	516.8414	537.2228
	6	-1.150609000	1.939662000	0.073226000				558.4699	580.9702	593.8628
	6	0.859263000	-0.044760000	0.009483000				613.8950	642.6804	680.4626
	6	1.206642000	1.330780000	-0.036110000				706.3417	730.3350	751.2164
	6	0.168039000	2.306057000	-0.067923000				792.7100	802.5361	803.6195
	6	2.557397000	1.685831000	-0.057252000				840.4267	849.7340	872.4895
	1	2.826535000	2.733715000	-0.091956000				886.1464	933.9675	951.2278
	6	3.545502000	0.713334000	-0.032327000				961.0514	1010.5093	1015.7901
	6	3.212497000	-0.630546000	0.007873000				1022.0695	1023.0125	1086.8471
	6	1.873387000	-1.029039000	0.023159000				1103.3716	1124.6508	1157.5251
	6	1.492161000	-2.413641000	0.035482000				1166.0595	1202.7130	1205.2025
	6	0.194529000	-2.782711000	0.014548000				1207.0370	1249.3628	1260.3035
	1	-0.080521000	-3.829849000	0.014145000				1269.0902	1317.1850	1331.5867
	1	2.276701000	-3.159525000	0.052363000				1361.6476	1399.2382	1438.7468
	1	-1.087389000	1.900551000	1.829602000				1450.1273	1468.5128	1477.1487
	1	-4.236142000	-1.500098000	-0.083867000				1515.2395	1536.2523	1551.7886
	1	-3.641409000	0.902407000	-0.026005000				1604.3122	1650.3904	1658.9599
	1	-2.467496000	-3.218705000	-0.048884000				1668.8279	1699.9013	3185.1692
	1	0.430842000	3.356327000	-0.117783000				3191.8173	3195.3018	3197.1091
	1	4.585888000	1.008324000	-0.046081000				3202.1651	3209.7150	3216.1319
	1	3.987710000	-1.385706000	0.021852000				3220.0711	3236.6406	3876.7301
	8	-2.178510000	2.822217000	-0.072308000						
	1	-1.841872000	3.721139000	-0.025796000						
TS7 (C ₁)	6	3.107906000	0.912005000	-0.070976000	0.90819	-690.473264	0.215068	-1057.8858	87.2025	111.0980
	6	2.711191000	-0.434636000	0.062361000	0.44890			193.9738	213.6053	259.0184
	6	1.337638000	-0.775076000	-0.003585000	0.30176			271.7973	297.0076	316.2922
	6	0.387660000	0.269352000	-0.000445000				386.1484	415.6782	436.2711
	6	0.800517000	1.625686000	-0.010708000				442.5378	470.2766	485.7307
	6	2.170369000	1.915292000	-0.070300000				514.5413	523.1034	526.3618

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	6	0.899627000	-2.132617000	-0.019746000				558.6037	563.4003	571.6038
	6	-1.000028000	-0.047434000	-0.001464000				614.7429	650.3186	700.8255
	6	-1.417815000	-1.400945000	-0.013732000				707.3284	720.3568	746.2581
	6	-0.420595000	-2.430124000	-0.026912000				779.4409	786.5050	820.5493
	6	-2.784505000	-1.689646000	-0.013021000				837.1057	860.0990	867.8349
	1	-3.103863000	-2.723859000	-0.023164000				884.8045	919.5384	940.1804
	6	-3.721406000	-0.669409000	0.000852000				974.5891	997.3639	1008.6730
	6	-3.319061000	0.657808000	0.011453000				1014.8038	1020.1373	1088.8273
	6	-1.964355000	0.991517000	0.008897000				1124.7074	1130.9024	1148.7274
	6	-1.513142000	2.353783000	0.013176000				1168.5183	1194.9372	1206.3182
	6	-0.195035000	2.653023000	0.000110000				1234.2826	1249.0674	1263.0301
	1	0.134006000	3.684605000	-0.004161000				1270.8544	1293.9747	1335.3527
	1	-2.256578000	3.140501000	0.022246000				1369.3039	1412.9800	1437.3262
	1	1.645324000	-2.914212000	-0.021886000				1440.5830	1464.1349	1471.1513
	1	4.165062000	1.142542000	-0.118024000				1509.0609	1539.2924	1550.9951
	1	2.724204000	-0.371188000	1.836173000				1609.5191	1650.0589	1656.1193
	1	2.488466000	2.948513000	-0.122063000				1667.8185	1691.1244	3190.5798
	1	-0.749198000	-3.461526000	-0.039922000				3192.0040	3194.7210	3200.0503
	1	-4.775919000	-0.909551000	0.002314000				3202.4155	3208.1593	3209.9295
	1	-4.056187000	1.450537000	0.020212000				3218.9046	3233.8640	3878.5526
8	3.601911000	-1.455752000	-0.098558000							
1	4.495596000	-1.131814000	0.040984000							
TS8 (C ₁)	6	-3.136005000	-0.013811000	0.082234000	1.00866 0.39801 0.28653	-690.469483	0.214904	-1150.4058	72.1018	151.0097
	6	-2.435948000	1.207069000	-0.034873000				175.3521	211.8943	244.9325
	6	-1.050917000	1.223707000	-0.023137000				259.0201	276.0079	334.7290
	6	-0.335360000	-0.002633000	0.000435000				365.4359	398.0069	417.0086
	6	-1.045121000	-1.233546000	-0.021793000				473.7106	491.2997	502.7800
	6	-2.428950000	-1.228887000	-0.024750000				515.8420	517.5254	537.4040
	6	-0.305353000	2.454478000	-0.040793000				555.6714	559.8672	576.9371
	6	1.084434000	0.001680000	0.005132000				612.2200	654.5240	695.3099
	6	1.792095000	1.229038000	0.002201000				700.4487	731.2538	778.7280
	6	1.042923000	2.454971000	-0.022701000				779.9603	785.5936	819.1328
	6	3.186094000	1.210810000	0.013453000				831.8501	847.6784	879.0286
	1	3.724756000	2.149953000	0.012642000				881.0678	910.7141	944.3972
	6	3.878595000	0.009629000	0.022023000				1002.1808	1003.7962	1008.3644
	6	3.192248000	-1.195667000	0.013413000				1014.7372	1018.3823	1022.5315
	6	1.798833000	-1.221941000	0.002361000				1112.0770	1134.6060	1143.7200
	6	1.056356000	-2.452555000	-0.022326000				1162.2740	1185.1904	1201.3520

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	6	-0.291600000	-2.460073000	-0.040195000				1208.5474	1236.1093	1261.1266
	1	-0.837826000	-3.394302000	-0.060902000				1272.3655	1325.8077	1334.6091
	1	1.610167000	-3.382964000	-0.028649000				1364.9891	1409.6496	1427.9778
	1	-0.856050000	3.386263000	-0.061943000				1457.0938	1466.8731	1477.4543
	1	-3.168872000	-0.001300000	1.749774000				1499.5314	1533.4514	1550.9775
	1	-2.991470000	2.137257000	-0.058695000				1620.2856	1646.1549	1663.8952
	1	-2.993246000	-2.151178000	-0.044137000				1675.2069	1703.3624	3187.7993
	1	1.590989000	3.388780000	-0.028966000				3191.0621	3192.0640	3194.2427
	1	4.959839000	0.012427000	0.030863000				3200.0904	3208.7595	3210.0951
	1	3.736248000	-2.131724000	0.012456000				3218.7565	3220.5665	3875.4580
	8	-4.487233000	-0.084248000	-0.130655000						
	1	-4.890612000	0.767160000	0.058696000						
TS9 (C ₁)	6	2.704785000	2.015182000	-0.045310000	0.68807 0.48318 0.28450	-690.477537	0.214234	-1209.9175	63.6084	72.6567
	6	2.732452000	0.629245000	-0.081902000				99.8624	151.8411	171.6121
	6	1.541598000	-0.094293000	-0.070339000				223.0300	252.1397	259.5891
	6	0.300326000	0.591275000	-0.023743000				339.4130	372.2323	405.5131
	6	0.286490000	2.006357000	0.011561000				427.8809	477.3989	501.6539
	6	1.498472000	2.697017000	0.000957000				507.4771	513.8726	518.2101
	6	1.490711000	-1.522073000	-0.108146000				548.2246	570.0155	595.2906
	6	-0.922344000	-0.138588000	-0.013916000				629.7556	689.7525	707.1127
	6	-0.913071000	-1.555296000	-0.046589000				739.5634	752.0130	785.8587
	6	0.356456000	-2.237239000	-0.084228000				803.4730	806.8178	822.1152
	6	-2.123288000	-2.246771000	-0.036363000				861.9276	873.7642	880.7159
	1	-2.113384000	-3.328804000	-0.062496000				914.8697	946.5733	955.1711
	6	-3.326880000	-1.559429000	0.006579000				1002.4219	1011.4263	1016.6212
	6	-3.345340000	-0.174006000	0.039923000				1022.1043	1022.5205	1091.7995
	6	-2.156259000	0.555226000	0.030809000				1101.9588	1123.3067	1126.3626
	6	-2.140880000	1.991746000	0.065125000				1158.6699	1192.4431	1201.6150
	6	-0.981387000	2.681087000	0.056144000				1234.4357	1241.8920	1258.6779
	1	-0.983747000	3.763439000	0.082069000				1268.6342	1294.0114	1319.8545
	1	-3.089934000	2.511610000	0.098711000				1356.5639	1398.1868	1408.8042
	1	2.549050000	-2.101264000	-0.167262000				1453.5671	1462.0418	1473.0414
	1	3.633332000	2.569211000	-0.054992000				1490.7160	1547.3591	1550.2926
	1	3.670468000	0.091056000	-0.121758000				1624.8578	1653.8026	1662.9171
	1	1.486562000	3.779224000	0.028100000				1676.3065	1703.0484	3192.0392
	1	0.371789000	-3.319678000	-0.100375000				3195.6432	3196.9873	3201.4848
	1	-4.258044000	-2.109203000	0.013815000				3202.8969	3206.8930	3209.9647
	1	-4.288090000	0.356999000	0.073455000				3220.4066	3221.5748	3798.8474

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TS10 (C ₁)	8	3.677388000	-2.668873000	0.115793000						
	1	3.591852000	-2.698243000	1.081026000						
	6	2.910343000	1.359697000	-0.068308000	0.84870	-690.477427	0.214194	-1235.2828	60.8904	73.5175
	6	2.648584000	0.006795000	-0.100727000	0.41220			101.7158	159.5455	169.9198
	6	1.369265000	-0.528674000	-0.072311000	0.27806			217.7672	247.4673	265.7358
	6	0.283000000	0.383689000	-0.032521000				349.4752	371.4997	409.3672
	6	0.527081000	1.779199000	-0.013762000				422.9121	470.3025	497.2633
	6	1.841656000	2.246734000	-0.032194000				507.8580	518.6489	525.2696
	6	1.102688000	-1.940044000	-0.089467000				544.2674	568.0639	597.1337
	6	-1.050461000	-0.111226000	-0.008196000				621.4954	703.7968	705.4875
	6	-1.288733000	-1.507105000	-0.023912000				732.9063	745.7560	782.8454
	6	-0.164683000	-2.401697000	-0.065852000				793.4843	820.9084	836.7208
	6	-2.604416000	-1.968973000	0.000382000				842.6540	859.8407	882.7270
	1	-2.788447000	-3.035672000	-0.012113000				886.0206	946.2450	986.4973
	6	-3.666314000	-1.078378000	0.039432000				989.3931	1012.8281	1019.8779
	6	-3.438800000	0.289107000	0.055352000				1025.9355	1028.1457	1086.9345
	6	-2.138842000	0.793692000	0.032067000				1109.8219	1125.2532	1140.9561
	6	-1.863413000	2.203817000	0.048331000				1167.2778	1184.2918	1203.2027
	6	-0.598381000	2.672027000	0.027234000				1217.8123	1247.7834	1265.3333
	1	-0.405610000	3.737230000	0.040400000				1272.7928	1284.8714	1322.4679
	1	-2.702073000	2.887897000	0.078239000				1354.6564	1399.8529	1423.5330
	1	1.948164000	-2.614639000	-0.124943000				1445.0161	1459.1462	1472.9759
	1	3.928637000	1.722908000	-0.081893000				1500.4180	1537.5238	1549.6892
	1	3.577212000	-0.767732000	-0.161976000				1615.3161	1650.8750	1659.5290
	1	2.024567000	3.313690000	-0.017776000				1676.7886	1707.2640	3190.3459
	1	-0.360469000	-3.466426000	-0.080780000				3193.7945	3194.7772	3196.7711
	1	-4.680388000	-1.453563000	0.057697000				3200.4762	3208.2320	3213.4390
	1	-4.271813000	0.979814000	0.086312000				3219.1384	3219.4645	3800.2114
	8	4.504481000	-1.617955000	0.119636000						
	1	4.482920000	-1.551825000	1.086461000						
TS11 (C ₁)	6	3.003925000	-0.000002000	-0.105383000	1.01328	-690.476477	0.214019	-1236.5507	51.9616	55.1580
	6	2.352395000	-1.213921000	-0.081718000	0.34827			117.5977	150.7245	202.7742
	6	0.955032000	-1.229544000	-0.051584000	0.25971			215.0813	249.1931	264.4769
	6	0.250069000	-0.000001000	-0.035768000				349.1273	361.6324	402.1305
	6	0.955034000	1.229542000	-0.051583000				454.7422	461.8372	505.3622
	6	2.352398000	1.213917000	-0.081716000				508.3042	517.7733	536.8149
	6	0.209562000	-2.457585000	-0.034491000				536.8760	549.5291	588.2346
	6	-1.173187000	0.000000000	-0.002019000				612.6786	699.2324	703.5880

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	6	-1.882468000	-1.225699000	0.014809000				733.5813	750.9709	778.4994
	6	-1.138934000	-2.454751000	-0.002720000				787.6718	824.9267	830.8939
	6	-3.276519000	-1.203381000	0.047528000				848.5701	882.2634	884.8379
	1	-3.817965000	-2.140700000	0.060263000				912.1315	920.5485	944.5738
	6	-3.964495000	0.000002000	0.063615000				986.6295	1009.1015	1014.0569
	6	-3.276517000	1.203384000	0.047527000				1018.8767	1021.3242	1092.9867
	6	-1.882466000	1.225701000	0.014809000				1106.0148	1118.6747	1137.7105
	6	-1.138931000	2.454751000	-0.002721000				1159.6328	1168.9638	1205.0216
	6	0.209565000	2.457584000	-0.034491000				1221.6892	1245.1362	1259.0480
	1	0.759372000	3.389921000	-0.048290000				1272.9315	1300.4187	1323.0544
	1	-1.690451000	3.386358000	0.009868000				1361.1854	1394.0395	1419.3494
	1	0.759368000	-3.389923000	-0.048290000				1450.5257	1460.7894	1469.0676
	1	4.209412000	-0.000009000	-0.158749000				1502.0225	1534.7889	1550.0165
	1	2.905879000	-2.143763000	-0.094654000				1609.7139	1655.4770	1657.4972
	1	2.905882000	2.143759000	-0.094652000				1679.2856	1707.3119	3192.4262
	1	-1.690456000	-3.386356000	0.009869000				3192.4640	3195.0882	3201.3804
	1	-5.045572000	0.000003000	0.088840000				3205.6936	3206.1666	3210.1068
	1	-3.817962000	2.140703000	0.060262000				3210.3890	3220.3350	3802.7225
	8	5.472239000	0.000005000	0.113695000						
	1	5.417806000	-0.000017000	1.081408000						
PC1 (C ₁)	6	2.556938000	2.091982000	-0.000271000	0.71563 0.43240 0.26987	-690.498744	0.218985	-6.8386	52.9644	74.3776
	6	2.643312000	0.707547000	-0.000414000				96.8243	100.6833	149.0704
	6	1.479888000	-0.060312000	-0.000335000				182.0525	219.1858	251.3251
	6	0.207147000	0.575235000	-0.000112000				255.8282	263.7233	356.4814
	6	0.139081000	1.988837000	0.000028000				403.6569	407.7354	461.8489
	6	1.324192000	2.725421000	-0.000053000				496.7225	506.6999	511.6052
	6	1.446639000	-1.478999000	-0.000462000				516.5652	547.1103	558.2437
	6	-0.987530000	-0.202594000	-0.000040000				593.7517	608.9912	683.9118
	6	-0.930092000	-1.620003000	-0.000181000				702.4523	742.8539	745.2942
	6	0.367648000	-2.259458000	-0.000384000				783.4826	809.3190	811.1642
	6	-2.114914000	-2.352727000	-0.000114000				831.9781	848.4573	876.8867
	1	-2.067261000	-3.434058000	-0.000222000				890.3544	942.4767	959.5317
	6	-3.342666000	-1.707251000	0.000094000				985.2946	1011.2551	1017.2466
	6	-3.410081000	-0.323642000	0.000236000				1021.1783	1024.4122	1101.8231
	6	-2.246496000	0.446466000	0.000172000				1112.7591	1123.1334	1155.4422
	6	-2.285602000	1.882882000	0.000316000				1185.0900	1199.3132	1225.2796
	6	-1.153388000	2.615923000	0.000248000				1239.8561	1262.4143	1267.4653
	1	-1.196818000	3.697706000	0.000355000				1310.5246	1350.4324	1374.5794

