Supplementary information

Optimised geometries in Cartesian coordinates (in angstroms) and total energies (in hartrees) at the B3LYP/aug-cc-pVTZ level of theory.

I' (D_{3h})

E=-1140.276969

P	1.595812	0.921342	0.000000
P	0.000000	-1.842685	0.000000
P	-1.595812	0.921342	0.000000
C	0.000000	1.594696	0.000000
C	1.381047	-0.797348	0.000000
C	-1.381047	-0.797348	0.000000
H	2.321541	-1.340342	0.000000
H	-2.321541	-1.340342	0.000000
H	0.000000	2.680684	0.000000

II' (C_{2v})

E=-1141.4491595

P	0.000000	1.587410	-0.980350
P	0.000000	-1.587410	-0.980350
P	0.000000	0.000000	1.709482
C	0.000000	0.000000	-1.671356
C	0.000000	-1.438508	0.726307
C	0.000000	1.438508	0.726307
H	0.000000	0.000000	-2.757616
H	0.000000	-2.376727	1.271841
H	-1.072381	0.000000	2.647330
H	0.000000	2.376727	1.271841
H	1.072381	0.000000	2.647330

III' (C_{2v})

E=-1142.6254106

P	0.000000	1.514494	-0.819388
P	0.000000	-1.514494	-0.819388
P	0.000000	0.000000	1.880528
C	0.000000	0.000000	-1.613608
C	0.000000	-1.407041	0.909995
C	0.000000	1.407041	0.909995
H	0.000000	0.000000	-2.700107
H	0.000000	-2.352045	1.447912
H	0.000000	2.352045	1.447912
H	1.064434	2.349197	-1.265076
H	-1.064434	2.349197	-1.265076

```
H    -1.064434    -2.349197    -1.265076
H     1.064434    -2.349197    -1.265076
```

IV' (C_s)

```
E=-1143.7968693

P     0.088569    -0.866987     1.519528
P     0.088569    -0.866987    -1.519528
P    -0.197633     1.713969     0.000000
C    -0.118419    -1.634824     0.000000
C     0.088569     0.842982     1.453753
C     0.088569     0.842982    -1.453753
H    -0.517225    -2.637346     0.000000
H    -1.463217     2.373286     0.000000
H     0.616903     2.869376     0.000000
H     0.324375     1.402493     2.346261
H     0.324375     1.402493    -2.346261
H    -0.896799    -1.441829     2.367941
H    -0.896799    -1.441829    -2.367941
H     1.231760    -1.266709     2.270186
H     1.231760    -1.266709    -2.270186
```

I' planar (D_{3h}, NImag=2)

```
E=-1143.7963647

P    -1.516128     0.875337     0.000000
P     1.516128     0.875337     0.000000
P     0.000000    -1.750674     0.000000
C     0.000000     1.670269     0.000000
C     1.446495    -0.835135     0.000000
C    -1.446495    -0.835135     0.000000
H     0.000000     2.750002     0.000000
H     2.381571    -1.375001     0.000000
H    -2.381571    -1.375001     0.000000
H    -2.333814     1.347428     1.065480
H    -2.333814     1.347428    -1.065480
H     2.333814     1.347428    -1.065480
H     2.333814     1.347428     1.065480
H     0.000000    -2.694856    -1.065480
H     0.000000    -2.694856     1.065480
```

I' TS (C_2, NImag=1)

```
E=-1143.7968224

P     0.000000     0.000000     1.769551
P     0.000000    -1.511416    -0.874453
P     0.000000     1.511416    -0.874453
C     0.000000     0.000000    -1.712831
```

```
H     0.000000     0.000000    -2.804127
H    -1.077718    -0.053652     2.727444
H     1.077718     0.053652     2.727444
C     0.289540    -1.417435     0.830947
C    -0.289540     1.417435     0.830947
H     0.761601    -2.274745     1.311156
H    -0.761601     2.274745     1.311156
H     0.986778    -2.413646    -1.392202
H    -0.986778     2.413646    -1.392202
H    -1.159232    -2.291912    -1.246370
H     1.159232     2.291912    -1.246370
```

