

MP2/aug-cc-pVDZ geometries in A

I

6	-0.115611	1.909638	0.000000
1	-0.157643	3.010218	0.000000
8	-1.134615	1.215092	0.000000
8	1.134615	1.469398	0.000000
1	1.130966	0.468172	0.000000
6	0.115611	-1.909638	0.000000
8	1.134615	-1.215092	0.000000
8	-1.134615	-1.469398	0.000000
1	-1.130966	-0.468172	0.000000
1	0.157643	-3.010218	0.000000

II

1	3.293609	0.279509	0.000053
6	2.190882	0.241949	0.000016
8	1.477674	1.236648	-0.000016
8	1.765564	-1.029739	0.000006
1	0.773782	-1.021779	-0.000018
1	-0.857912	1.093840	-0.000011
6	-1.465194	0.176882	-0.000008
8	-0.998898	-0.957060	-0.000009
8	-2.783757	0.443825	0.000008
1	-3.248271	-0.413943	0.000014

III

1	-3.294644	0.561641	-0.049044
6	-2.218650	0.328579	-0.017713
8	-1.339404	1.178876	0.034694
8	-2.027955	-1.002777	-0.045517
1	-1.062971	-1.174288	-0.016216
1	2.596939	-1.434291	0.011192
6	2.155602	-0.422952	0.003656
8	2.783958	0.612960	-0.063629
8	0.800463	-0.511403	0.082924
1	0.402462	0.391924	0.070638

IV

1	-0.910814	-1.097933	-0.000011
6	-1.669351	-0.300338	-0.000007
8	-2.874294	-0.429980	-0.000190
8	-1.038387	0.924461	0.000254
1	-1.739953	1.601208	0.000295
1	3.322216	-0.340314	-0.000045
6	2.221479	-0.271135	-0.000022
8	1.471998	-1.235067	0.000138
8	1.835970	1.019725	-0.000199
1	0.853491	1.032766	-0.000093

V

1	1.084540	-0.972728	-0.000003
6	1.736610	-0.085295	-0.000002
8	1.340605	1.068490	-0.000033
8	3.043679	-0.446552	0.000038
1	3.558484	0.381511	0.000036
1	-1.084540	0.972728	-0.000062
6	-1.736610	0.085295	-0.000022
8	-1.340604	-1.068489	-0.000039
8	-3.043679	0.446551	0.000046
1	-3.558484	-0.381512	0.000078

VI

1	-1.135695	1.006941	0.000070
6	-1.751933	0.094050	0.000025
8	-1.313176	-1.043077	0.000023
8	-3.069108	0.412432	-0.000030
1	-3.558312	-0.431103	-0.000069
1	1.077767	-0.961277	0.000000
6	1.896894	-0.224921	-0.000004
8	3.087674	-0.467234	-0.000020
8	1.371263	1.038378	0.000011
1	2.133252	1.646676	0.000007

RIMP2/TZVPP geometries in a.u.

I

C	0.220568	-3.574435	-0.000003
H	0.312560	-5.633628	0.000022
O	2.125269	-2.270742	-0.000014
O	-2.120265	-2.757460	-0.000006
H	-2.122422	-0.872425	-0.000001
C	-0.220568	3.574435	0.000004
O	-2.125269	2.270742	0.000014
O	2.120265	2.757460	0.000006
H	2.122422	0.872425	0.000000
H	-0.312560	5.633628	-0.000018

II

H	6.196698	0.525308	0.000101
C	4.132307	0.458494	0.000030
O	2.801989	2.321265	-0.000031
O	3.332352	-1.921968	0.000019
H	1.469348	-1.909879	-0.000033
H	-1.636535	2.043252	-0.000026
C	-2.771227	0.326846	-0.000015
O	-1.892953	-1.792411	-0.000034
O	-5.239023	0.830591	0.000021
H	-6.116830	-0.776540	0.000035

III

H	-6.197567	1.057634	-0.091330
C	-4.184147	0.620324	-0.033338
O	-2.538180	2.209397	0.064444
O	-3.823042	-1.870888	-0.085303
H	-2.009156	-2.188345	-0.030188
H	4.892766	-2.685081	0.020967
C	4.069360	-0.791947	0.006665
O	5.245484	1.144490	-0.119021
O	1.529979	-0.958968	0.154771
H	0.777443	0.734084	0.133683

IV

H	-1.994562	-1.690967	-1.608038
C	-3.354293	-0.145191	-1.654385
O	-5.387856	-0.131206	-2.656794
O	-2.389640	1.865380	-0.359729
H	-3.644640	3.195698	-0.44164
H	5.189128	-1.221154	2.144372
C	3.313640	-0.883556	1.351601
O	2.134080	-2.420515	0.142615
O	2.533897	1.449007	1.912254
H	0.858349	1.666947	1.170025

V

H	2.065830	-1.814638	-0.000005
C	3.286941	-0.155118	-0.000003
O	2.546795	2.003171	-0.000066
O	5.732521	-0.834964	0.000077
H	6.700946	0.718393	0.000064
H	-2.065831	1.814639	-0.000115
C	-3.286941	0.155118	-0.000043
O	-2.546793	-2.003170	-0.00007
O	-5.732521	0.834963	0.000089
H	-6.700945	-0.718395	0.000149

VI

H	-2.162316	1.879596	0.000137
C	-3.317087	0.172873	0.000047
O	-2.497521	-1.954633	0.000026
O	-5.782176	0.771022	-0.000049
H	-6.700382	-0.812894	-0.000134
H	2.061638	-1.796904	0.000002
C	3.591650	-0.416281	-0.000002
O	5.819603	-0.867250	-0.000044
O	2.603216	1.945132	0.000052
H	4.030904	3.091018	0.000030