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	E_{elec}^{0K} (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
	1	-3.254200000	2.366516000	0.000480000				1398.9790	1449.8392	1459.6948
	1	3.954147000	-2.278521000	-0.756509000				1468.4110	1477.3017	1544.2076
	1	3.462764000	2.682416000	-0.000333000				1551.7017	1617.3158	1623.7044
	1	3.603621000	0.208871000	-0.000579000				1646.3617	1661.4328	1676.7216
	1	1.269113000	3.806628000	0.000055000				1701.1685	3189.9934	3191.5791
	1	0.423235000	-3.341260000	-0.000502000				3195.8438	3196.9611	3202.6548
	1	-4.253810000	-2.289718000	0.000146000				3209.4577	3210.9786	3220.1896
	1	-4.370862000	0.174950000	0.000398000				3223.3124	3850.9510	3943.2705
	8	4.538817000	-2.186475000	0.000699000						
	1	3.955090000	-2.277567000	0.758747000						
PC2 (C ₁)	6	-2.707206000	1.795850000	-0.000559000	0.77796 0.40691 0.26750	-690.498079	0.218901	-8.6825	35.4484	52.9670
	6	-2.587086000	0.432522000	-0.000775000				95.7561	99.3196	151.8289
	6	-1.411103000	-0.286019000	-0.000708000				166.5684	216.6776	247.0064
	6	-0.217511000	0.488706000	-0.000316000				253.6322	263.4486	361.5305
	6	-0.285346000	1.905163000	-0.000056000				409.6295	410.5303	462.1210
	6	-1.528984000	2.538852000	-0.000179000				494.2337	502.3741	510.2501
	6	-1.323911000	-1.720674000	-0.000973000				522.5668	546.0916	548.9551
	6	1.044028000	-0.168550000	-0.000168000				587.6181	607.8477	701.5657
	6	1.105508000	-1.583618000	-0.000414000				702.2621	733.4513	745.7259
	6	-0.121262000	-2.332190000	-0.000821000				783.1781	804.5507	809.5284
	6	2.353495000	-2.206168000	-0.000239000				835.0672	848.7328	874.5497
	1	2.402458000	-3.287539000	-0.000422000				885.8101	944.4984	973.4797
	6	3.518642000	-1.454891000	0.000172000				980.8684	1011.7837	1014.9587
	6	3.464330000	-0.069554000	0.000412000				1017.6072	1029.5044	1105.9079
	6	2.237614000	0.593756000	0.000247000				1121.8807	1134.6805	1164.5637
	6	2.141146000	2.027310000	0.000490000				1179.1561	1201.6994	1210.7128
	6	0.944257000	2.649490000	0.000343000				1247.4447	1266.7288	1272.6727
	1	0.886720000	3.730569000	0.000535000				1321.6283	1343.1812	1396.1339
	1	3.058932000	2.601494000	0.000804000				1409.5752	1441.1746	1454.8920
	1	-2.244686000	-2.288923000	-0.001255000				1466.0351	1492.6101	1516.5366
	1	-3.671452000	2.285945000	-0.000631000				1548.2062	1614.8231	1617.8167
	1	-4.549971000	-1.311250000	0.758161000				1641.3666	1662.1032	1675.1117
	1	-1.572535000	3.620784000	0.000022000				1705.3316	3191.8858	3194.7143
	1	-0.058831000	-3.413029000	-0.000995000				3195.1714	3197.2511	3201.9946
	1	4.478172000	-1.953649000	0.000310000				3209.7421	3211.6516	3217.1711
	1	4.377629000	0.511605000	0.000734000				3219.9597	3849.5702	3941.6969
	8	-4.788293000	-1.855368000	0.002640000						
	1	-4.559758000	-1.312971000	-0.757113000						

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PC3 (C ₁)	6	2.893154000	0.596570000	-0.000100000	0.98380	-690.498107	0.219070	14.4382	41.3264	88.0208
	6	2.479798000	-0.707438000	-0.000103000	0.33303			100.0216	105.4034	149.5462
	6	1.097098000	-0.939607000	-0.000071000	0.24909			185.7239	216.7513	249.1484
	6	0.207769000	0.165653000	-0.000035000	265.0363			274.9306	365.1577	
	6	0.706715000	1.494069000	-0.000031000	400.4767			415.4606	461.5724	
	6	2.092288000	1.705249000	-0.000064000	504.9619			506.2403	509.4145	
	6	0.554275000	-2.269271000	-0.000074000	525.8712			537.3511	546.9296	
	6	-1.198322000	-0.059733000	-0.000002000	582.9659			606.8709	698.4720	
	6	-1.705847000	-1.382083000	-0.000006000	701.3907			732.3438	753.1506	
	6	-0.778383000	-2.478406000	-0.000043000	785.5014			800.7468	827.3466	
	6	-3.086340000	-1.580939000	0.000026000	836.3443			836.5875	884.9537	
	1	-3.472132000	-2.592434000	0.000022000	897.7143			913.4826	949.3413	
	6	-3.956970000	-0.502411000	0.000062000	995.9054			1012.1889	1017.1087	
	6	-3.467448000	0.794511000	0.000066000	1019.3872			1022.1924	1098.2347	
	6	-2.094180000	1.037313000	0.000035000	1116.2034			1133.9787	1152.1770	
	6	-1.556249000	2.368843000	0.000038000	1170.8575			1205.4368	1215.3820	
	6	-0.225196000	2.587069000	0.000008000	1258.1580			1263.3155	1274.0880	
	1	0.168791000	3.595304000	0.000011000	1316.4668			1359.4348	1380.5981	
	1	-2.249376000	3.200649000	0.000067000	1420.4565			1440.4604	1459.6760	
	1	1.244602000	-3.102936000	-0.000102000	1464.1282			1501.5472	1537.9524	
	1	5.396516000	-0.130052000	-0.757561000	1548.6570			1579.9211	1620.3472	
	1	3.180538000	-1.533163000	-0.000126000	1649.6407			1659.1754	1683.1101	
	1	2.490301000	2.711943000	-0.000065000	1707.2226			3191.0513	3191.7043	
	1	-1.176486000	-3.485296000	-0.000046000	3193.7291			3197.0312	3198.1558	
	1	-5.024636000	-0.673701000	0.000086000	3200.0551			3208.9283	3209.7434	
	1	-4.150339000	1.634518000	0.000094000	3219.3553			3852.1662	3944.3098	
	8	5.802873000	-0.558879000	0.000193000						
	1	5.396256000	-0.130139000	0.757856000						
P1 (C _s)	6	-3.217009000	-1.149748000	0.000012000	0.75382	-689.981249	0.213434	89.3635	130.0755	170.9351
	6	-2.875549000	0.195236000	0.000041000	0.53104			235.2698	256.5123	313.6507
	6	-1.536385000	0.576603000	0.000022000	0.31156			325.9044	358.2824	383.8488
	6	-0.522424000	-0.410559000	-0.000008000	398.6533			441.7094	444.3091	
	6	-0.883727000	-1.779607000	-0.000024000	503.5020			508.3679	524.1503	
	6	-2.235104000	-2.126494000	-0.000024000	528.9669			569.7983	594.0103	
	6	-1.136346000	1.962186000	0.000008000	611.7447			627.9202	675.3275	
	6	0.851228000	-0.038137000	-0.000011000	707.2255			730.7914	751.4286	
	6	1.207464000	1.332245000	-0.000038000	790.1767			802.9325	804.1081	
	6	0.167255000	2.319609000	-0.000065000	841.5773			852.0782	875.1198	

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	6	2.559030000	1.676987000	-0.000013000			887.0884	933.7073	951.0263
	1	2.837558000	2.723091000	-0.000024000			961.8123	1008.7440	1013.7485
	6	3.539987000	0.696186000	0.000032000			1019.7900	1023.5077	1090.4850
	6	3.197774000	-0.646341000	0.000037000			1103.7896	1125.1008	1155.3845
	6	1.857064000	-1.033062000	0.000015000			1171.5421	1202.4108	1206.9238
	6	1.460210000	-2.413906000	0.000008000			1209.7573	1253.4865	1262.8848
	6	0.158604000	-2.768414000	-0.000022000			1269.8488	1315.4409	1337.6888
	1	-0.128182000	-3.812442000	-0.000045000			1362.9832	1406.2901	1442.4782
	1	2.236450000	-3.168692000	0.000025000			1460.1468	1469.3442	1479.3329
	1	-4.259713000	-1.436241000	0.000018000			1521.9182	1555.0635	1557.6839
	1	-3.640934000	0.957294000	0.000090000			1627.2848	1662.7485	1665.6104
	1	-2.508528000	-3.174090000	-0.000051000			1686.5754	1715.3938	3180.8374
	1	0.445087000	3.367761000	-0.000191000			3191.1052	3194.3921	3196.7640
	1	4.582581000	0.983935000	0.000065000			3201.5351	3209.1513	3215.8363
	1	3.967533000	-1.407228000	0.000058000			3219.2247	3236.7465	3876.4423
	8	-2.159755000	2.857382000	0.000007000					
	1	-1.806234000	3.750852000	0.000185000					
P2 (C _s)	6	-3.129469000	0.887520000	-0.000011000	-689.980036	0.213215	88.2844	118.5844	198.0886
	6	-2.726452000	-0.440437000	-0.000005000			217.4738	263.0774	273.2519
	6	-1.367319000	-0.775925000	0.000005000			320.8435	355.0337	391.8849
	6	-0.414115000	0.268496000	0.000003000			423.9647	440.7834	458.6723
	6	-0.827168000	1.623969000	0.000006000			490.3090	509.4773	525.4112
	6	-2.190721000	1.905641000	0.000002000			528.3623	557.4498	560.3834
	6	-0.921250000	-2.139124000	0.000014000			616.1726	637.1809	703.5191
	6	0.974734000	-0.048037000	0.000000000			705.3518	718.5606	741.3830
	6	1.393913000	-1.401118000	0.000002000			780.3442	785.1713	819.0915
	6	0.396285000	-2.433495000	0.000012000			837.0011	855.8032	870.2856
	6	2.759636000	-1.688945000	-0.000004000			884.2324	920.8486	938.5762
	1	3.079632000	-2.722994000	-0.000001000			966.2480	997.2040	1008.0550
	6	3.696090000	-0.667961000	-0.000009000			1013.3040	1019.6956	1091.3436
	6	3.292688000	0.658877000	-0.000006000			1127.1261	1129.1938	1147.7635
	6	1.938503000	0.991445000	-0.000002000			1170.0958	1194.7034	1206.1897
	6	1.486930000	2.355974000	0.000003000			1237.2730	1250.0701	1269.3412
	6	0.171648000	2.654957000	0.000008000			1272.5330	1306.2314	1334.7572
	1	-0.158376000	3.686267000	0.000013000			1374.4900	1410.0432	1439.8098
	1	2.231373000	3.141783000	0.000006000			1446.8066	1464.5535	1478.4636
	1	-1.664946000	-2.922607000	0.000022000			1505.8953	1550.1636	1569.1369
	1	-4.187210000	1.122958000	-0.000033000			1626.9458	1664.8192	1670.9868

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	1	-2.519253000	2.936973000	0.000001000				1679.7997	1709.2650	3184.3214
	1	0.727617000	-3.464126000	0.000023000				3191.2251	3194.3611	3199.3170
	1	4.750772000	-0.907395000	-0.000016000				3202.1741	3207.4170	3209.6611
	1	4.029276000	1.452123000	-0.000006000				3218.7068	3233.5804	3882.7319
	8	-3.622023000	-1.464907000	-0.000044000						
	1	-4.516304000	-1.114755000	0.000240000						
P3 (C _s)	6	-3.153111000	0.017198000	-0.000060000	1.01945	-689.979802	0.212969	75.6476	151.6790	183.9678
	6	-2.472391000	-1.191748000	-0.000012000	0.40245			218.2379	249.1962	269.8043
	6	-1.078563000	-1.216732000	-0.000014000	0.28854			342.7249	355.1875	373.9000
	6	-0.362793000	0.003555000	-0.000017000				405.5372	422.2199	479.2857
	6	-1.071499000	1.230757000	-0.000041000				508.6814	509.9972	516.4659
	6	-2.462193000	1.221100000	-0.000030000				541.8922	557.2128	574.6911
	6	-0.338471000	-2.448482000	0.000004000				577.8974	633.5113	642.3311
	6	1.058676000	-0.002112000	-0.000010000				701.9880	733.1431	778.3284
	6	1.763433000	-1.230064000	-0.000012000				780.3567	782.7667	821.3573
	6	1.011187000	-2.453300000	0.000005000				834.1850	844.7031	881.6412
	6	3.158432000	-1.213229000	0.000000000				888.3106	910.2982	942.5767
	1	3.696341000	-2.152849000	0.000008000				1005.3202	1006.4309	1012.0907
	6	3.851402000	-0.012905000	0.000023000				1015.4698	1016.0637	1024.0877
	6	3.166402000	1.193333000	0.000010000				1112.1357	1136.0284	1148.9571
	6	1.772696000	1.220822000	-0.000005000				1164.8345	1191.6866	1202.2467
	6	1.029126000	2.450716000	0.000023000				1208.1555	1240.8527	1263.2719
	6	-0.319748000	2.457057000	0.000005000				1272.7948	1335.0852	1347.4346
	1	-0.865905000	3.391686000	0.000046000				1364.3240	1410.4159	1430.9361
	1	1.581911000	3.381812000	0.000046000				1459.6050	1472.4529	1492.0751
	1	-0.891004000	-3.379584000	0.000014000				1504.9646	1549.1657	1556.3890
	1	-3.024450000	-2.125213000	-0.000067000				1631.8589	1662.7062	1674.6240
	1	-3.022417000	2.146494000	-0.000042000				1684.0504	1710.7256	3179.2710
	1	1.556041000	-3.389047000	0.000001000				3189.8139	3191.0030	3193.4279
	1	4.932744000	-0.016568000	0.000036000				3199.4292	3207.6693	3209.0496
	1	3.711560000	2.128764000	0.000030000				3214.6904	3219.7712	3881.3678
	8	-4.513383000	0.082793000	0.000023000						
	1	-4.883263000	-0.803640000	0.000531000						
P4 (C _s)	6	3.520684000	-0.108889000	-0.000184000	1.04980	-614.135517	0.195828	96.4759	150.4939	216.5043
	6	2.814006000	-1.301848000	-0.000323000	0.56069			248.0052	263.3750	355.0368
	6	1.420408000	-1.288647000	-0.000255000	0.36549			400.7233	407.6627	460.9825
	6	0.724444000	-0.048727000	-0.000042000				495.2079	506.4333	510.7008
	6	1.460404000	1.160552000	0.000098000				515.0658	547.0770	556.6464

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	6	2.854667000	1.106867000	0.000024000				594.1193	608.0862	682.2470
	6	0.604029000	-2.448940000	-0.000386000				701.9716	742.2339	742.4898
	6	-0.700487000	-0.024133000	0.000030000				779.3152	802.5909	811.2496
	6	-1.444665000	-1.231772000	-0.000113000				831.4716	843.2679	874.2634
	6	-0.727030000	-2.487599000	-0.000331000				888.6216	936.8272	945.3944
	6	-2.837013000	-1.174748000	-0.000037000				985.8960	1008.2048	1012.3648
	1	-3.402648000	-2.097508000	-0.000147000				1017.4345	1021.1765	1099.0388
	6	-3.493431000	0.047127000	0.000175000				1113.5411	1120.2553	1154.5277
	6	-2.775524000	1.231977000	0.000315000				1183.6182	1199.0198	1222.7201
	6	-1.380312000	1.218491000	0.000245000				1239.5405	1263.0323	1266.4295
	6	-0.607963000	2.430311000	0.000385000				1310.3843	1348.1366	1375.0891
	6	0.740723000	2.403935000	0.000315000				1399.6683	1449.3463	1459.1416
	1	1.310166000	3.324692000	0.000422000				1468.3622	1477.9035	1544.9004
	1	-1.139246000	3.373591000	0.000551000				1551.8582	1623.7355	1646.2695
	1	4.601823000	-0.127429000	-0.000239000				1662.3586	1675.8682	1700.9931
	1	3.330345000	-2.251827000	-0.000485000				3190.5093	3191.9191	3195.7574
	1	3.415340000	2.032879000	0.000131000				3197.1376	3202.8383	3209.6947
	1	-1.286282000	-3.415211000	-0.000444000				3210.8642	3219.9874	3224.5654
	1	-4.574523000	0.074182000	0.000232000						
	1	-3.292617000	2.182896000	0.000481000						
P5 (C _s)	6	-3.549551000	0.165477000	0.000016000	1.03016 0.56894 0.36652	-614.134818	0.195915	96.9952	153.7686	210.7916
	6	-2.767791000	1.288663000	0.000003000				252.7932	261.8101	360.2830
	6	-1.390427000	1.318537000	-0.000006000				408.9913	410.4897	461.7888
	6	-0.740922000	0.053405000	-0.000006000				494.4694	500.2994	508.9002
	6	-1.506012000	-1.140152000	-0.000003000				521.3651	542.7649	547.9889
	6	-2.900004000	-1.066777000	0.000009000				587.1562	607.6906	700.4353
	6	-0.598317000	2.517052000	-0.000012000				701.4949	731.0979	745.3836
	6	0.680570000	-0.005632000	-0.000005000				781.0442	804.4727	808.3749
	6	1.439561000	1.190548000	0.000001000				834.7113	840.6412	872.8949
	6	0.749105000	2.451190000	-0.000006000				883.0410	940.8676	972.9912
	6	2.831849000	1.108246000	0.000010000				980.5072	1008.7986	1013.1268
	1	3.413559000	2.021156000	0.000016000				1015.0000	1017.6519	1105.5027
	6	3.467381000	-0.123962000	0.000012000				1120.1183	1134.2505	1164.4523
	6	2.729761000	-1.297725000	0.000004000				1173.0947	1200.9943	1209.5024
	6	1.335419000	-1.261584000	-0.000004000				1246.0612	1266.5501	1272.1174
	6	0.536851000	-2.456102000	-0.000010000				1321.4394	1341.6499	1396.2169
	6	-0.811063000	-2.398165000	-0.000008000				1407.8606	1441.2978	1455.0566
	1	-1.399887000	-3.306692000	-0.000012000				1465.4612	1493.7850	1516.6046