$HPCH_2$ (C_s)

```
E=-381.2725742

C     0.056558     1.071834     0.000000
P     0.056558    -0.595635     0.000000
H     1.001168     1.601678     0.000000
H    -0.829821     1.691571     0.000000
H    -1.359065    -0.789730     0.000000
```

H_3PCH_2 (C_s)

```
E=-382.4359378

P    -0.013849    -0.477953     0.000000
C    -0.013849     1.199902     0.000000
H     1.112376    -1.385217     0.000000
H    -0.685244    -1.008751     1.116978
H    -0.685244    -1.008751    -1.116978
H     0.274470     1.686298     0.921685
H     0.274470     1.686298    -0.921685
```

Benzene (D_{6h})

```
E=-232.335571

C     0.000000     1.391033     0.000000
C     1.204670     0.695517     0.000000
C     1.204670    -0.695517     0.000000
C     0.000000    -1.391033     0.000000
C    -1.204670    -0.695517     0.000000
C    -1.204670     0.695517     0.000000
H     2.141581     1.236442     0.000000
H     2.141581    -1.236442     0.000000
H     0.000000    -2.472884     0.000000
H    -2.141581    -1.236442     0.000000
H    -2.141581     1.236442     0.000000
H     0.000000     2.472884     0.000000
```

Optimised geometries in Cartesian coordinates (in angstroms) and total energies (in hartrees) at the B3LYP/cc-pVDZ level of theory.

I

E=-1611.9392974

P	0.122064	-1.838287	0.000000
P	-1.653089	0.813516	0.000000
P	1.531103	1.024915	0.000000
C	-1.368985	-0.935647	0.000000
C	-2.689895	-1.773826	0.000000
C	-3.517773	-1.431835	1.263427
C	1.494931	-0.717694	0.000000
C	2.881293	-1.442636	0.000000
C	2.998691	-2.330450	1.263475
C	-0.125819	1.653475	0.000000
C	-0.191269	3.216519	0.000000
C	0.518817	3.762204	1.263515
C	-2.448400	-3.297228	0.000000
C	-3.517773	-1.431835	-1.263427
C	-1.631308	3.769033	0.000000
C	0.518816	3.762204	-1.263515
C	4.080048	-0.471928	0.000000
C	2.998691	-2.330449	-1.263475
H	-3.421789	-3.814190	0.000000
H	-2.198054	3.452473	-0.889032
H	5.014398	-1.056505	0.000000
H	-2.952475	-1.669692	-2.178907
H	-2.952475	-1.669692	2.178908
H	-3.789727	-0.366151	-1.299351
H	-3.789727	-0.366150	1.299351
H	-4.450073	-2.020891	1.273678
H	-4.450073	-2.020890	-1.273678
H	-1.890787	-3.629799	-0.888965
H	-1.890787	-3.629799	0.888966
H	0.474445	4.864140	-1.274612
H	0.474444	4.864140	1.274611
H	1.577836	3.465208	-1.299114
H	1.577836	3.465207	1.299114
H	0.030414	3.390695	-2.178786
H	0.030415	3.390694	2.178786
H	-1.592297	4.870488	0.000000
H	-2.198053	3.452472	0.889033
H	2.211793	-3.098852	1.298767
H	2.211793	-3.098851	-1.298766
H	2.921234	-1.721839	-2.178825
H	2.921234	-1.721839	2.178825
H	3.975043	-2.843199	-1.274507
H	3.975043	-2.843199	1.274508
H	4.089417	0.177212	-0.888995
H	4.089417	0.177212	0.888995

