

Expansion coefficients of the PES's. $R_{CP}^{ref} = 3.035778$ bohr, $R_{CH}^{ref} = 2.045660$ bohr, $\theta^{ref} = 180$ deg.

i	j	k	C_{ijk}	i	j	k	C_{ijk}	i	j	k	C_{ijk}
A' surface											
0	0	0	0.000000	1	0	0	0.000000	0	1	0	0.000000
2	0	0	0.23972 ^a	1	1	0	-0.009736	0	2	0	0.183407
0	0	2	0.026190	2	1	0	-0.000126	1	2	0	0.001210
0	3	0	-0.185303	3	0	0	-0.222544	1	0	2	-0.010489
0	1	2	-0.007543	1	3	0	-0.001824	0	4	0	0.129448
3	1	0	0.000597	2	2	0	-0.002955	0	0	4	-0.001871
1	1	2	0.009421	2	0	2	-0.012486	0	2	2	-0.000782
4	0	0	0.126870	3	2	0	0.001745	2	3	0	0.002086
1	4	0	0.001407	0	5	0	-0.076746	5	0	0	-0.057673
1	0	4	0.003641	0	1	4	-0.000876	3	0	2	0.013728
4	1	0	0.000177	0	6	0	0.027051	0	0	6	-0.000176
4	0	2	-0.037240	6	0	0	0.016619	1	0	6	0.000364
5	0	2	0.050926	0	1	6	-0.001111	0	0	8	-0.000152
0	1	8	0.000156	0	0	10	0.000039				
A'' surface											
0	0	0	0.000000	1	0	0	0.000000	0	1	0	0.000000
2	0	0	0.23972 ^a	1	1	0	-0.009736	0	2	0	0.183407
0	0	2	0.027907	2	1	0	-0.000126	1	2	0	0.001210
0	3	0	-0.185303	3	0	0	-0.222544	1	0	2	-0.035634
0	1	2	-0.005380	1	3	0	-0.001824	0	4	0	0.129448
3	1	0	0.000597	2	2	0	-0.002955	0	0	4	0.000996
1	1	2	0.007676	2	0	2	0.007886	4	0	0	0.126870
2	3	0	0.002086	1	4	0	0.001407	0	5	0	-0.076746
5	0	0	-0.057673	1	0	4	0.003285	0	1	4	-0.002798
4	1	0	0.000177	3	2	0	0.001745	0	6	0	0.027051
0	0	6	0.000415	6	0	0	0.016619	0	0	8	-0.000248
0	0	10	0.000021								

^a Modified value. The ab initio value is 0.235018

A' surface

```

0 0 0 0.0000000000 1 0 0 0.0000000000 0 1 0 0.0000000000
2 0 0 0.23972 1 1 0 -0.0097364429 0 2 0 0.1834066138
0 0 2 0.0261899821 2 1 0 -0.0001256414 1 2 0 0.0012102763
0 3 0 -0.1853028315 3 0 0 -0.2225443326 1 0 2 -0.0104891335
0 1 2 -0.0075430467 1 3 0 -0.0018239383 0 4 0 0.1294482914
3 1 0 0.0005966156 2 2 0 -0.0029545634 0 0 4 -0.0018713277
1 1 2 0.0094212203 2 0 2 -0.0124864816 0 2 2 -0.0007817559
4 0 0 0.1268698112 3 2 0 0.0017447348 2 3 0 0.0020861910
1 4 0 0.0014065365 0 5 0 -0.0767460012 5 0 0 -0.0576734660
1 0 4 0.0036414800 0 1 4 -0.0008760901 3 0 2 0.0137280311
4 1 0 0.0001771017 0 6 0 0.0270510987 0 0 6 -0.0001755484
4 0 2 -0.0372396781 6 0 0 0.0166187940 1 0 6 0.0003640789
5 0 2 0.0509262237 0 1 6 -0.0011108842 0 0 8 -0.0001522771
0 1 8 0.0001564864 0 0 10 0.0000393494
3.0357783832 2.0456298823 3.1415926169

```

A'' surface

```

0 0 0 0.0000000001 1 0 0 0.0000000000 0 1 0 0.0000000000
2 0 0 0.23972 1 1 0 -0.0097364429 0 2 0 0.1834066138
0 0 2 0.0279065295 2 1 0 -0.0001256414 1 2 0 0.0012102763
0 3 0 -0.1853028315 3 0 0 -0.2225443326 1 0 2 -0.0356342197
0 1 2 -0.0053795189 1 3 0 -0.0018239383 0 4 0 0.1294482914
3 1 0 0.0005966156 2 2 0 -0.0029545634 0 0 4 0.0009966769
1 1 2 0.0076760723 2 0 2 0.0078860210 4 0 0 0.1268698112
2 3 0 0.0020861910 1 4 0 0.0014065365 0 5 0 -0.0767460012
5 0 0 -0.0576734660 1 0 4 0.0032849260 0 1 4 -0.0027975688
4 1 0 0.0001771017 3 2 0 0.0017447348 0 6 0 0.0270510987
0 0 6 0.0004148904 6 0 0 0.0166187940 0 0 8 -0.0002482159
0 0 10 0.0000206242
3.0357783832 2.0456298823 3.1415926169

```