Species	Cartesian coordinate (Å)				Rotational constants (GHz)	$E_{elec}^{0\text{ K}}$ (Hartree)	ZPE (Hartree)	Unscaled vibrational frequencies (cm ⁻¹)		
	1	1.045838000	-3.411564000	-0.000015000				1548.1199	1614.8595	1641.2990
	1	-1.111933000	3.468650000	-0.000025000				1662.1196	1674.9941	1705.5479
	1	-4.629684000	0.222302000	0.000033000				3191.6173	3193.3873	3194.5029
	1	-3.478080000	-1.982497000	0.000014000				3196.6334	3201.5366	3209.6112
	1	1.342011000	3.357050000	-0.000007000				3211.2483	3219.0997	3219.4795
	1	4.547859000	-0.169752000	0.000020000						
	1	3.231852000	-2.256771000	0.000004000						
P6 (C _{2v})	6	-3.486581000	0.000036000	0.000164000	1.01614 0.57844 0.36861	-614.135514	0.195658	99.1492	147.7314	212.8605
	6	-2.867202000	-1.219356000	0.000162000				245.0583	272.8436	362.8209
	6	-1.465767000	-1.231766000	0.000097000				395.3927	413.3424	460.5304
	6	-0.761942000	0.000015000	0.000036000				503.9356	504.5429	508.5703
	6	-1.465735000	1.231684000	0.000043000	523.5407			533.4406	546.4702	
	6	-2.867399000	1.219313000	0.000108000	579.9993			605.8168	693.1212	
	6	-0.718426000	-2.458520000	0.000088000	699.7161			728.7729	752.6941	
	6	0.662096000	0.000013000	-0.000031000	779.1626			799.5831	820.0155	
	6	1.373002000	-1.225200000	-0.000039000	826.0399			835.7175	883.7820	
	6	0.630527000	-2.454583000	0.000023000	891.4477			898.5282	942.5240	
	6	2.767505000	-1.202867000	-0.000106000	994.9716			1007.6163	1011.2243	
	1	3.308620000	-2.140535000	-0.000111000	1017.0968			1017.5414	1094.4215	
	6	3.456368000	0.000049000	-0.000164000	1114.6436			1133.1835	1150.6006	
	6	2.767527000	1.202923000	-0.000157000	1167.8923			1204.3379	1212.4906	
	6	1.372970000	1.225237000	-0.000091000	1257.1430			1261.4383	1272.8870	
	6	0.630487000	2.454553000	-0.000083000	1314.6847			1358.7458	1379.1444	
	6	-0.718510000	2.458414000	-0.000019000	1418.0308			1438.6096	1458.3206	
	1	-1.267436000	3.391431000	-0.000013000	1462.1865			1500.3180	1535.3535	
	1	1.182803000	3.385851000	-0.000129000	1548.7026			1580.4501	1650.0796	
	1	-1.267385000	-3.391511000	0.000136000	1657.5439			1681.0765	1705.5237	
	1	-3.419889000	-2.150326000	0.000209000	3191.5809			3191.6067	3194.4072	
	1	-3.419513000	2.150614000	0.000114000	3195.9621			3197.3454	3200.6164	
	1	1.182911000	-3.385841000	0.000017000	3209.3482			3209.6128	3220.0852	
	1	4.537740000	0.000041000	-0.000215000						
	1	3.308623000	2.140601000	-0.000203000						

Frequencies in the parentheses (“()”) are collected from experimental works.

Table S2: Calculated total rate constants, k_{tot} , of the Pyrene + OH $\rightarrow$ products over the range of temperature 200 – 2000 K at different pressures, e.g., $P = 7.6 - 76000$ Torr, including the HIR treatments, Eckart quantum tunneling effects. Units are in $\text{cm}^3/\text{molecule/s}$. $k_{\text{tot}}(T, P)$ values at different pressures are fitted as the double modified Arrhenius formats based on the ROCBS-QB3//M06-2X PES.

<i>T</i> (K)	7.6 Torr	76 Torr	760 Torr	7600 Torr	76000 Torr
200	2.70E-10	2.71E-10	2.75E-10	3.03E-10	3.46E-10
240	1.74E-10	1.74E-10	1.77E-10	2.00E-10	2.59E-10
250	1.51E-10	1.51E-10	1.54E-10	1.73E-10	2.31E-10
275	1.01E-10	1.02E-10	1.03E-10	1.15E-10	1.62E-10
298	6.80E-11	6.80E-11	6.88E-11	7.56E-11	1.09E-10
300	6.56E-11	6.56E-11	6.63E-11	7.29E-11	1.05E-10
325	4.17E-11	4.18E-11	4.21E-11	4.57E-11	6.61E-11
340	3.18E-11	3.18E-11	3.21E-11	3.46E-11	4.99E-11
400	1.15E-11	1.15E-11	1.16E-11	1.23E-11	1.74E-11
500	3.87E-12	3.88E-12	3.88E-12	4.02E-12	5.09E-12
600	3.77E-12	3.77E-12	3.78E-12	3.79E-12	4.07E-12
700	5.73E-12	5.73E-12	5.71E-12	5.73E-12	5.84E-12
800	8.94E-12	8.94E-12	8.95E-12	8.97E-12	8.98E-12
900	1.34E-11	1.34E-11	1.34E-11	1.34E-11	1.34E-11
1000	1.92E-11	1.91E-11	1.91E-11	1.91E-11	1.92E-11
1100	2.64E-11	2.64E-11	2.64E-11	2.64E-11	2.64E-11
1200	3.52E-11	3.52E-11	3.53E-11	3.52E-11	3.53E-11
1300	4.57E-11	4.58E-11	4.58E-11	4.59E-11	4.58E-11
1400	5.82E-11	5.81E-11	5.82E-11	5.82E-11	5.82E-11
1500	7.25E-11	7.25E-11	7.24E-11	7.24E-11	7.25E-11
1600	8.89E-11	8.89E-11	8.89E-11	8.89E-11	8.88E-11
1700	1.07E-10	1.07E-10	1.07E-10	1.07E-10	1.07E-10
1800	1.28E-10	1.28E-10	1.28E-10	1.28E-10	1.28E-10
1900	1.51E-10	1.51E-10	1.51E-10	1.51E-10	1.51E-10
2000	1.76E-10	1.76E-10	1.76E-10	1.76E-10	1.76E-10

- $k(T) = 4.62 \times 10^{25} \times T^{-13.11} \times \exp[-2334.3 \text{ K}/T] + 3.90 \times 10^{-21} \times T^{3.23} \times \exp[-33.4 \text{ K}/T]$
($\text{cm}^3/\text{molecule/s}$) ($T = 200 - 2000 \text{ K}$ & $P = 7.6 \text{ Torr}$; error $\sim 1.4 \%$).
- $k(T) = 5.45 \times 10^{25} \times T^{-13.13} \times \exp[-2339.8 \text{ K}/T] + 3.39 \times 10^{-21} \times T^{3.25} \times \exp[-13.7 \text{ K}/T]$
($\text{cm}^3/\text{molecule/s}$) ($T = 200 - 2000 \text{ K}$ & $P = 76 \text{ Torr}$; error $\sim 1.4 \%$).
- $k(T) = 6.10 \times 10^{25} \times T^{-13.15} \times \exp[-2340.9 \text{ K}/T] + 3.59 \times 10^{-21} \times T^{3.24} \times \exp[-21.6 \text{ K}/T]$
($\text{cm}^3/\text{molecule/s}$) ($T = 200 - 2000 \text{ K}$ & $P = 760 \text{ Torr}$; error $\sim 1.4 \%$).
- $k(T) = 2.59 \times 10^{27} \times T^{-13.71} \times \exp[-2474.4 \text{ K}/T] + 1.38 \times 10^{-21} \times T^{3.36} \times \exp[119.7 \text{ K}/T]$
($\text{cm}^3/\text{molecule/s}$) ($T = 200 - 2000 \text{ K}$ & $P = 7600 \text{ Torr}$; error $\sim 1.8 \%$).

- $k(T) = 6.01 \times 10^{31} \times T^{-15.13} \times \exp[-2958.1 \text{ K}/T] + 1.04 \times 10^{-22} \times T^{3.68} \times \exp[509.6 \text{ K}/T]$
(cm³/molecule/s) ($T = 200 - 2000 \text{ K}$ & $P = 76000 \text{ Torr}$; error $\sim 2.1 \%$).

Table S3: The calculated Eckart tunneling factor via tight transition state channels over the wide temperature range of 200 – 2000 K based on the ROCBS-QB3//M06-2X PES.

T (K)	via TS1	via TS2	via TS3	via TS4	via TS5	via TS6	via TS7	via TS8	via TS9	via TS10	via TS11
200	1.12	1.19	1.66	1.95	1.95	22.50	15.50	50.00	13.10	14.50	17.50
240	1.07	1.13	1.42	1.58	1.58	7.65	6.13	11.80	6.45	6.96	7.76
250	1.06	1.11	1.38	1.52	1.52	6.38	5.24	9.34	5.66	6.08	6.69
275	1.05	1.09	1.31	1.41	1.42	4.47	3.84	5.92	4.32	4.59	4.93
298	1.04	1.07	1.26	1.34	1.35	3.51	3.10	4.38	3.55	3.75	3.96
300	1.04	1.07	1.25	1.34	1.34	3.44	3.05	4.28	3.50	3.69	3.89
325	1.03	1.06	1.21	1.28	1.28	2.83	2.56	3.37	2.96	3.10	3.23
340	1.02	1.05	1.19	1.26	1.26	2.57	2.36	3.00	2.72	2.84	2.95
400	1.01	1.03	1.14	1.18	1.18	1.96	1.85	2.17	2.12	2.19	2.23
500	1.00	1.01	1.09	1.12	1.12	1.53	1.48	1.63	1.66	1.70	1.71
600	1.00	1.01	1.06	1.08	1.08	1.35	1.31	1.40	1.45	1.47	1.48
700	1.00	1.00	1.05	1.06	1.06	1.25	1.22	1.29	1.33	1.34	1.35
800	1.00	1.00	1.04	1.05	1.05	1.19	1.17	1.21	1.25	1.27	1.27
900	1.00	1.00	1.03	1.04	1.04	1.15	1.13	1.17	1.20	1.21	1.21
1000	1.00	1.00	1.02	1.03	1.03	1.12	1.11	1.14	1.17	1.18	1.17
1100	1.00	1.00	1.02	1.03	1.03	1.10	1.09	1.11	1.14	1.15	1.15
1200	1.00	1.00	1.02	1.02	1.02	1.08	1.07	1.09	1.12	1.13	1.13
1300	1.00	1.00	1.01	1.02	1.02	1.07	1.06	1.08	1.11	1.11	1.11
1400	1.00	1.00	1.01	1.02	1.02	1.06	1.05	1.07	1.09	1.10	1.10
1500	1.00	1.00	1.01	1.02	1.02	1.05	1.05	1.06	1.08	1.09	1.09
1600	1.00	1.00	1.01	1.01	1.01	1.05	1.04	1.05	1.07	1.08	1.08
1700	1.00	1.00	1.01	1.01	1.01	1.04	1.04	1.05	1.07	1.07	1.07
1800	1.00	1.00	1.01	1.01	1.01	1.04	1.03	1.04	1.06	1.06	1.06
1900	1.00	1.00	1.01	1.01	1.01	1.03	1.03	1.04	1.06	1.06	1.06
2000	1.00	1.00	1.01	1.01	1.01	1.03	1.03	1.04	1.05	1.05	1.05

Table S4: Individual and total rate constants for Pyrene + OH → Products (cm³/molecule/s) at different pressures (7.6, 76, 760, 7600 and 76000 Torr) based on the ROCBS-QB3//M06-2X PES. (“Unc.” stands for the uncertainty). Units are in cm³/molecule/s.

<i>P</i> = 7.6 Torr																
<i>T</i> (K)	RC	unc.(%)	I1	unc.(%)	I2	unc.(%)	I3	unc.(%)	I4	unc.(%)	I5	unc.(%)	P1 + H	unc.(%)	P2 + H	unc.(%)
200	2.24E-16	1.20E+01	1.36E-10	2.10E-05	1.34E-10	2.10E-05	9.02E-14	3.10E-02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
240	1.68E-16	1.70E+01	8.75E-11	3.20E-05	8.64E-11	3.20E-05	7.47E-14	3.80E-02	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
250	2.80E-17	1.00E+02	7.58E-11	3.70E-05	7.50E-11	3.70E-05	6.90E-14	4.10E-02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
275	8.40E-17	3.30E+01	5.07E-11	5.50E-05	5.05E-11	5.50E-05	5.73E-14	4.90E-02	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
298	2.80E-17	1.00E+02	3.38E-11	8.30E-05	3.38E-11	8.30E-05	4.69E-14	6.00E-02	2.24E-16	1.20E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
300	2.80E-17	1.00E+02	3.26E-11	8.60E-05	3.27E-11	8.60E-05	4.64E-14	6.00E-02	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
325	2.80E-17	1.00E+02	2.06E-11	1.40E-04	2.07E-11	1.40E-04	3.66E-14	7.70E-02	1.68E-16	1.70E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
340	5.61E-17	5.00E+01	1.56E-11	1.80E-04	1.58E-11	1.80E-04	3.48E-14	8.10E-02	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
400	2.80E-17	1.00E+02	5.31E-12	5.30E-04	5.47E-12	5.10E-04	1.83E-14	1.50E-01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
500	2.81E-17	1.00E+02	1.06E-12	2.70E-03	1.14E-12	2.50E-03	4.75E-15	5.90E-01	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
600	2.82E-17	1.00E+02	2.53E-13	1.10E-02	2.98E-13	9.50E-03	6.77E-16	4.20E+00	2.82E-17	1.00E+02	2.82E-17	1.00E+02	2.82E-17	1.00E+02	2.82E-17	1.00E+02
700	2.84E-17	1.00E+02	6.35E-14	4.50E-02	1.06E-13	2.70E-02	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02
800	2.86E-17	1.00E+02	1.04E-14	2.80E-01	4.36E-14	6.60E-02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	1.15E-16	2.50E+01	8.59E-17	3.30E+01
900	2.89E-17	1.00E+02	9.84E-16	2.90E+00	1.86E-14	1.60E-01	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02	7.23E-16	4.00E+00	9.55E-16	3.00E+00
1000	2.93E-17	1.00E+02	2.93E-17	1.00E+02	3.52E-15	8.30E-01	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.35E-15	1.20E+00	1.94E-15	1.50E+00
1100	2.99E-17	1.00E+02	2.99E-17	1.00E+02	2.99E-16	1.00E+01	2.99E-17	1.00E+02	2.99E-17	1.00E+02	2.99E-17	1.00E+02	1.85E-15	1.60E+00	1.97E-15	1.50E+00
1200	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	8.83E-16	3.40E+00	7.62E-16	4.00E+00
1300	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	4.68E-16	6.70E+00	6.55E-16	4.80E+00
1400	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	1.28E-16	2.50E+01	3.21E-16	1.00E+01
1500	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	1.32E-16	2.50E+01	2.32E-16	1.40E+01
1600	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	2.05E-16	1.70E+01	2.40E-16	1.40E+01
1700	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	7.10E-17	5.00E+01
1800	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	1.85E-16	2.00E+01	7.39E-17	5.00E+01
1900	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	1.16E-16	3.30E+01	1.54E-16	2.50E+01
2000	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	2.02E-16	2.00E+01	4.03E-17	1.00E+02
<i>T</i> (K)	P3 + H	unc.(%)	P4 + H ₂ O	unc.(%)	P5 + H ₂ O	unc.(%)	P6 + H ₂ O	unc.(%)	k _{tot}							
200	2.80E-17	1.00E+02	3.09E-14	9.10E-02	2.82E-14	9.90E-02	1.00E-14	2.80E-01	2.70E-10							
240	2.80E-17	1.00E+02	5.41E-14	5.20E-02	4.87E-14	5.80E-02	1.95E-14	1.40E-01	1.74E-10							
250	2.80E-17	1.00E+02	5.94E-14	4.70E-02	5.63E-14	5.00E-02	2.40E-14	1.20E-01	1.51E-10							
275	2.80E-17	1.00E+02	8.47E-14	3.30E-02	7.43E-14	3.80E-02	3.43E-14	8.20E-02	1.01E-10							
298	2.80E-17	1.00E+02	1.11E-13	2.50E-02	1.00E-13	2.80E-02	5.15E-14	5.40E-02	6.80E-11							
300	2.80E-17	1.00E+02	1.14E-13	2.50E-02	1.05E-13	2.70E-02	4.94E-14	5.70E-02	6.56E-11							
325	2.80E-17	1.00E+02	1.46E-13	1.90E-02	1.35E-13	2.10E-02	6.94E-14	4.00E-02	4.17E-11							
340	2.80E-17	1.00E+02	1.74E-13	1.60E-02	1.58E-13	1.80E-02	8.31E-14	3.40E-02	3.18E-11							
400	2.80E-17	1.00E+02	3.00E-13	9.30E-03	2.86E-13	9.80E-03	1.60E-13	1.80E-02	1.15E-11							
500	2.81E-17	1.00E+02	6.70E-13	4.20E-03	6.21E-13	4.50E-03	3.79E-13	7.40E-03	3.87E-12							
600	2.82E-17	1.00E+02	1.27E-12	2.20E-03	1.18E-12	2.40E-03	7.65E-13	3.70E-03	3.77E-12							