II

E=-1613.1001803

P	-0.911180	-1.627902	-0.268030
P	-1.023521	1.524336	-0.288297
P	1.101089	0.029678	1.043628
C	-1.726738	-0.081210	0.003722
C	-3.290647	-0.099190	0.042096
C	-3.770958	0.763282	1.233270
C	0.759233	-1.459985	0.162360
C	1.840736	-2.517645	-0.140365
C	2.424822	-3.073473	1.180833
C	0.644585	1.495045	0.165372
C	1.643770	2.630377	-0.136889
C	2.196017	3.214623	1.185538
C	0.960408	3.771077	-0.915741
C	2.821910	2.108310	-0.991663
C	-3.858221	-1.519703	0.242662
C	-3.892397	0.469366	-1.265767
C	2.985761	-1.908141	-0.981949
C	1.245129	-3.697124	-0.933509
H	-4.954937	-1.466384	0.344794
H	0.560727	3.421223	-1.880132
H	3.742060	-2.676726	-1.216590
H	-3.576890	-0.131627	-2.133688
H	-3.372114	0.374782	2.184464
H	-3.576299	1.509033	-1.441709
H	-3.439928	1.809276	1.132397
H	-4.872986	0.760553	1.294788
H	-4.994980	0.456243	-1.221497
H	-3.634830	-2.181664	-0.607795
H	-3.456823	-1.993149	1.153258
H	3.522158	2.928653	-1.225097
H	2.908406	4.031988	0.982058
H	3.397429	1.327571	-0.468653
H	2.733360	2.456638	1.779755
H	2.459790	1.682096	-1.939958
H	1.380497	3.616475	1.807219
H	1.693110	4.568964	-1.119113
H	0.127014	4.210616	-0.346548
H	1.636568	-3.542218	1.790712
H	0.442666	-4.201323	-0.373542
H	0.825817	-3.366914	-1.896528
H	2.898130	-2.283579	1.788020
H	2.033803	-4.438770	-1.140911
H	3.199108	-3.832179	0.975783
H	2.602531	-1.499260	-1.929566
H	3.503703	-1.094822	-0.448006
H	0.364502	0.005813	2.273271
H	2.452144	0.083357	1.473486

III

E=-1614.2565775

P	-1.658756	0.465237	-0.185508
P	0.438343	-1.799523	-0.077952
P	1.273817	1.175569	-0.099869
C	-1.196955	-1.237217	-0.104676
C	-2.357432	-2.269389	0.037126
C	-1.890720	-3.702623	-0.292626
C	-0.394500	1.652402	-0.134595
C	-0.767403	3.154048	0.048548
C	0.316907	4.076686	-0.549818
C	1.636615	-0.551185	-0.121275
C	3.138027	-0.956306	0.017249
C	3.566436	-0.900516	1.503855
C	4.058382	-0.018935	-0.798116
C	3.387370	-2.389047	-0.500869
C	-2.087765	3.492471	-0.678279
C	-0.925223	3.487134	1.550831
C	-3.525043	-1.941942	-0.922829
C	-2.891608	-2.269111	1.490533
H	-2.511743	0.679139	-1.320986
H	-2.653389	0.742823	0.819655
H	1.963932	1.802310	1.002635
H	2.002299	1.836021	-1.143106
H	-2.022106	3.264727	-1.754114
H	-2.950129	2.945981	-0.262725
H	-2.313430	4.566138	-0.570191
H	-1.716618	2.875024	2.013233
H	-1.189307	4.548730	1.702898
H	0.010398	3.290799	2.099220
H	0.018467	5.131390	-0.432763
H	1.290096	3.966359	-0.044258
H	0.462388	3.881583	-1.624240
H	3.773644	-0.003391	-1.862506
H	4.049683	1.018364	-0.424344
H	5.102167	-0.367075	-0.730789
H	2.969954	-1.605949	2.103232
H	4.632677	-1.163220	1.620125
H	3.425086	0.105589	1.931934
H	3.094633	-2.487505	-1.558179
H	2.828017	-3.141794	0.072729
H	4.459904	-2.630306	-0.414626
H	-3.728004	-2.980863	1.603691
H	-2.094981	-2.558136	2.193753
H	-3.262308	-1.276199	1.793228
H	-2.745046	-4.394041	-0.205113
H	-1.494527	-3.771174	-1.317953
H	-1.105204	-4.051690	0.393148

H	-4.306702	-2.715661	-0.845646
H	-4.010830	-0.980111	-0.688849
H	-3.182615	-1.905927	-1.969517

IV

E=-1615.4150232

P	-0.055981	-1.744163	0.002720
P	-1.477351	0.918769	0.037760
P	1.532085	0.818696	-0.164854
C	-1.518879	-0.815911	0.138141
C	-2.887795	-1.543470	-0.012970
C	-3.268386	-1.717401	-1.502721
C	1.464236	-0.918270	-0.164367
C	2.781748	-1.726069	0.027262
C	3.965496	-1.026434	-0.675875
C	0.049024	1.725792	-0.164317
C	0.105775	3.271343	0.018737
C	1.327926	3.869108	-0.712313
C	-2.842938	-2.936636	0.652752
C	-4.009024	-0.751843	0.696262
C	-1.146274	3.939857	-0.590518
C	0.193381	3.654129	1.516005
C	2.659593	-3.130315	-0.604776
C	3.125391	-1.884331	1.528043
H	2.363831	1.268411	-1.242836
H	2.398966	1.276104	0.900922
H	-2.403462	1.344210	-0.979438
H	-0.220130	-2.719730	-1.045399
H	-2.183985	1.509762	1.146782
H	0.044715	-2.693144	1.081876
H	-3.828608	-3.424645	0.576105
H	-2.118668	-3.611696	0.168008
H	-2.580940	-2.859221	1.719794
H	-4.238691	-2.233251	-1.614818
H	-3.347674	-0.741677	-2.009061
H	-2.509637	-2.310059	-2.039219
H	-4.963906	-1.298023	0.620885
H	-3.779269	-0.608110	1.763858
H	-4.176461	0.239271	0.243629
H	3.610262	-3.678682	-0.497407
H	1.884851	-3.745380	-0.118391
H	2.421317	-3.063322	-1.678078
H	4.878626	-1.635053	-0.569893
H	3.767876	-0.889875	-1.750865
H	4.192030	-0.040061	-0.238381
H	4.059949	-2.455625	1.670872
H	3.255983	-0.901657	2.009593
H	2.323350	-2.415058	2.066122
H	1.324611	4.967298	-0.614967

```
H      2.283734     3.518399    -0.289624
H      1.313372     3.620068    -1.785196
H      0.234472     4.749682     1.651105
H     -0.680548     3.280805     2.074238
H      1.094840     3.225131     1.982426
H     -1.076255     5.035946    -0.492896
H     -1.246379     3.695812    -1.659973
H     -2.075119     3.636532    -0.080240
```

Optimised geometries in Cartesian coordinates (in angstroms) and total energies (in hartrees) at the B3LYP/cc-pVDZ(-PP) level of theory.

V' (C_{3v})

```
E=-1548.3503148

Mo     0.000000     0.000000     0.349926
P     -1.662259     0.959706    -1.494224
P      0.000000    -1.919411    -1.494224
P      1.662259     0.959706    -1.494224
O      2.205422    -1.273301     2.238738
O      0.000000     2.546602     2.238738
O     -2.205422    -1.273301     2.238738
C      1.400023    -0.808304     1.557916
C      0.000000     1.616608     1.557916
C     -1.400023    -0.808304     1.557916
C     -1.373842    -0.793188    -1.410083
C      1.373842    -0.793188    -1.410083
C      0.000000     1.586376    -1.410083
H      0.000000     2.678314    -1.282499
H     -2.319488    -1.339157    -1.282499
H      2.319488    -1.339157    -1.282499
```