700	2.84E-17	1.00E+02	2.17E-12	1.30E-03	2.02E-12	1.40E-03	1.38E-12	2.10E-03	5.73E-12							
800	2.86E-17	1.00E+02	3.42E-12	8.40E-04	3.19E-12	9.00E-04	2.28E-12	1.30E-03	8.94E-12							
900	1.74E-16	1.70E+01	5.10E-12	5.70E-04	4.79E-12	6.00E-04	3.46E-12	8.40E-04	1.34E-11							
1000	4.99E-16	5.90E+00	7.28E-12	4.00E-04	6.84E-12	4.30E-04	5.04E-12	5.80E-04	1.92E-11							
1100	3.88E-16	7.70E+00	9.97E-12	3.00E-04	9.36E-12	3.20E-04	7.05E-12	4.20E-04	2.64E-11							
1200	1.22E-16	2.50E+01	1.32E-11	2.30E-04	1.25E-11	2.40E-04	9.48E-12	3.20E-04	3.52E-11							
1300	1.25E-16	2.50E+01	1.71E-11	1.80E-04	1.62E-11	1.90E-04	1.24E-11	2.50E-04	4.57E-11							
1400	9.62E-17	3.30E+01	2.18E-11	1.50E-04	2.06E-11	1.60E-04	1.59E-11	2.00E-04	5.82E-11							
1500	3.31E-17	1.00E+02	2.70E-11	1.20E-04	2.56E-11	1.30E-04	1.99E-11	1.70E-04	7.25E-11							
1600	3.42E-17	1.00E+02	3.30E-11	1.00E-04	3.14E-11	1.10E-04	2.44E-11	1.40E-04	8.89E-11							
1700	7.10E-17	5.00E+01	3.99E-11	8.90E-05	3.79E-11	9.40E-05	2.96E-11	1.20E-04	1.07E-10							
1800	3.70E-17	1.00E+02	4.74E-11	7.80E-05	4.51E-11	8.20E-05	3.54E-11	1.00E-04	1.28E-10							
1900	3.86E-17	1.00E+02	5.57E-11	6.90E-05	5.32E-11	7.30E-05	4.18E-11	9.20E-05	1.51E-10							
2000	4.03E-17	1.00E+02	6.51E-11	6.20E-05	6.20E-11	6.50E-05	4.90E-11	8.20E-05	1.76E-10							
P = 76 Torr																
T (K)	RC	unc.(%)	I1	unc.(%)	I2	unc.(%)	I3	unc.(%)	I4	unc.(%)	I5	unc.(%)	P1 + H	unc.(%)	P2 + H	unc.(%)
200	2.10E-15	1.30E+00	1.36E-10	2.10E-05	1.34E-10	2.10E-05	8.91E-14	3.10E-02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
240	1.29E-15	2.20E+00	8.76E-11	3.20E-05	8.65E-11	3.20E-05	7.33E-14	3.80E-02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
250	7.84E-16	3.60E+00	7.59E-11	3.70E-05	7.52E-11	3.70E-05	6.90E-14	4.10E-02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
275	5.04E-16	5.60E+00	5.09E-11	5.50E-05	5.05E-11	5.50E-05	5.73E-14	4.90E-02	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
298	2.24E-16	1.20E+01	3.38E-11	8.30E-05	3.38E-11	8.30E-05	4.75E-14	5.90E-02	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
300	4.76E-16	5.90E+00	3.26E-11	8.60E-05	3.26E-11	8.60E-05	4.54E-14	6.20E-02	1.40E-16	2.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
325	1.40E-16	2.00E+01	2.06E-11	1.40E-04	2.08E-11	1.40E-04	3.72E-14	7.50E-02	1.40E-16	2.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
340	5.61E-17	5.00E+01	1.56E-11	1.80E-04	1.58E-11	1.80E-04	3.13E-14	9.00E-02	1.40E-16	2.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
400	2.81E-17	1.00E+02	5.32E-12	5.30E-04	5.46E-12	5.10E-04	1.91E-14	1.50E-01	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
500	2.81E-17	1.00E+02	1.07E-12	2.60E-03	1.14E-12	2.50E-03	7.74E-15	3.60E-01	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
600	2.83E-17	1.00E+02	2.67E-13	1.10E-02	2.86E-13	9.90E-03	1.78E-15	1.60E+00	2.83E-17	1.00E+02	2.83E-17	1.00E+02	2.83E-17	1.00E+02	2.83E-17	1.00E+02
700	2.84E-17	1.00E+02	7.56E-14	3.80E-02	8.90E-14	3.20E-02	3.41E-16	8.30E+00	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02
800	2.86E-17	1.00E+02	2.06E-14	1.40E-01	3.57E-14	8.00E-02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02
900	2.89E-17	1.00E+02	4.05E-15	7.10E-01	1.72E-14	1.70E-01	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02	1.16E-16	2.50E+01	1.74E-16	1.70E+01
1000	2.93E-17	1.00E+02	3.23E-16	9.10E+00	8.04E-15	3.60E-01	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.64E-16	1.10E+01	4.99E-16	5.90E+00
1100	2.98E-17	1.00E+02	8.95E-17	3.30E+01	2.69E-15	1.10E+00	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02	8.65E-16	3.40E+00	6.56E-16	4.50E+00
1200	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.96E-16	7.70E+00	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	8.53E-16	3.60E+00	9.14E-16	3.30E+00
1300	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	4.99E-16	6.20E+00	6.86E-16	4.50E+00
1400	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-16	1.00E+01	1.28E-16	2.50E+01
1500	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	5.29E-16	6.20E+00	3.97E-16	8.30E+00
1600	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.08E-16	1.10E+01	3.76E-16	9.10E+00
1700	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	1.42E-16	2.50E+01	3.91E-16	9.10E+00
1800	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	2.96E-16	1.20E+01	2.22E-16	1.70E+01
1900	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.09E-16	1.20E+01	4.63E-16	8.30E+00
2000	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	1.61E-16	2.50E+01	2.02E-16	2.00E+01
T (K)	P3 + H	unc.(%)	P4 + H₂O	unc.(%)	P5 + H₂O	unc.(%)	P6 + H₂O	unc.(%)	k_tot							
200	2.80E-17	1.00E+02	2.94E-14	9.50E-02	2.90E-14	9.70E-02	1.00E-14	2.80E-01	2.71E-10							
240	2.80E-17	1.00E+02	5.38E-14	5.20E-02	5.06E-14	5.50E-02	2.07E-14	1.40E-01	1.74E-10							

250	2.80E-17	1.00E+02	5.96E-14	4.70E-02	5.57E-14	5.00E-02	2.38E-14	1.20E-01	1.51E-10							
275	2.80E-17	1.00E+02	8.43E-14	3.30E-02	7.65E-14	3.70E-02	3.38E-14	8.30E-02	1.02E-10							
298	2.80E-17	1.00E+02	1.09E-13	2.60E-02	1.01E-13	2.80E-02	4.96E-14	5.70E-02	6.80E-11							
300	2.80E-17	1.00E+02	1.13E-13	2.50E-02	1.06E-13	2.60E-02	4.98E-14	5.60E-02	6.56E-11							
325	2.80E-17	1.00E+02	1.51E-13	1.90E-02	1.38E-13	2.00E-02	6.86E-14	4.10E-02	4.18E-11							
340	2.80E-17	1.00E+02	1.73E-13	1.60E-02	1.58E-13	1.80E-02	7.97E-14	3.50E-02	3.18E-11							
400	2.81E-17	1.00E+02	3.03E-13	9.30E-03	2.83E-13	9.90E-03	1.59E-13	1.80E-02	1.15E-11							
500	2.81E-17	1.00E+02	6.70E-13	4.20E-03	6.18E-13	4.60E-03	3.83E-13	7.30E-03	3.88E-12							
600	2.83E-17	1.00E+02	1.27E-12	2.20E-03	1.18E-12	2.40E-03	7.74E-13	3.70E-03	3.77E-12							
700	2.84E-17	1.00E+02	2.17E-12	1.30E-03	2.01E-12	1.40E-03	1.38E-12	2.10E-03	5.73E-12							
800	2.86E-17	1.00E+02	3.41E-12	8.40E-04	3.20E-12	8.90E-04	2.28E-12	1.30E-03	8.94E-12							
900	5.79E-17	5.00E+01	5.12E-12	5.60E-04	4.80E-12	6.00E-04	3.49E-12	8.30E-04	1.34E-11							
1000	1.17E-16	2.50E+01	7.26E-12	4.00E-04	6.83E-12	4.30E-04	5.04E-12	5.80E-04	1.91E-11							
1100	3.28E-16	9.10E+00	9.96E-12	3.00E-04	9.40E-12	3.20E-04	7.05E-12	4.20E-04	2.64E-11							
1200	1.22E-16	2.50E+01	1.32E-11	2.30E-04	1.25E-11	2.40E-04	9.47E-12	3.20E-04	3.52E-11							
1300	1.25E-16	2.50E+01	1.72E-11	1.80E-04	1.62E-11	1.90E-04	1.24E-11	2.50E-04	4.58E-11							
1400	9.62E-17	3.30E+01	2.17E-11	1.50E-04	2.06E-11	1.60E-04	1.59E-11	2.00E-04	5.81E-11							
1500	1.32E-16	2.50E+01	2.71E-11	1.20E-04	2.56E-11	1.30E-04	1.98E-11	1.70E-04	7.25E-11							
1600	6.84E-17	5.00E+01	3.31E-11	1.00E-04	3.14E-11	1.10E-04	2.45E-11	1.40E-04	8.89E-11							
1700	7.10E-17	5.00E+01	3.98E-11	8.90E-05	3.79E-11	9.40E-05	2.96E-11	1.20E-04	1.07E-10							
1800	1.11E-16	3.30E+01	4.74E-11	7.80E-05	4.52E-11	8.20E-05	3.54E-11	1.00E-04	1.28E-10							
1900	7.71E-17	5.00E+01	5.59E-11	6.90E-05	5.32E-11	7.30E-05	4.19E-11	9.20E-05	1.51E-10							
2000	2.02E-16	2.00E+01	6.51E-11	6.20E-05	6.20E-11	6.50E-05	4.90E-11	8.20E-05	1.76E-10							
P = 760 Torr																
T (K)	RC	unc.(%)	I1	unc.(%)	I2	unc.(%)	I3	unc.(%)	I4	unc.(%)	I5	unc.(%)	P1 + H	unc.(%)	P2 + H	unc.(%)
200	2.29E-14	1.20E-01	1.39E-10	2.00E-05	1.37E-10	2.10E-05	8.86E-14	3.20E-02	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
240	1.22E-14	2.30E-01	8.92E-11	3.10E-05	8.81E-11	3.20E-05	7.62E-14	3.70E-02	8.40E-17	3.30E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
250	1.03E-14	2.70E-01	7.71E-11	3.60E-05	7.64E-11	3.70E-05	6.96E-14	4.00E-02	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
275	5.21E-15	5.40E-01	5.15E-11	5.40E-05	5.12E-11	5.50E-05	5.92E-14	4.70E-02	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
298	2.97E-15	9.40E-01	3.42E-11	8.20E-05	3.42E-11	8.20E-05	4.66E-14	6.00E-02	2.52E-16	1.10E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
300	3.47E-15	8.10E-01	3.30E-11	8.50E-05	3.30E-11	8.50E-05	4.63E-14	6.10E-02	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
325	1.23E-15	2.30E+00	2.08E-11	1.30E-04	2.09E-11	1.30E-04	3.79E-14	7.40E-02	1.68E-16	1.70E+01	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
340	6.45E-16	4.30E+00	1.58E-11	1.80E-04	1.59E-11	1.80E-04	3.29E-14	8.50E-02	3.64E-16	7.70E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
400	5.61E-17	5.00E+01	5.36E-12	5.20E-04	5.49E-12	5.10E-04	1.97E-14	1.40E-01	1.40E-16	2.00E+01	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
500	2.81E-17	1.00E+02	1.07E-12	2.60E-03	1.14E-12	2.50E-03	7.76E-15	3.60E-01	1.69E-16	1.70E+01	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
600	2.82E-17	1.00E+02	2.71E-13	1.00E-02	2.87E-13	9.80E-03	3.11E-15	9.10E-01	2.82E-17	1.00E+02	2.82E-17	1.00E+02	2.82E-17	1.00E+02	2.82E-17	1.00E+02
700	2.84E-17	1.00E+02	7.86E-14	3.60E-02	8.39E-14	3.40E-02	1.05E-15	2.70E+00	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02
800	2.86E-17	1.00E+02	2.41E-14	1.20E-01	3.06E-14	9.40E-02	2.00E-16	1.40E+01	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02
900	2.89E-17	1.00E+02	8.91E-15	3.20E-01	1.27E-14	2.30E-01	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02
1000	2.93E-17	1.00E+02	2.58E-15	1.10E+00	6.63E-15	4.40E-01	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02
1100	2.98E-17	1.00E+02	6.57E-16	4.50E+00	3.64E-15	8.20E-01	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02
1200	3.05E-17	1.00E+02	6.09E-17	5.00E+01	1.89E-15	1.60E+00	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	6.09E-17	5.00E+01
1300	3.12E-17	1.00E+02	3.12E-17	1.00E+02	7.80E-16	4.00E+00	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	1.25E-16	2.50E+01	1.25E-16	2.50E+01
1400	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-16	1.00E+01	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.53E-16	9.10E+00	3.21E-16	1.00E+01
1500	3.31E-17	1.00E+02	3.31E-17	1.00E+02	1.65E-16	2.00E+01	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	9.92E-17	3.30E+01	2.65E-16	1.20E+01

1600	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	2.74E-16	1.20E+01	2.05E-16	1.70E+01
1700	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	4.26E-16	8.30E+00	2.13E-16	1.70E+01
1800	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.33E-16	1.10E+01	2.96E-16	1.20E+01
1900	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	1.93E-16	2.00E+01	1.54E-16	2.50E+01
2000	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-16	1.00E+01	2.42E-16	1.70E+01
T (K)	P3 + H	unc.(%)	P4 + H ₂ O	unc.(%)	P5 + H ₂ O	unc.(%)	P6 + H ₂ O	unc.(%)	k_tot							
200	2.80E-17	1.00E+02	2.93E-14	9.60E-02	2.79E-14	1.00E-01	9.63E-15	2.90E-01	2.75E-10							
240	2.80E-17	1.00E+02	5.20E-14	5.40E-02	5.04E-14	5.60E-02	2.10E-14	1.30E-01	1.77E-10							
250	2.80E-17	1.00E+02	5.97E-14	4.70E-02	5.59E-14	5.00E-02	2.39E-14	1.20E-01	1.54E-10							
275	2.80E-17	1.00E+02	8.42E-14	3.30E-02	7.86E-14	3.60E-02	3.51E-14	8.00E-02	1.03E-10							
298	2.80E-17	1.00E+02	1.08E-13	2.60E-02	1.01E-13	2.80E-02	4.91E-14	5.70E-02	6.88E-11							
300	2.80E-17	1.00E+02	1.14E-13	2.50E-02	1.03E-13	2.70E-02	4.92E-14	5.70E-02	6.63E-11							
325	2.80E-17	1.00E+02	1.45E-13	1.90E-02	1.41E-13	2.00E-02	6.85E-14	4.10E-02	4.21E-11							
340	2.80E-17	1.00E+02	1.67E-13	1.70E-02	1.57E-13	1.80E-02	8.38E-14	3.30E-02	3.21E-11							
400	2.81E-17	1.00E+02	3.07E-13	9.10E-03	2.82E-13	1.00E-02	1.57E-13	1.80E-02	1.16E-11							
500	2.81E-17	1.00E+02	6.61E-13	4.30E-03	6.24E-13	4.50E-03	3.83E-13	7.30E-03	3.88E-12							
600	2.82E-17	1.00E+02	1.26E-12	2.20E-03	1.19E-12	2.40E-03	7.77E-13	3.60E-03	3.78E-12							
700	2.84E-17	1.00E+02	2.16E-12	1.30E-03	2.00E-12	1.40E-03	1.39E-12	2.00E-03	5.71E-12							
800	2.86E-17	1.00E+02	3.43E-12	8.40E-04	3.21E-12	8.90E-04	2.26E-12	1.30E-03	8.95E-12							
900	2.89E-17	1.00E+02	5.07E-12	5.70E-04	4.78E-12	6.10E-04	3.48E-12	8.30E-04	1.34E-11							
1000	2.93E-17	1.00E+02	7.28E-12	4.00E-04	6.79E-12	4.30E-04	5.04E-12	5.80E-04	1.91E-11							
1100	2.98E-17	1.00E+02	9.95E-12	3.00E-04	9.40E-12	3.20E-04	7.02E-12	4.20E-04	2.64E-11							
1200	3.05E-17	1.00E+02	1.33E-11	2.30E-04	1.25E-11	2.40E-04	9.50E-12	3.20E-04	3.53E-11							
1300	3.12E-17	1.00E+02	1.72E-11	1.80E-04	1.62E-11	1.90E-04	1.24E-11	2.50E-04	4.58E-11							
1400	9.62E-17	3.30E+01	2.18E-11	1.50E-04	2.06E-11	1.60E-04	1.59E-11	2.00E-04	5.82E-11							
1500	1.65E-16	2.00E+01	2.71E-11	1.20E-04	2.56E-11	1.30E-04	1.98E-11	1.70E-04	7.24E-11							
1600	6.85E-17	5.00E+01	3.31E-11	1.00E-04	3.14E-11	1.10E-04	2.44E-11	1.40E-04	8.89E-11							
1700	3.55E-17	1.00E+02	3.99E-11	8.90E-05	3.79E-11	9.40E-05	2.96E-11	1.20E-04	1.07E-10							
1800	7.39E-17	5.00E+01	4.74E-11	7.80E-05	4.51E-11	8.20E-05	3.54E-11	1.00E-04	1.28E-10							
1900	3.86E-17	1.00E+02	5.58E-11	6.90E-05	5.31E-11	7.30E-05	4.18E-11	9.20E-05	1.51E-10							
2000	1.21E-16	3.30E+01	6.51E-11	6.20E-05	6.19E-11	6.50E-05	4.90E-11	8.20E-05	1.76E-10							
P = 7600 Torr																
T (K)	RC	unc.(%)	I1	unc.(%)	I2	unc.(%)	I3	unc.(%)	I4	unc.(%)	I5	unc.(%)	P1 + H	unc.(%)	P2 + H	unc.(%)
200	4.84E-13	5.80E-03	1.53E-10	1.80E-05	1.50E-10	1.90E-05	9.96E-14	2.80E-02	1.40E-16	2.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
240	1.85E-13	1.50E-02	1.01E-10	2.80E-05	9.88E-11	2.80E-05	8.87E-14	3.20E-02	1.40E-16	2.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
250	1.47E-13	1.90E-02	8.68E-11	3.20E-05	8.57E-11	3.30E-05	8.55E-14	3.30E-02	2.24E-16	1.20E+01	1.12E-16	2.50E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
275	7.28E-14	3.80E-02	5.74E-11	4.90E-05	5.70E-11	4.90E-05	7.29E-14	3.80E-02	1.68E-16	1.70E+01	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
298	3.81E-14	7.30E-02	3.77E-11	7.40E-05	3.76E-11	7.50E-05	5.76E-14	4.90E-02	3.08E-16	9.10E+00	8.40E-17	3.30E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
300	3.51E-14	8.00E-02	3.63E-11	7.70E-05	3.62E-11	7.70E-05	5.69E-14	4.90E-02	3.08E-16	9.10E+00	8.41E-17	3.30E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
325	1.55E-14	1.80E-01	2.26E-11	1.20E-04	2.27E-11	1.20E-04	4.51E-14	6.20E-02	3.08E-16	9.10E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02	2.80E-17	1.00E+02
340	1.04E-14	2.70E-01	1.70E-11	1.70E-04	1.72E-11	1.60E-04	3.78E-14	7.40E-02	3.64E-16	7.70E+00	8.41E-17	3.30E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
400	1.26E-15	2.20E+00	5.71E-12	4.90E-04	5.88E-12	4.80E-04	2.21E-14	1.30E-01	4.77E-16	5.90E+00	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
500	5.62E-17	5.00E+01	1.15E-12	2.50E-03	1.20E-12	2.30E-03	9.00E-15	3.10E-01	3.38E-16	8.30E+00	2.81E-17	1.00E+02	2.81E-17	1.00E+02	2.81E-17	1.00E+02
600	2.82E-17	1.00E+02	2.82E-13	1.00E-02	3.04E-13	9.30E-03	3.75E-15	7.50E-01	1.13E-16	2.50E+01	2.82E-17	1.00E+02	2.82E-17	1.00E+02	2.82E-17	1.00E+02