VI' (C_s)

```
E=-1549.5122671

Mo     0.037718     0.453817     0.000000
P     -1.481447    -2.153782     0.000000
P      1.052093    -1.259400     1.638208
P      1.052093    -1.259400    -1.638208
O      1.052093     2.617800     2.070297
O      1.052093     2.617800    -2.070297
O     -2.854956     1.734133     0.000000
C     -1.782240     1.301186     0.000000
C      1.719095    -1.356431     0.000000
C     -0.708045    -1.399712     1.388090
C     -0.708045    -1.399712    -1.388090
C      0.681774     1.809054     1.329826
C      0.681774     1.809054    -1.329826
H     -2.860210    -1.816062     0.000000
```

H	-1.569589	-3.595611	0.000000
H	2.807330	-1.208172	0.000000
H	-1.301255	-1.345113	2.306149
H	-1.301255	-1.345113	-2.306149

VII' (Cs)

E=-1550.6702613

Mo	-0.032093	0.539130	0.000000
P	-0.488088	-1.992048	1.500563
P	-0.488088	-1.992048	-1.500563
P	2.084592	-0.840995	0.000000
O	-1.613137	1.955554	2.340206
O	-1.613137	1.955554	-2.340206
O	1.817132	3.082502	0.000000
C	-1.328502	-1.581023	0.000000
C	1.152061	2.129594	0.000000
C	1.026893	-1.121387	1.418519
C	1.026893	-1.121387	-1.418519
C	-1.040203	1.450613	1.464912
C	-1.040203	1.450613	-1.464912
H	-2.409190	-1.757879	0.000000
H	1.528810	-0.953387	2.377328
H	1.528810	-0.953387	-2.377328
H	-0.434456	-3.397091	1.858915
H	-0.434456	-3.397091	-1.858915
H	-1.283183	-1.499640	2.566818
H	-1.283183	-1.499640	-2.566818

VIII' (C_{3v})

E=-1551.8174705

Mo	0.000000	0.000000	0.629959
P	-1.517013	-0.875848	-1.725796
P	1.517013	-0.875848	-1.725796
P	0.000000	1.751696	-1.725796
O	2.239881	-1.293196	2.403568
O	0.000000	2.586392	2.403568
O	-2.239881	-1.293196	2.403568
C	1.393158	-0.804340	1.761795
C	0.000000	1.608680	1.761795
C	-1.393158	-0.804340	1.761795
C	-1.409342	0.813684	-1.236902
C	0.000000	-1.627368	-1.236902
C	1.409342	0.813684	-1.236902
H	-2.357563	1.361140	-1.208695
H	0.000000	-2.722279	-1.208695
H	2.357563	1.361140	-1.208695
H	0.000000	2.973064	-1.011885

H	-2.574749	-1.486532	-1.011885
H	2.574749	-1.486532	-1.011885
H	0.000000	2.259716	-3.089814
H	-1.956971	-1.129858	-3.089814
H	1.956971	-1.129858	-3.089814