700	2.84E-17	1.00E+02	8.26E-14	3.40E-02	9.13E-14	3.10E-02	1.51E-15	1.90E+00	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02
800	2.86E-17	1.00E+02	2.85E-14	1.00E-01	3.21E-14	8.90E-02	6.01E-16	4.80E+00	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02
900	2.89E-17	1.00E+02	1.02E-14	2.80E-01	1.24E-14	2.30E-01	2.03E-16	1.40E+01	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02
1000	2.93E-17	1.00E+02	4.52E-15	6.50E-01	6.95E-15	4.20E-01	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02	2.93E-17	1.00E+02
1100	2.98E-17	1.00E+02	1.61E-15	1.90E+00	3.70E-15	8.10E-01	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02	2.98E-17	1.00E+02
1200	3.05E-17	1.00E+02	5.79E-16	5.30E+00	1.71E-15	1.80E+00	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02
1300	3.12E-17	1.00E+02	3.43E-16	9.10E+00	1.47E-15	2.10E+00	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02
1400	3.21E-17	1.00E+02	1.28E-16	2.50E+01	8.34E-16	3.80E+00	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02
1500	3.31E-17	1.00E+02	3.31E-17	1.00E+02	6.61E-16	5.00E+00	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02
1600	3.42E-17	1.00E+02	3.42E-17	1.00E+02	5.48E-16	6.20E+00	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	1.03E-16	3.30E+01
1700	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.91E-16	9.10E+00	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02
1800	3.70E-17	1.00E+02	3.70E-17	1.00E+02	4.07E-16	9.10E+00	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02
1900	3.86E-17	1.00E+02	3.86E-17	1.00E+02	5.79E-16	6.70E+00	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02
2000	4.03E-17	1.00E+02	4.03E-17	1.00E+02	6.45E-16	6.20E+00	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	1.61E-16	2.50E+01	1.61E-16	2.50E+01
T (K)	P3 + H	unc.(%)	P4 + H₂O	unc.(%)	P5 + H₂O	unc.(%)	P6 + H₂O	unc.(%)	k_tot							
200	2.80E-17	1.00E+02	3.07E-14	9.10E-02	2.69E-14	1.00E-01	1.09E-14	2.60E-01	3.03E-10							
240	2.80E-17	1.00E+02	5.19E-14	5.40E-02	4.99E-14	5.60E-02	2.09E-14	1.30E-01	2.00E-10							
250	2.80E-17	1.00E+02	6.00E-14	4.70E-02	5.60E-14	5.00E-02	2.39E-14	1.20E-01	1.73E-10							
275	2.80E-17	1.00E+02	8.32E-14	3.40E-02	7.64E-14	3.70E-02	3.22E-14	8.70E-02	1.15E-10							
298	2.80E-17	1.00E+02	1.07E-13	2.60E-02	1.03E-13	2.70E-02	4.69E-14	6.00E-02	7.56E-11							
300	2.80E-17	1.00E+02	1.12E-13	2.50E-02	1.04E-13	2.70E-02	4.99E-14	5.60E-02	7.29E-11							
325	2.80E-17	1.00E+02	1.48E-13	1.90E-02	1.35E-13	2.10E-02	6.53E-14	4.30E-02	4.57E-11							
340	2.80E-17	1.00E+02	1.73E-13	1.60E-02	1.62E-13	1.70E-02	8.13E-14	3.40E-02	3.46E-11							
400	2.81E-17	1.00E+02	3.02E-13	9.30E-03	2.78E-13	1.00E-02	1.55E-13	1.80E-02	1.23E-11							
500	2.81E-17	1.00E+02	6.61E-13	4.30E-03	6.19E-13	4.50E-03	3.87E-13	7.30E-03	4.02E-12							
600	2.82E-17	1.00E+02	1.26E-12	2.20E-03	1.17E-12	2.40E-03	7.77E-13	3.60E-03	3.79E-12							
700	2.84E-17	1.00E+02	2.16E-12	1.30E-03	2.01E-12	1.40E-03	1.38E-12	2.10E-03	5.73E-12							
800	2.86E-17	1.00E+02	3.43E-12	8.40E-04	3.20E-12	9.00E-04	2.28E-12	1.30E-03	8.97E-12							
900	2.89E-17	1.00E+02	5.11E-12	5.70E-04	4.81E-12	6.00E-04	3.47E-12	8.30E-04	1.34E-11							
1000	2.93E-17	1.00E+02	7.28E-12	4.00E-04	6.81E-12	4.30E-04	5.03E-12	5.80E-04	1.91E-11							
1100	2.98E-17	1.00E+02	9.95E-12	3.00E-04	9.38E-12	3.20E-04	7.03E-12	4.20E-04	2.64E-11							
1200	3.05E-17	1.00E+02	1.33E-11	2.30E-04	1.25E-11	2.40E-04	9.45E-12	3.20E-04	3.52E-11							
1300	3.12E-17	1.00E+02	1.72E-11	1.80E-04	1.62E-11	1.90E-04	1.24E-11	2.50E-04	4.59E-11							
1400	3.21E-17	1.00E+02	2.18E-11	1.50E-04	2.06E-11	1.60E-04	1.58E-11	2.00E-04	5.82E-11							
1500	3.31E-17	1.00E+02	2.70E-11	1.20E-04	2.57E-11	1.30E-04	1.98E-11	1.70E-04	7.24E-11							
1600	3.42E-17	1.00E+02	3.31E-11	1.00E-04	3.14E-11	1.10E-04	2.44E-11	1.40E-04	8.89E-11							
1700	3.55E-17	1.00E+02	3.98E-11	8.90E-05	3.79E-11	9.40E-05	2.97E-11	1.20E-04	1.07E-10							
1800	7.39E-17	5.00E+01	4.74E-11	7.80E-05	4.51E-11	8.20E-05	3.55E-11	1.00E-04	1.28E-10							
1900	3.86E-17	1.00E+02	5.59E-11	6.90E-05	5.32E-11	7.20E-05	4.19E-11	9.20E-05	1.51E-10							
2000	4.03E-17	1.00E+02	6.50E-11	6.20E-05	6.20E-11	6.50E-05	4.90E-11	8.20E-05	1.76E-10							
P = 76000 Torr																
T (K)	RC	unc.(%)	I1	unc.(%)	I2	unc.(%)	I3	unc.(%)	I4	unc.(%)	I5	unc.(%)	P1 + H	unc.(%)	P2 + H	unc.(%)
200	1.50E-11	1.90E-04	1.69E-10	1.70E-05	1.62E-10	1.70E-05	1.20E-13	2.30E-02	3.36E-16	8.30E+00	5.60E-17	5.00E+01	2.80E-17	1.00E+02	2.80E-17	1.00E+02
240	3.45E-12	8.10E-04	1.28E-10	2.20E-05	1.27E-10	2.20E-05	1.73E-13	1.60E-02	1.48E-15	1.90E+00	4.76E-16	5.90E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02

250	2.36E-12	1.20E-03	1.15E-10	2.40E-05	1.14E-10	2.50E-05	1.75E-13	1.60E-02	1.46E-15	1.90E+00	5.04E-16	5.60E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02
275	1.03E-12	2.70E-03	8.03E-11	3.50E-05	8.04E-11	3.50E-05	1.69E-13	1.70E-02	2.05E-15	1.40E+00	6.72E-16	4.20E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02
298	4.73E-13	5.90E-03	5.39E-11	5.20E-05	5.44E-11	5.20E-05	1.44E-13	1.90E-02	2.13E-15	1.30E+00	4.48E-16	6.20E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02
300	4.41E-13	6.30E-03	5.20E-11	5.40E-05	5.24E-11	5.30E-05	1.46E-13	1.90E-02	2.86E-15	9.80E-01	7.29E-16	3.80E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02
325	1.83E-13	1.50E-02	3.25E-11	8.60E-05	3.30E-11	8.50E-05	1.15E-13	2.40E-02	2.78E-15	1.00E+00	6.73E-16	4.20E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02
340	1.12E-13	2.50E-02	2.43E-11	1.20E-04	2.50E-11	1.10E-04	9.87E-14	2.80E-02	2.61E-15	1.10E+00	6.45E-16	4.30E+00	2.80E-17	1.00E+02	2.80E-17	1.00E+02
400	1.27E-14	2.20E-01	8.12E-12	3.50E-04	8.48E-12	3.30E-04	5.53E-14	5.10E-02	2.50E-15	1.10E+00	6.17E-16	4.50E+00	2.81E-17	1.00E+02	2.81E-17	1.00E+02
500	6.19E-16	4.50E+00	1.62E-12	1.70E-03	1.77E-12	1.60E-03	1.86E-14	1.50E-01	1.58E-15	1.80E+00	1.97E-16	1.40E+01	2.81E-17	1.00E+02	2.81E-17	1.00E+02
600	2.82E-17	1.00E+02	4.02E-13	7.00E-03	4.46E-13	6.30E-03	6.66E-15	4.20E-01	9.03E-16	3.10E+00	1.41E-16	2.00E+01	2.82E-17	1.00E+02	2.82E-17	1.00E+02
700	2.84E-17	1.00E+02	1.18E-13	2.40E-02	1.35E-13	2.10E-02	2.87E-15	9.90E-01	2.27E-16	1.20E+01	2.84E-17	1.00E+02	2.84E-17	1.00E+02	2.84E-17	1.00E+02
800	2.86E-17	1.00E+02	4.02E-14	7.10E-02	4.51E-14	6.30E-02	1.09E-15	2.60E+00	5.72E-17	5.00E+01	2.86E-17	1.00E+02	2.86E-17	1.00E+02	2.86E-17	1.00E+02
900	2.89E-17	1.00E+02	1.55E-14	1.90E-01	1.84E-14	1.60E-01	4.92E-16	5.90E+00	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02	2.89E-17	1.00E+02
1000	2.94E-17	1.00E+02	6.93E-15	4.20E-01	7.63E-15	3.80E-01	2.64E-16	1.10E+01	2.94E-17	1.00E+02	2.94E-17	1.00E+02	2.94E-17	1.00E+02	2.94E-17	1.00E+02
1100	2.99E-17	1.00E+02	2.57E-15	1.20E+00	3.41E-15	8.80E-01	1.49E-16	2.00E+01	2.99E-17	1.00E+02	2.99E-17	1.00E+02	2.99E-17	1.00E+02	2.99E-17	1.00E+02
1200	3.05E-17	1.00E+02	1.62E-15	1.90E+00	1.80E-15	1.70E+00	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02	3.05E-17	1.00E+02
1300	3.12E-17	1.00E+02	8.12E-16	3.80E+00	8.43E-16	3.70E+00	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02	3.12E-17	1.00E+02
1400	3.21E-17	1.00E+02	6.74E-16	4.80E+00	8.34E-16	3.80E+00	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02	3.21E-17	1.00E+02
1500	3.31E-17	1.00E+02	2.65E-16	1.20E+01	3.31E-16	1.00E+01	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02	3.31E-17	1.00E+02
1600	3.42E-17	1.00E+02	3.08E-16	1.10E+01	4.45E-16	7.70E+00	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02	3.42E-17	1.00E+02
1700	3.55E-17	1.00E+02	1.78E-16	2.00E+01	6.75E-16	5.30E+00	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02	3.55E-17	1.00E+02
1800	3.70E-17	1.00E+02	1.48E-16	2.50E+01	1.85E-16	2.00E+01	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02	3.70E-17	1.00E+02
1900	3.86E-17	1.00E+02	2.31E-16	1.70E+01	3.86E-16	1.00E+01	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02	3.86E-17	1.00E+02
2000	4.03E-17	1.00E+02	2.02E-16	2.00E+01	5.24E-16	7.70E+00	4.03E-17	1.00E+02	4.03E-17	1.00E+02	4.03E-17	1.00E+02	1.21E-16	3.30E+01	4.03E-17	1.00E+02
T (K)	P3 + H	unc.(%)	P4 + H ₂ O	unc.(%)	P5 + H ₂ O	unc.(%)	P6 + H ₂ O	unc.(%)	k_tot							
200	2.80E-17	1.00E+02	3.08E-14	9.10E-02	2.98E-14	9.40E-02	1.03E-14	2.70E-01	3.46E-10							
240	2.80E-17	1.00E+02	5.42E-14	5.20E-02	4.89E-14	5.70E-02	2.01E-14	1.40E-01	2.59E-10							
250	2.80E-17	1.00E+02	6.08E-14	4.60E-02	5.72E-14	4.90E-02	2.45E-14	1.10E-01	2.31E-10							
275	2.80E-17	1.00E+02	8.39E-14	3.30E-02	7.80E-14	3.60E-02	3.32E-14	8.40E-02	1.62E-10							
298	2.80E-17	1.00E+02	1.11E-13	2.50E-02	1.03E-13	2.70E-02	4.96E-14	5.60E-02	1.09E-10							
300	2.80E-17	1.00E+02	1.15E-13	2.40E-02	1.04E-13	2.70E-02	4.96E-14	5.70E-02	1.05E-10							
325	2.80E-17	1.00E+02	1.44E-13	1.90E-02	1.38E-13	2.00E-02	6.61E-14	4.20E-02	6.61E-11							
340	2.80E-17	1.00E+02	1.71E-13	1.60E-02	1.62E-13	1.70E-02	8.32E-14	3.40E-02	4.99E-11							
400	2.81E-17	1.00E+02	3.04E-13	9.20E-03	2.87E-13	9.80E-03	1.56E-13	1.80E-02	1.74E-11							
500	2.81E-17	1.00E+02	6.69E-13	4.20E-03	6.26E-13	4.50E-03	3.82E-13	7.40E-03	5.09E-12							
600	2.82E-17	1.00E+02	1.26E-12	2.20E-03	1.18E-12	2.40E-03	7.74E-13	3.60E-03	4.07E-12							
700	2.84E-17	1.00E+02	2.17E-12	1.30E-03	2.02E-12	1.40E-03	1.39E-12	2.00E-03	5.84E-12							
800	2.86E-17	1.00E+02	3.42E-12	8.40E-04	3.21E-12	8.90E-04	2.27E-12	1.30E-03	8.98E-12							
900	2.89E-17	1.00E+02	5.10E-12	5.70E-04	4.80E-12	6.00E-04	3.46E-12	8.40E-04	1.34E-11							
1000	2.94E-17	1.00E+02	7.27E-12	4.00E-04	6.83E-12	4.30E-04	5.05E-12	5.80E-04	1.92E-11							
1100	2.99E-17	1.00E+02	9.97E-12	3.00E-04	9.38E-12	3.20E-04	7.04E-12	4.20E-04	2.64E-11							
1200	3.05E-17	1.00E+02	1.33E-11	2.30E-04	1.25E-11	2.40E-04	9.49E-12	3.20E-04	3.53E-11							
1300	3.12E-17	1.00E+02	1.72E-11	1.80E-04	1.63E-11	1.90E-04	1.24E-11	2.50E-04	4.58E-11							
1400	3.21E-17	1.00E+02	2.18E-11	1.50E-04	2.06E-11	1.60E-04	1.59E-11	2.00E-04	5.82E-11							
1500	3.31E-17	1.00E+02	2.71E-11	1.20E-04	2.56E-11	1.30E-04	1.98E-11	1.70E-04	7.25E-11							
1600	3.42E-17	1.00E+02	3.30E-11	1.00E-04	3.14E-11	1.10E-04	2.44E-11	1.40E-04	8.88E-11							

1700	3.55E-17	1.00E+02	3.99E-11	8.90E-05	3.79E-11	9.40E-05	2.95E-11	1.20E-04	1.07E-10							
1800	7.39E-17	5.00E+01	4.74E-11	7.80E-05	4.51E-11	8.20E-05	3.55E-11	1.00E-04	1.28E-10							
1900	3.86E-17	1.00E+02	5.59E-11	6.90E-05	5.32E-11	7.20E-05	4.19E-11	9.20E-05	1.51E-10							
2000	4.03E-17	1.00E+02	6.50E-11	6.20E-05	6.20E-11	6.50E-05	4.90E-11	8.20E-05	1.76E-10							

Table S5: Calculated branching ratios for each species of Pyrene + OH → products reactions at $P = 760$ Torr based on the ROCBS-QB3//M06-2X PES.