V

E=-2020.0894539

Mo	-0.000147	0.002693	0.966097
P	1.613601	0.983213	-0.922951
P	0.047297	-1.895988	-0.909485
P	-1.661929	0.899795	-0.924113
O	-2.318651	-0.815146	2.944229
O	1.883361	-1.579201	2.942601
O	0.440499	2.430655	2.932415
C	-0.049005	1.646327	-0.854133
C	1.452694	-0.786711	-0.849707
C	-1.405270	-0.871144	-0.845907
C	-2.742802	-1.702885	-0.896444
C	-2.991420	-2.030714	-2.390082
C	-1.479645	-0.519188	2.203915
C	-0.100477	3.220647	-0.905511
C	-0.251117	3.600523	-2.400219
C	1.199939	-1.007930	2.203590
C	0.283473	1.551098	2.196646
C	-3.968227	-0.923878	-0.367371
C	-2.660790	-3.026218	-0.102204
C	1.182411	3.892780	-0.366515
C	-1.294550	3.811703	-0.121907
C	2.842426	-1.527887	-0.897964
C	3.254213	-1.576282	-2.391007
C	2.781816	-2.979858	-0.371877
C	3.944851	-0.793340	-0.101882
H	1.051889	4.986216	-0.403382
H	-3.837602	-0.604550	0.676597
H	3.791470	-3.417995	-0.423965
H	-1.243575	3.558393	0.946850
H	0.588932	3.211828	-2.997880
H	-2.265519	3.470414	-0.508329
H	-1.184703	3.198817	-2.824709
H	-0.269173	4.697210	-2.511171
H	-1.273446	4.909937	-0.209431
H	1.387056	3.616590	0.677810
H	2.071261	3.649222	-0.966228
H	-3.618359	-3.562924	-0.197818
H	-3.929926	-2.598422	-2.501121
H	-1.870925	-3.694874	-0.473226
H	-2.173197	-2.636218	-2.810676
H	-2.481368	-2.845524	0.967660

H	-3.076687	-1.110822	-2.990586
H	-4.850360	-1.582975	-0.406669
H	-4.197677	-0.034760	-0.972335
H	3.373141	-0.563923	-2.808237
H	4.139137	0.219234	-0.483681
H	3.690089	-0.714065	0.964820
H	2.500832	-2.106489	-2.995479
H	4.885347	-1.361759	-0.182273
H	4.214299	-2.106842	-2.501266
H	2.450907	-3.028333	0.675521
H	2.117014	-3.618525	-0.971121

VI

E= -2021.256768

Mo	0.077988	-0.026083	1.013713
P	0.889591	-1.640275	-0.816919
P	1.016506	1.600187	-0.751687
P	-1.535489	0.089623	-1.579451
O	1.303276	-2.134265	3.011874
O	-2.642437	-0.111071	2.613805
O	1.265173	2.032223	3.093541
C	1.683109	-0.046367	-0.934719
C	3.250630	-0.081514	-1.033741
C	3.923880	0.885141	-0.033265
C	0.843721	-1.375755	2.263503
C	-0.769177	1.475583	-0.784871
C	-1.581742	2.812962	-0.723578
C	-2.870608	2.652557	0.111015
C	-0.884376	-1.369379	-0.813141
C	-1.762748	-2.667990	-0.791700
C	-1.237074	-3.660315	0.266633
C	-1.958366	3.252819	-2.158389
C	-0.758299	3.944715	-0.073836
C	-1.635793	-0.067880	2.039276
C	0.833908	1.286749	2.316862
C	3.622076	0.341092	-2.475657
C	3.840133	-1.484725	-0.777413
C	-1.715559	-3.343922	-2.182465
C	-3.236489	-2.367291	-0.441392
H	4.938807	-1.429463	-0.842233
H	-0.404911	3.667052	0.930803
H	-3.779976	-3.315813	-0.304660
H	3.679964	0.610255	1.004315
H	3.157236	-0.328822	-3.217058
H	3.620477	1.930940	-0.188710
H	3.287207	1.368499	-2.690563
H	4.714965	0.302360	-2.617666
H	5.018437	0.837168	-0.153760
H	3.581043	-1.862547	0.223977

H	3.502464	-2.225227	-1.518302
H	-3.447595	3.591524	0.090253
H	-2.490572	4.218192	-2.141162
H	-3.535836	1.861038	-0.268240
H	-2.627741	2.528345	-2.654872
H	-2.634350	2.419207	1.158441
H	-1.061089	3.369901	-2.787087
H	-1.392408	4.840117	0.026794
H	0.118023	4.224980	-0.676960
H	-0.690467	-3.656021	-2.437814
H	-0.186974	-3.939703	0.095182
H	-1.313479	-3.235726	1.278446
H	-2.067710	-2.664763	-2.977802
H	-1.835782	-4.584790	0.233287
H	-2.359695	-4.238831	-2.204131
H	-3.327209	-1.791760	0.492050
H	-3.761367	-1.821013	-1.241863
H	-2.925177	0.162501	-1.333434
H	-1.542332	0.100908	-3.024819