T (K)	RC	I1	I2	I3	I4	I5	P1 + H	P2 + H	P3 + H	P4 + H ₂ O	P5 + H ₂ O	P6 + H ₂ O
200	0.01	50.39	49.55	0.03	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00
240	0.01	50.25	49.63	0.04	0.00	0.00	0.00	0.00	0.00	0.03	0.03	0.01
250	0.01	50.17	49.69	0.05	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.02
275	0.01	50.00	49.75	0.06	0.00	0.00	0.00	0.00	0.00	0.08	0.08	0.03
298	0.00	49.77	49.78	0.07	0.00	0.00	0.00	0.00	0.00	0.16	0.15	0.07
300	0.01	49.76	49.76	0.07	0.00	0.00	0.00	0.00	0.00	0.17	0.16	0.07
325	0.00	49.43	49.64	0.09	0.00	0.00	0.00	0.00	0.00	0.34	0.33	0.16
340	0.00	49.09	49.53	0.10	0.00	0.00	0.00	0.00	0.00	0.52	0.49	0.26
400	0.00	46.12	47.28	0.17	0.00	0.00	0.00	0.00	0.00	2.65	2.43	1.35
500	0.00	27.44	29.40	0.20	0.00	0.00	0.00	0.00	0.00	17.02	16.07	9.86
600	0.00	7.16	7.59	0.08	0.00	0.00	0.00	0.00	0.00	33.24	31.36	20.56
700	0.00	1.37	1.47	0.02	0.00	0.00	0.00	0.00	0.00	37.85	35.03	24.25
800	0.00	0.27	0.34	0.00	0.00	0.00	0.00	0.00	0.00	38.29	35.89	25.21
900	0.00	0.07	0.09	0.00	0.00	0.00	0.00	0.00	0.00	38.00	35.81	26.03
1000	0.00	0.01	0.03	0.00	0.00	0.00	0.00	0.00	0.00	38.08	35.49	26.38
1100	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	37.74	35.62	26.62
1200	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	37.61	35.43	26.96
1300	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.52	35.36	27.12
1400	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.40	35.37	27.23
1500	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.35	35.30	27.35
1600	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.23	35.31	27.46
1700	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.15	35.28	27.57
1800	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.07	35.26	27.66
1900	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.04	35.22	27.74
2000	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	37.00	35.18	27.82

Table S6: Acute and chronic toxicity classification (mg/L).

Classification	Acute toxicity ^a	Chronic toxicity ^b
Not harmful	$LC_{50} > 100$ or $EC_{50} > 100$	$ChV > 10$
Harmful	$10 < LC_{50} < 100$ or $10 < EC_{50} < 100$	$1 < ChV < 10$
Toxic	$1 < LC_{50} < 10$ or $1 < EC_{50} < 10$	$0.1 < ChV < 1$
Very toxic	$LC_{50} < 1$ or $EC_{50} < 1$	$ChV < 0.1$

^aCriteria set by the European Union (Annex VI of Directive 67/548/EEC³).

^bCriteria set by the Chinese hazard evaluation guidelines for new chemical substances (HJ/T 154 – 2004)⁴.

Table S7: Rate constants for typical PAHs (Poly Aromatic Hydrocarbons) + OH reactions in gas and condensed phases under ambient conditions.

Species	Rate constant at ambient condition (Unit in cm ³ /molecule/s)	
	Gas phase	Condensed phase (water)
Benzene	$1.3 \times 10^{-12.5}$	$1.3 \times 10^{-11.6}$
Naphthalene	$2.2 \times 10^{-11.5}$	$1.6 \times 10^{-11.7}$
Pyrene	6.9×10^{-11} (This work)	---

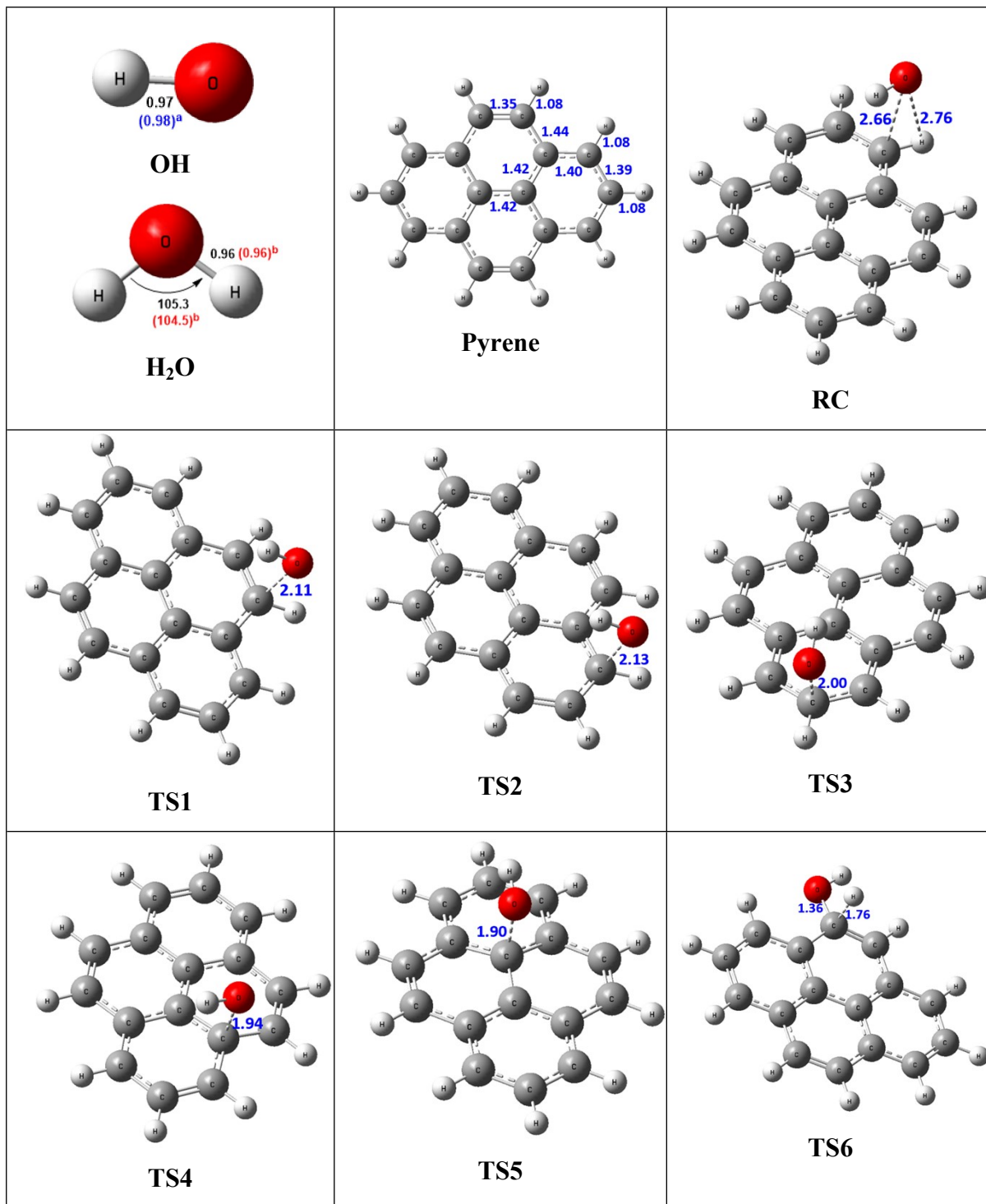
Table S8: Predicted thermochemical data of the adducts and products at 298 K.

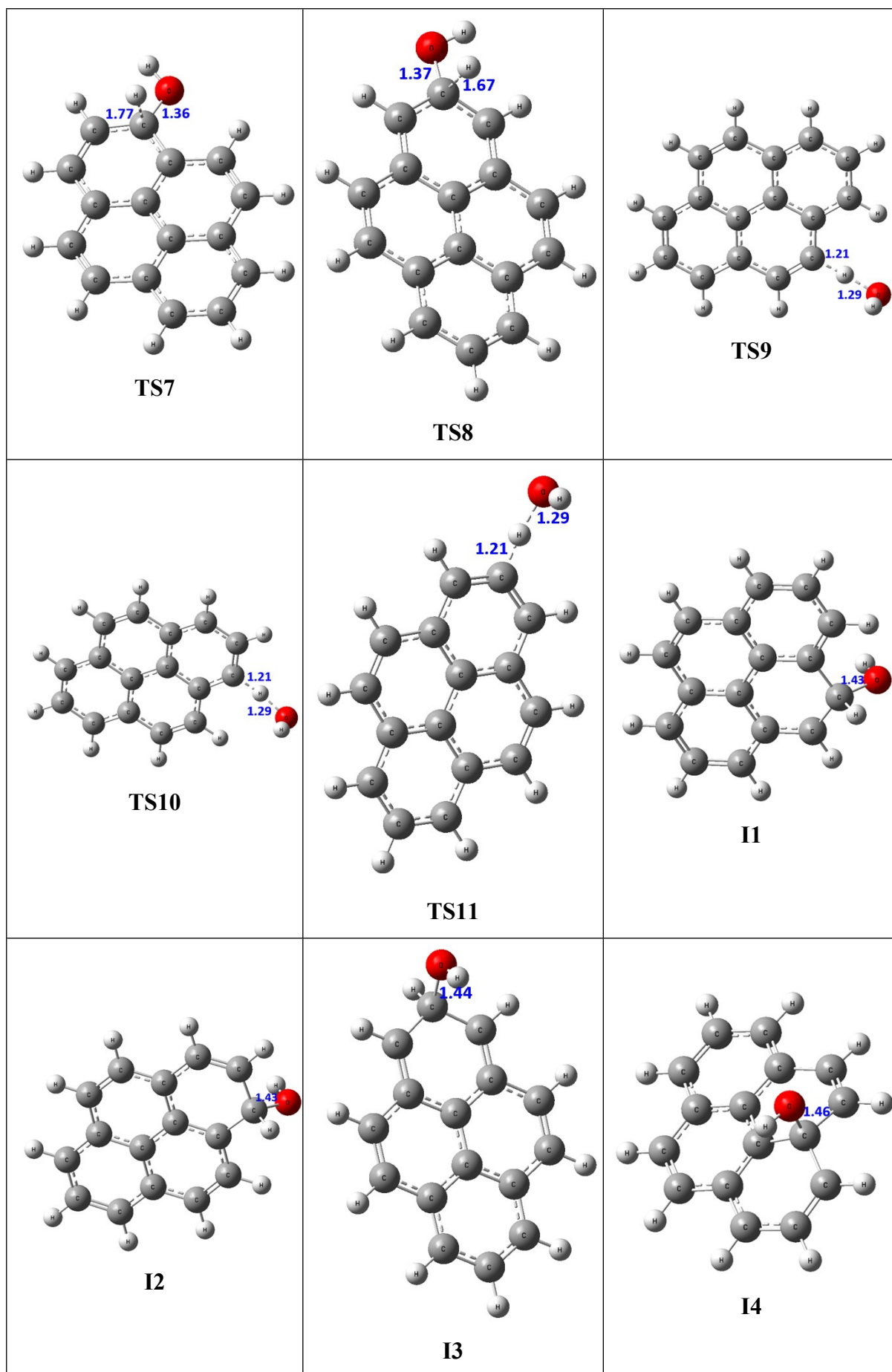
Species	$\Delta_f H^{298\text{ K}}$ (kcal/mol) ^[a]	$S^{298\text{ K}}$ (cal/mol/K)	$C_p^{298\text{ K}}$ (cal/mol/K)
I1	42.6	109.9	54.3
I2	36.9	109.5	54.1
I3	50.5	109.7	54.8
I4	59.3	109.0	54.9
I5	62.4	108.8	54.1
P1	13.4	103.9	53.4
P2	14.3	104.3	53.0
P3	14.0	103.8	52.4
P4	119.1	99.3	46.8
P5	120.0	99.2	46.7
P6	119.3	99.3	46.9

^a The calculations in this work were performed using the atomization method at the CBS-QB3 level.

Table S9: Relative energies with respect to the isolated reactants for the primary transition states of the reaction between pyrene and OH radicals in the gas phase and in water (SMD model⁸), calculated at the ROCBS-QB3//M06-2X/aug-cc-pVTZ level.

Species	Relative energy in gas-phase (kcal/mol)	Relative energy in water (kcal/mol)
TS1	-2.9	-2.5
TS2	-2.8	-2.5
TS3	-0.2	0.5
TS4	2.2	2.4
TS5	2.7	2.5
TS9	2.7	N/A
TS10	2.8	4.6
TS11	3.3	N/A





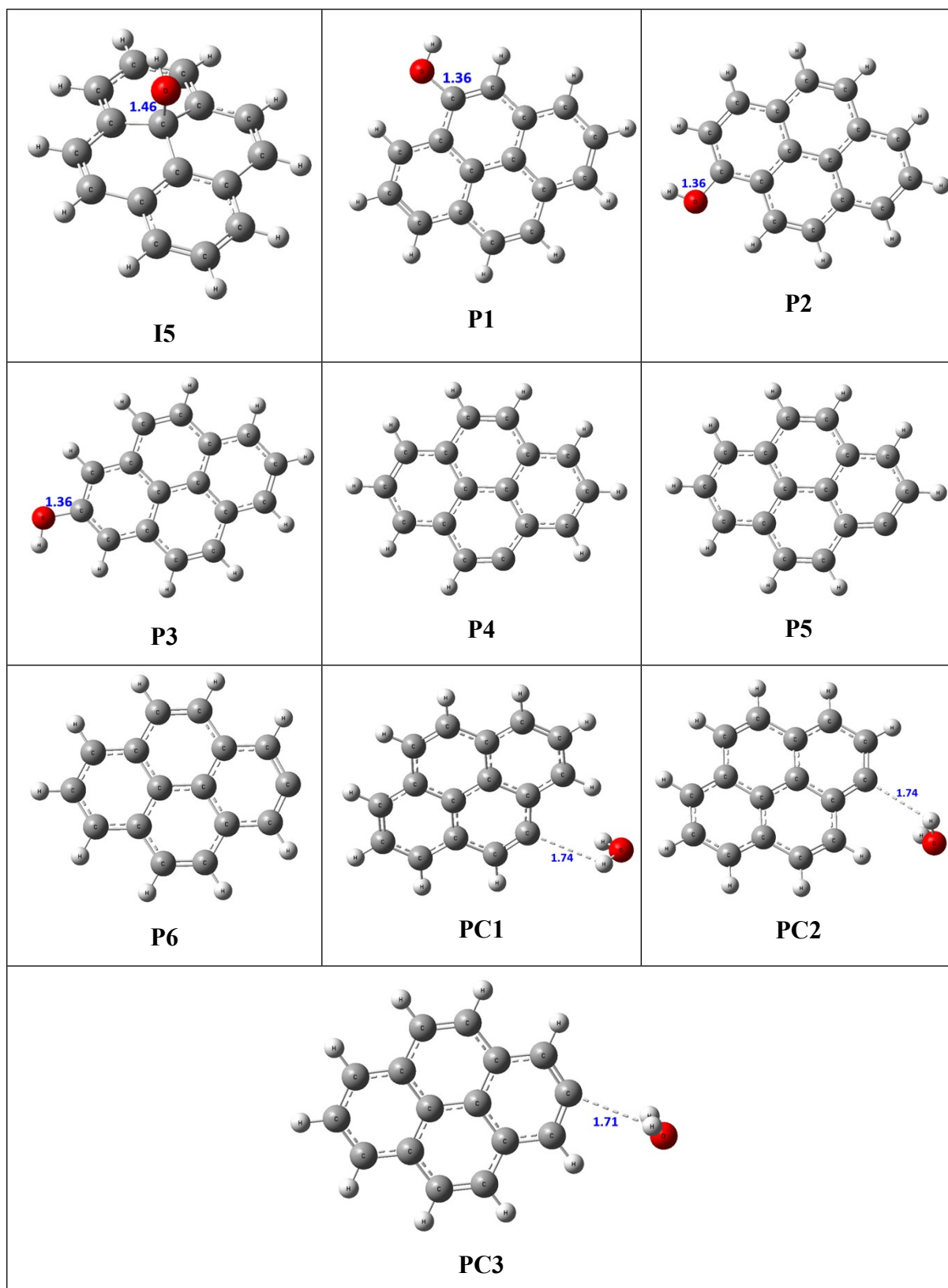


Figure S1: M06-2X/aug-cc-pVTZ optimized geometries for the species involved in the Pyrene + OH reaction. All structures were obtained for the lowest-energy conformer of a given species. Bond lengths and bond angles are in Å and degree (°), respectively. ^{a, b} obtained from Huber *et al.*¹, Hoy *et al.*⁹, respectively.