VII

E=-2022.4156728

Mo	0.009344	-0.164413	1.022705
P	-1.509051	0.876635	-1.323815
P	1.439648	1.045590	-1.293374
P	0.102798	-1.785539	-0.909160
O	0.215256	-2.655751	2.923719
O	-2.409843	0.724257	2.842754
O	2.248414	1.166100	2.805917
C	-1.418401	-0.823889	-0.862715
C	0.135879	-1.744317	2.203518
C	-2.738972	-1.667630	-0.941089
C	-3.971746	-0.843329	-0.511614
C	-0.083746	1.712899	-0.658669
C	1.511197	-0.664281	-0.864858
C	2.913831	-1.366046	-0.940582
C	2.967232	-2.592337	-0.004851
C	-2.662908	-2.892118	-0.004115
C	-2.953761	-2.156759	-2.392701
C	-0.208102	3.271318	-0.471046
C	1.138208	3.894882	-0.048097
C	-1.216278	3.583310	0.654948
C	-0.667679	3.960288	-1.776784
C	-1.501518	0.413139	2.183935
C	1.408183	0.672540	2.168062
C	4.054596	-0.419091	-0.508376
C	3.180449	-1.826574	-2.392706
H	-4.855156	-1.500130	-0.469306
H	2.832354	-2.294178	1.045086

H	0.980791	4.953995	0.210016
H	-2.562638	-2.580263	1.045848
H	-3.001541	-1.314519	-3.103826
H	-1.814872	-3.550278	-0.244370
H	-2.133458	-2.818818	-2.712018
H	-3.898809	-2.718691	-2.480498
H	-3.584031	-3.488931	-0.104398
H	-3.837023	-0.397302	0.485959
H	-4.215890	-0.040359	-1.227744
H	5.001461	-0.980677	-0.467441
H	4.175351	-2.295113	-2.478384
H	4.214753	0.407491	-1.221384
H	3.150138	-0.979672	-3.099146
H	3.873689	0.006473	0.491043
H	2.428371	-2.562561	-2.718204
H	3.947490	-3.086317	-0.103720
H	2.196195	-3.338704	-0.246233
H	-1.681180	3.645970	-2.079247
H	-2.217515	3.168815	0.463499
H	-0.866134	3.176334	1.613760
H	0.015451	3.741705	-2.614491
H	-1.333143	4.674410	0.758800
H	-0.698300	5.054926	-1.649009
H	1.560782	3.394852	0.836580
H	1.886475	3.876294	-0.857630
H	2.475236	1.726392	-0.623327
H	1.780449	1.390951	-2.665526
H	-1.839699	1.148597	-2.712081
H	-2.622377	1.485474	-0.703662

VIII

E=-2023.5662246

Mo	-0.008055	0.002127	1.086846
P	-0.413619	-1.668609	-1.302747
P	1.674830	0.471373	-1.267610
P	-1.227867	1.199200	-1.303798
O	2.459184	0.742506	2.871130
O	-0.611766	-2.483070	2.899690
O	-1.889946	1.748480	2.885192
C	1.208612	-1.171394	-0.769277
C	2.335181	-2.269691	-0.749730
C	1.859706	-3.512827	0.032151
C	-1.608831	-0.458630	-0.778739
C	-3.122350	-0.890564	-0.768462
C	-3.983648	0.190925	-0.080942
C	1.523640	0.458644	2.223453
C	0.415658	1.627668	-0.777898
C	0.794844	3.154196	-0.757496
C	2.179487	3.356139	-0.104792