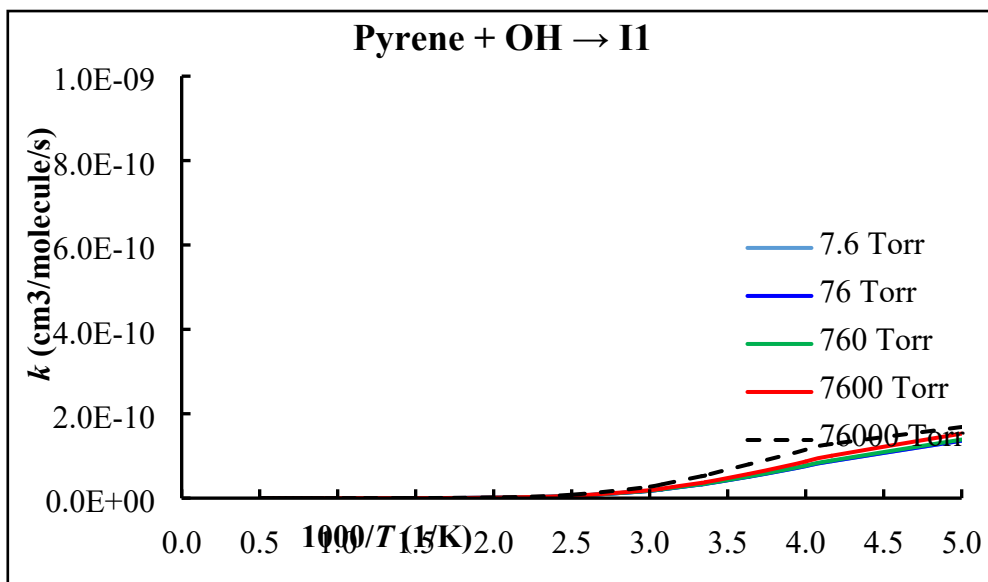


Figure S2: Predicted rate coefficients, $k(T, P)$, for the Pyrene + OH → **I1** as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.

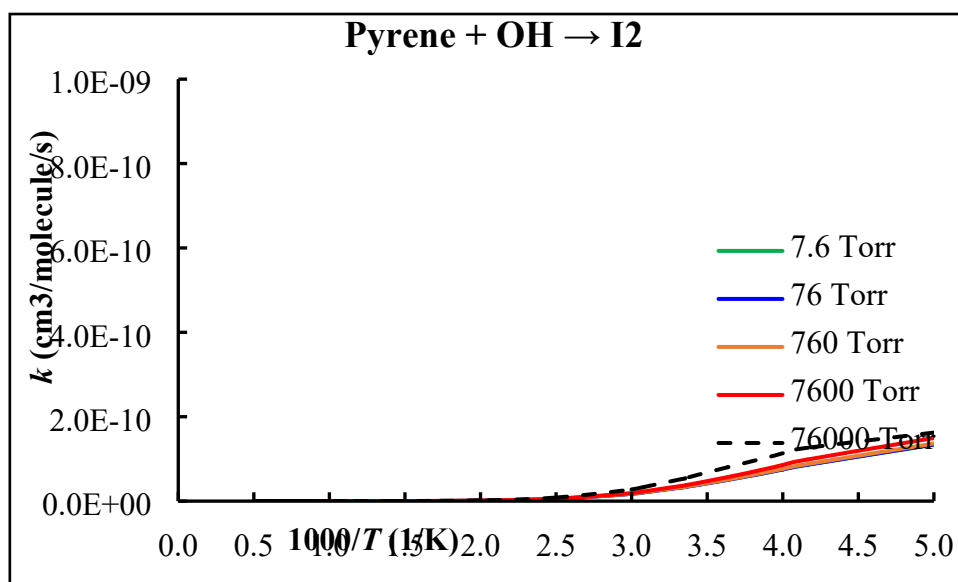


Figure S3: Predicted rate coefficients, $k(T, P)$, for the Pyrene + OH → **I2** as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.

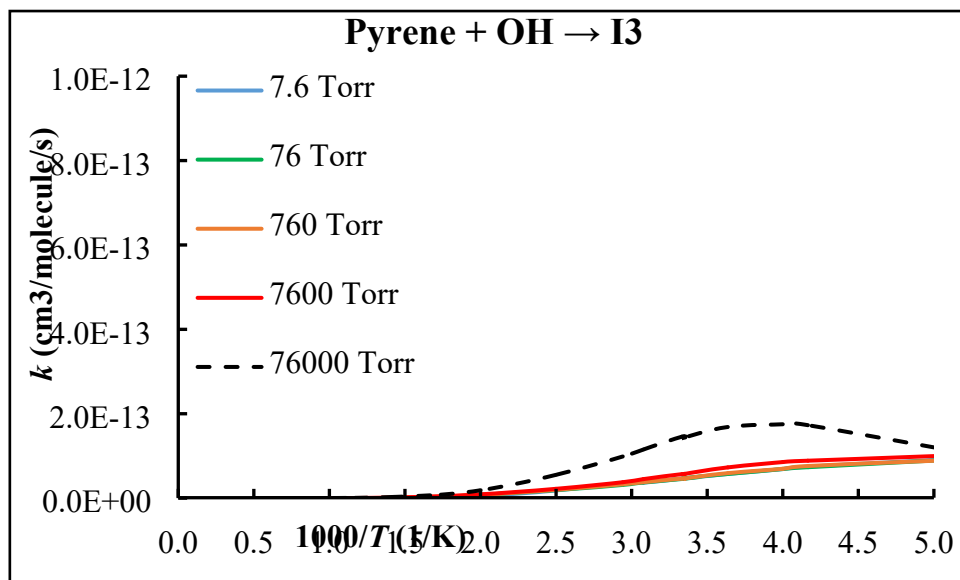


Figure S4: Predicted rate coefficients, $k(T, P)$, for the Pyrene + OH → I3 as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.

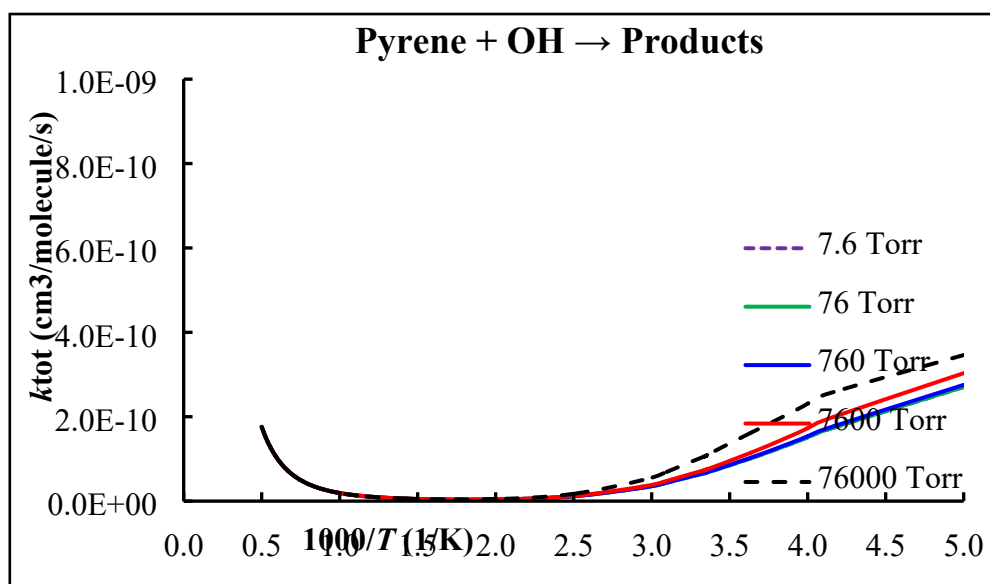


Figure S5: Calculated overall rate coefficients, $k_{tot}(T, P)$, for the Pyrene + OH → Products as functions of temperature at different pressures (e.g., 7.6, 76, 760, 7600, and 76000 Torr) based on the ROCBS-QB3//M06-2X PES.

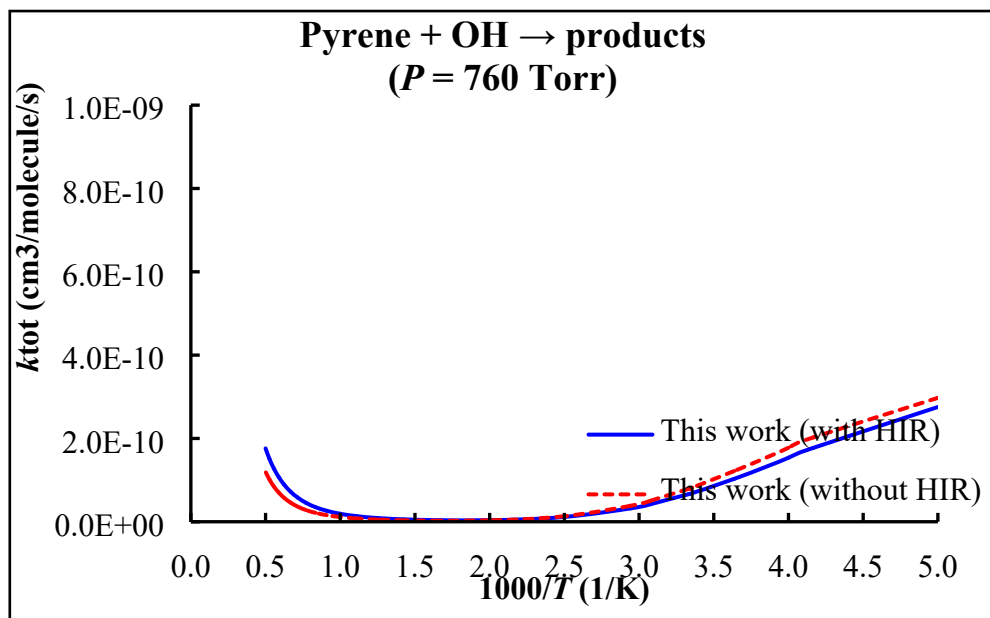
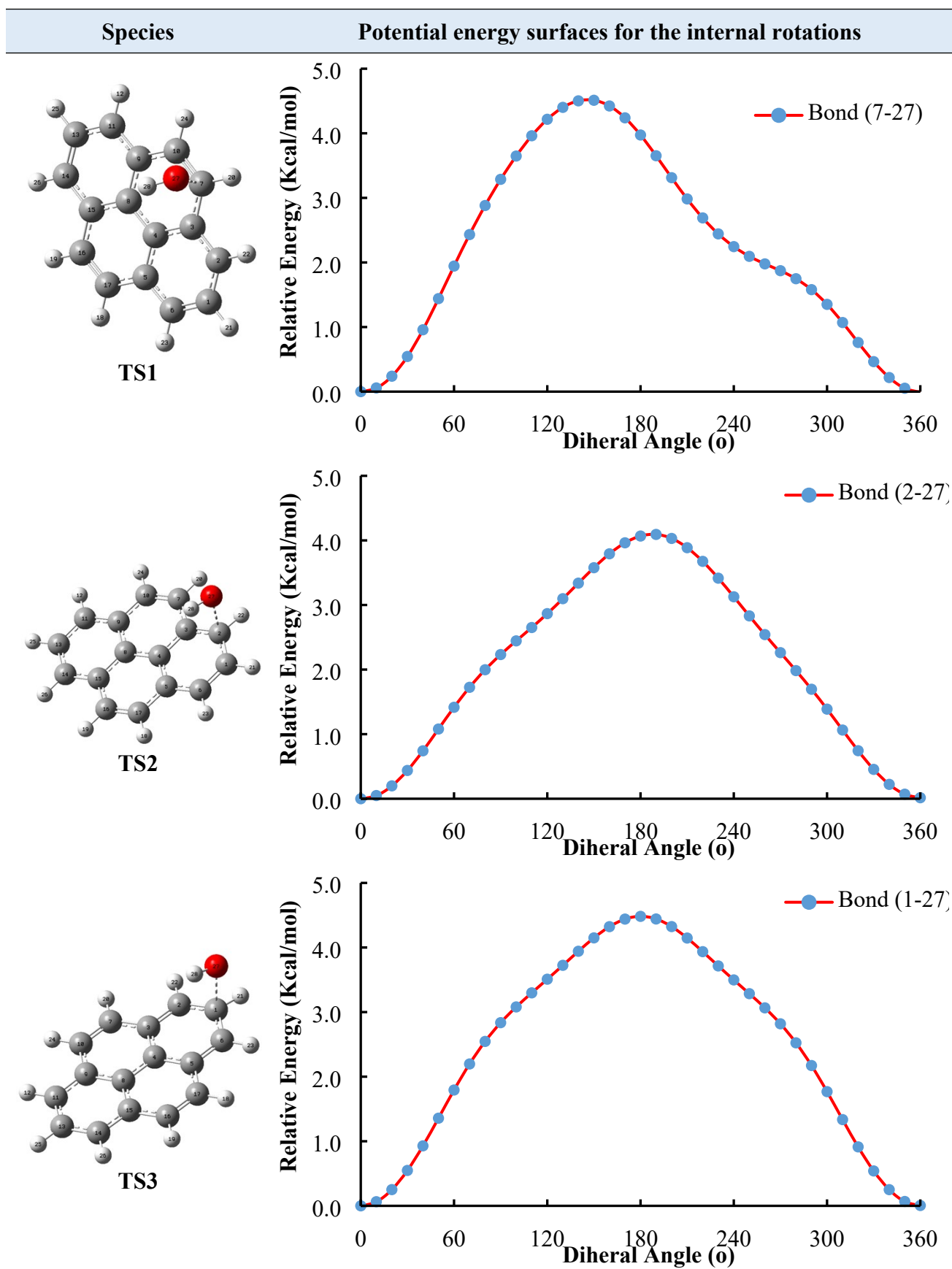
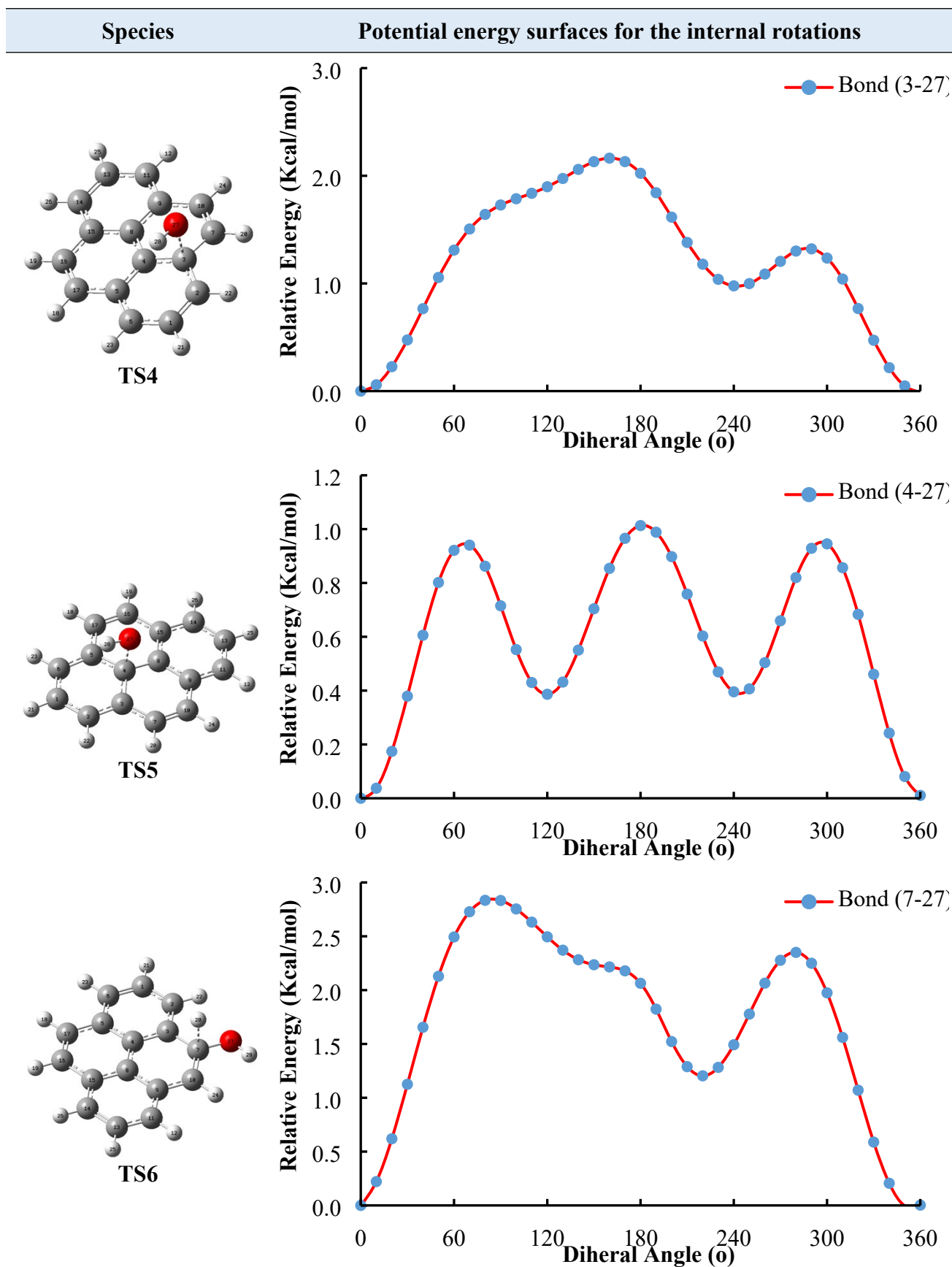
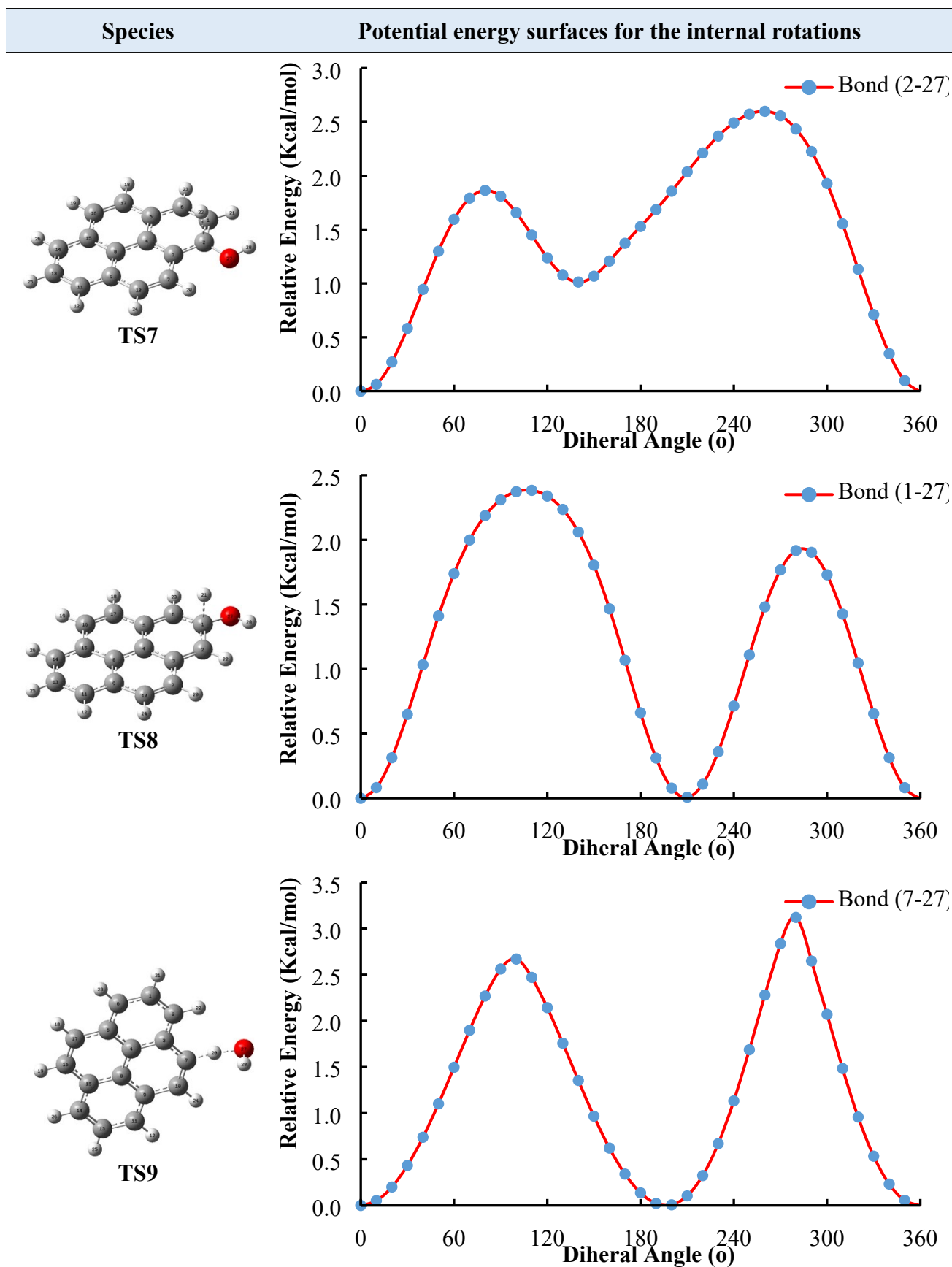
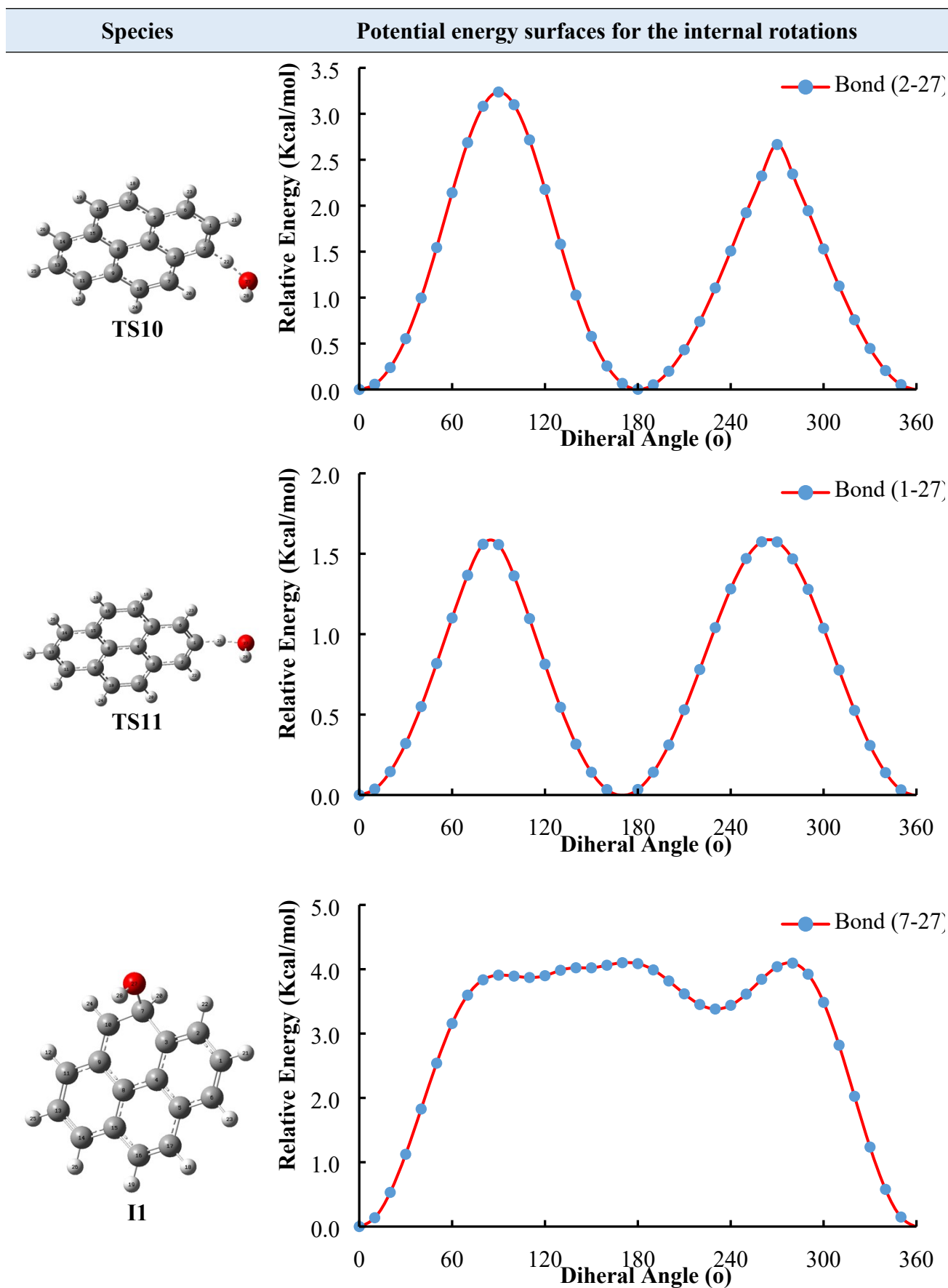


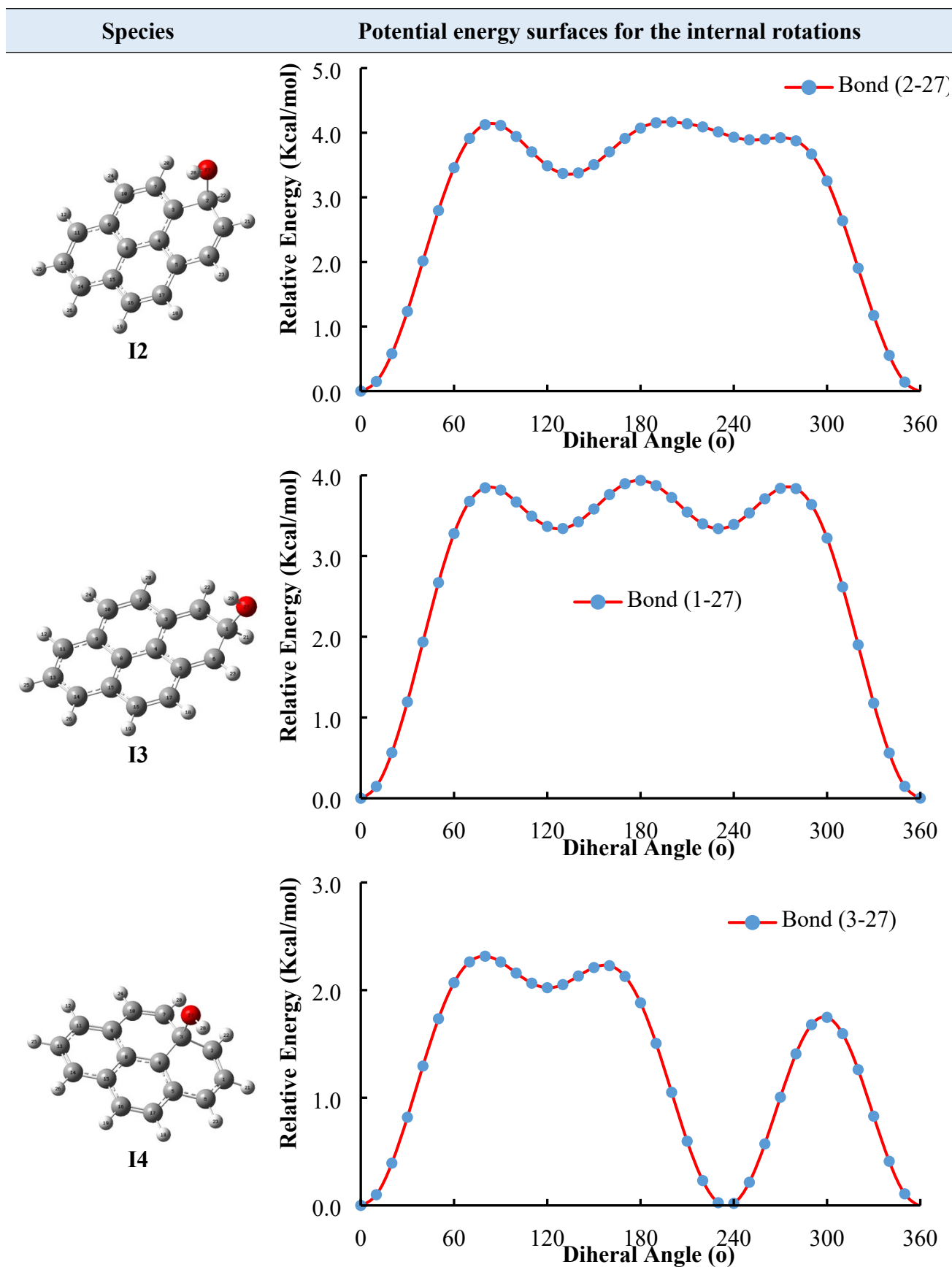
Figure S6: Calculated overall rate constant, k_{tot} , for the Pyrene + OH $\rightarrow$ products reaction at $P = 760$ Torr as a function of temperature with (solid line) and without (dashed line) HIR treatment, based on the ROCBS-QB3//M06-2X PES.

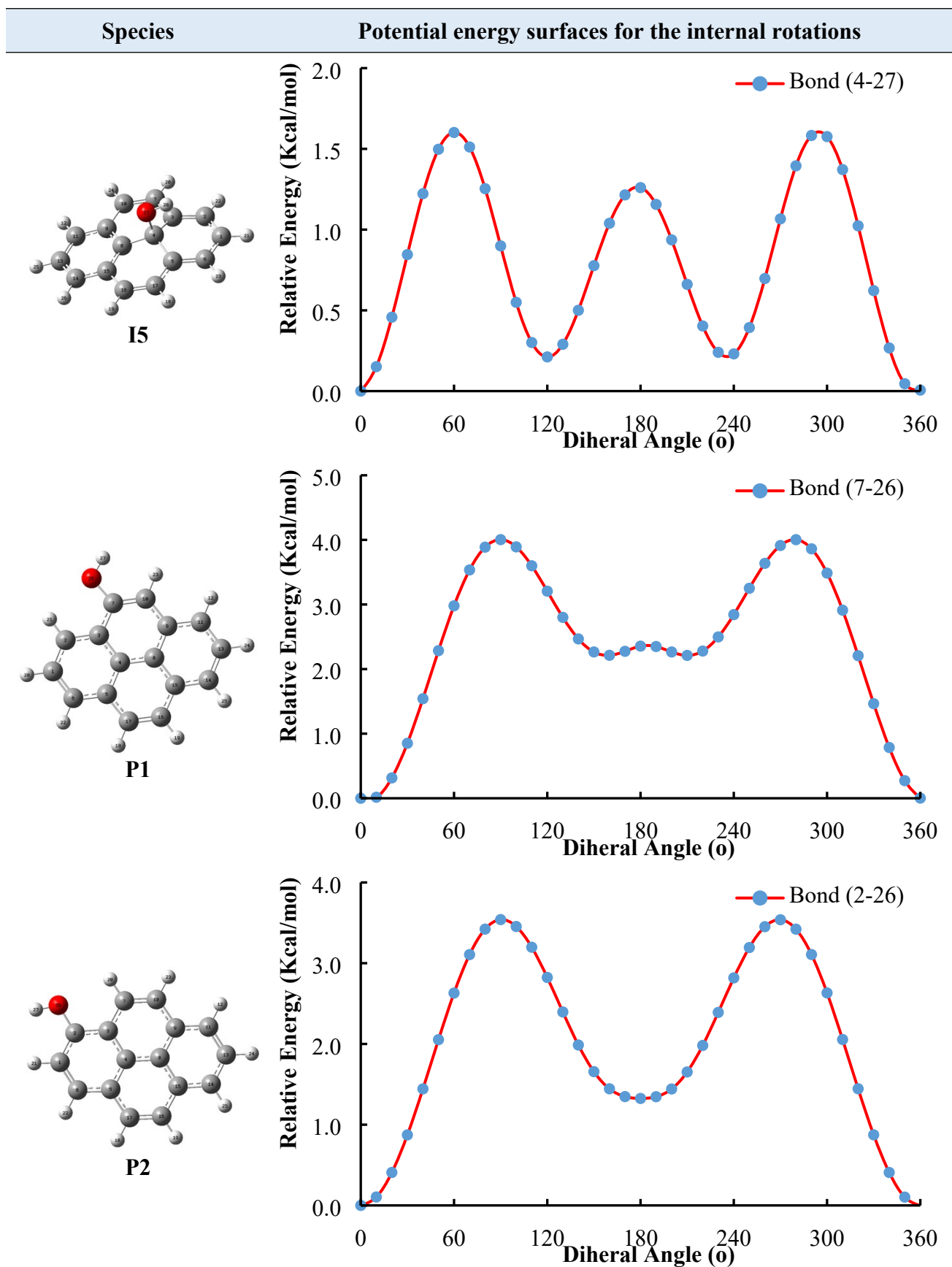












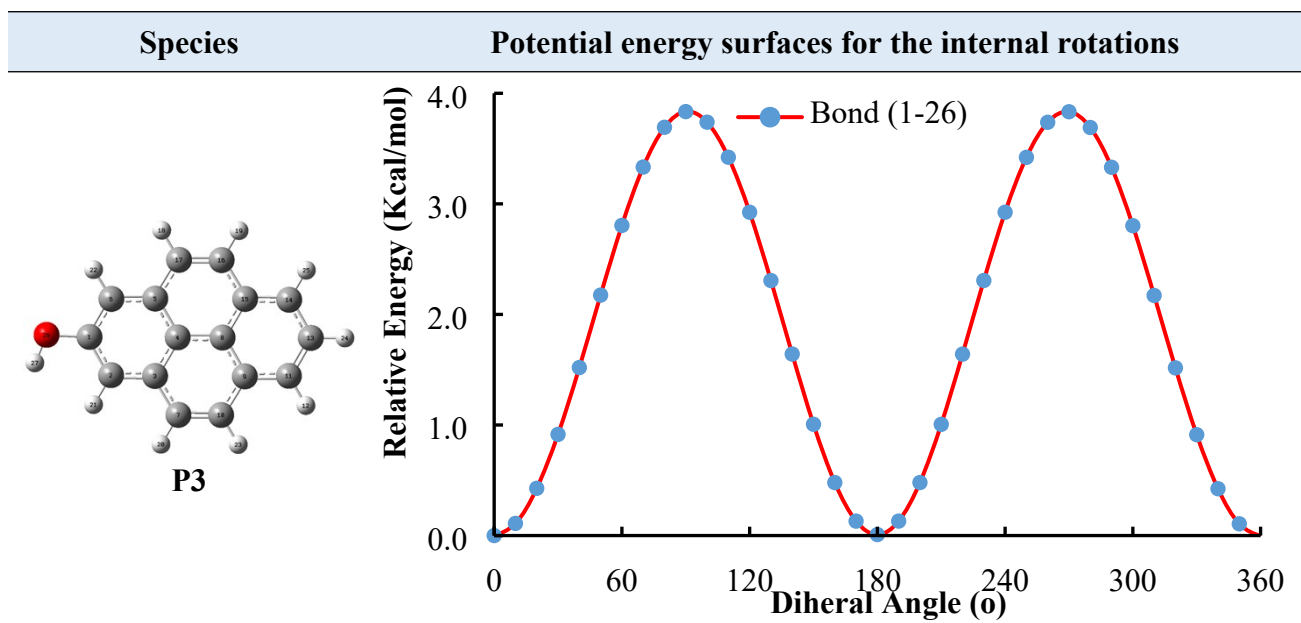


Figure S7: Hindrance potentials for the species involved in the Pyrene + OH reaction, calculated at M06-2X/cc-pVDZ level of theory.

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