C	-0.386512	-1.546324	2.232472
C	-1.175221	1.093486	2.226056
C	3.590809	-1.737017	-0.026759
C	2.729600	-2.699857	-2.181464
C	-0.224352	3.944276	0.090417
C	0.828579	3.747160	-2.184696
C	-3.301967	-2.190453	0.044506
C	-3.657123	-1.117120	-2.200819
H	2.696513	-4.222069	0.133645
H	2.242364	2.861149	0.875792
H	-5.013080	-0.182556	0.037329
H	3.346374	-1.342951	0.970601
H	1.874247	-3.126171	-2.732103
H	4.105165	-0.948301	-0.599625
H	3.118235	-1.852963	-2.771410
H	3.517471	-3.470903	-2.153667
H	4.317603	-2.555703	0.094421
H	1.506853	-3.244031	1.037817
H	1.053245	-4.057309	-0.484747
H	0.107604	4.990670	0.181699
H	1.114387	4.811824	-2.157815
H	-1.225646	3.974294	-0.368128
H	-0.156140	3.686796	-2.678202
H	-0.321366	3.517161	1.098274
H	1.557458	3.225148	-2.827000
H	2.360196	4.432754	0.041273
H	3.002027	2.986844	-0.739341
H	-3.110565	-1.921734	-2.720823
H	-2.823882	-3.060849	-0.432935
H	-2.895508	-2.087185	1.060510
H	-3.576646	-0.206000	-2.816961
H	-4.374676	-2.428996	0.121135
H	-4.721004	-1.406516	-2.178179
H	-3.593343	0.445532	0.915254
H	-4.056253	1.115844	-0.676211
H	-2.111268	2.067226	-0.635246
H	-1.573927	1.528146	-2.681102
H	-0.523220	-2.127463	-2.681691
H	-0.723156	-2.870909	-0.639270
H	2.842566	0.802243	-0.555642
H	2.179068	0.613185	-2.628827

$Mo(CO)_3(C_6H_6)$ (C_{3v})

E=-640.3855864

Mo	-0.118444	-0.000051	0.000126
O	-1.966277	-1.723437	-1.879040
O	-1.969898	-0.764694	2.430039
O	-1.964567	2.490298	-0.553974
C	1.801836	-0.362193	-1.371433

C	1.805184	-1.374927	-0.360006
C	1.800750	-1.008228	1.000239
C	1.805273	0.374132	1.371151
C	1.801810	1.368907	0.373507
C	1.805839	0.999306	-1.009158
C	-1.307468	-1.078935	-1.175475
C	-1.309692	-0.478052	1.520959
C	-1.306917	1.557984	-0.347409
H	1.803133	1.770527	-1.779478
H	1.798899	-0.646464	-2.424021
H	1.802946	-2.427453	-0.643692
H	1.795559	-1.777445	1.772815
H	1.803509	0.655235	2.424367
H	1.796858	2.422411	0.654252

$Mo(CO)_3(C_6H_6)$ TS (C_{3v}, NImag=1)

E= -640.3853113

Mo	0.000000	0.000000	0.118565
O	0.000000	2.549971	1.965165
O	-2.208340	-1.274986	1.965165
O	2.208340	-1.274986	1.965165
C	0.000000	1.594699	1.308162
C	-1.381050	-0.797350	1.308162
C	1.381050	-0.797350	1.308162
C	1.223721	-0.706516	-1.787596
C	0.000000	1.413031	-1.787596
C	-1.223721	-0.706516	-1.787596
C	0.000000	-1.426085	-1.817839
C	1.235026	0.713043	-1.817839
C	-1.235026	0.713043	-1.817839
H	0.000000	-2.515443	-1.823590
H	2.178438	1.257722	-1.823590
H	-2.178438	1.257722	-1.823590
H	-2.168447	-1.251954	-1.773998
H	2.168447	-1.251954	-1.773998
H	0.000000	2.503907	-1.773998