Supporting Information

for

A computational study of base-catalyzed reactions of cyclic 1,2-diones: cyclobutane-1,2-dione

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Detailed computational results and plot of MP2, SCS-MP2 and M06-2X vs. CEPA ΔG_{rel} values, pertinent structural data, and Cartesian coordinates of all stationary structures.

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Table S1: Relative Gibbs free energies excluding bulk solvation[a].

	M06-2X	MP2	SCS-MP2	E_C	CEPA/1
IDC	-19.2	-17.6	-15.1	-18.1	-14.4
TS1	-12.9	-12.7	-9.3	-13.0	-8.2
Int1	-25.3	-23.6	-23.4	-25.1	-21.4
TS2	-8.4	-9.3	-6.9	-6.8	-1.8
P1a	-33.9	-29.0	-29.7	-27.6	-24.9
2	-52.2	-48.2	-49.5	-47.8	-44.0
TS3a	-6.9	-4.0	-1.8	-3.0	0.2
P2	-63.4	-61.2	-63.6	-63.0	-60.3
TS4	-7.2	-6.0	-3.4	-6.0	-1.4
Int4	-9.0	-5.9	-3.0	-5.6	-1.0
TS5	10.6	15.0	17.4	13.0	18.5
P3a	-50.6	-45.0	-44.4	-45.0	-42.5
Int2a	-43.6	-38.0	-39.0	-40.2	-36.5
P2a	-59.6	-56.6	-58.2	-57.9	-54.6

[a] ΔG (kcal mol^{-1}) with respect to separated reactants **1**·$(H_2O)_2$ + $[OH(H_2O)_4]^-$. All geometries optimized with M06-2X/6-31+G(d,p). For M06-2X, MP2, and SCS-MP2 single point calculations the 6-311+G(2df,2p) basis set was used; LPNO-CEPA calculations were done with the def2-QZVPP basis set; $E_C = E$[MP2/6-311+G(2df,2p)] + E{[CCSD(T) – MP2]/6-31+G(d)}.

Table S2: Relative electronic, ZPE and thermal and solvation energies[a].

	M06-2X	MP2	SCS-MP2	E_C	CEPA	dG-corr	ΔG_{solv}
IDC	-35.2	-33.6	-31.1	-34.1	-30.4	17.9	21.7
TS1	-30.5	-30.3	-26.8	-30.6	-25.7	19.4	19.3
Int1	-44.4	-42.7	-42.5	-44.2	-40.5	21.0	19.2
TS2	-25.5	-26.3	-24.0	-23.9	-18.9	19.0	16.2
P1a	-50.7	-45.8	-46.6	-44.5	-41.7	18.8	18.6
2	-73.0	-69.1	-70.3	-68.6	-64.9	22.7	19.6
TS3a	-21.2	-18.2	-16.1	-17.3	-14.0	16.2	19.7
P2	-81.1	-78.9	-81.3	-80.7	-78.0	19.6	23.7
TS4	-28.6	-27.4	-24.8	-27.3	-22.7	23.3	23.6
Int4	-30.8	-27.7	-24.8	-27.4	-22.8	23.7	23.7
TS5	-9.7	-5.3	-2.9	-7.3	-1.8	22.2	23.7
P3a	-71.3	-65.7	-65.1	-65.7	-63.2	22.6	21.3
Int2a	-64.2	-58.6	-59.7	-60.9	-57.2	22.5	18.1
P2a	-80.7	-77.6	-79.3	-79.0	-75.7	23.0	19.3

[a] ΔG (kcal mol^{-1}) with respect to separated reactants **1**·$(H_2O)_2$ + $[OH(H_2O)_4]^-$. All geometries optimized with M06-2X/6-31+G(d,p). For M06-2X, MP2, and SCS-MP2 single point calculations the 6-311+G(2df,2p) basis set was used; LPNO-CEPA calculations were done with the def2-QZVPP basis set; $E_C = E$[MP2/6-311+G(2df,2p)] + E{[CCSD(T) – MP2]/6-31+G(d)}; dG-corr from unscaled M06-2X/6-31+G(d,p) frequencies and ZPE corrections; ΔG_{solv} calculated by SMD M06-2X/6-31G(d).

Table S3: Selected calculated structural parameters[a].

	1·$(H_2O)_2$	**TS1**	**Int1**	**TS2**	**2**
C1-O1	1.198	1.234	1.322	1.254	1.246
C1-C2	1.572	1.560	1.564	1.466	1.514
C2-O2	1.198	1.205	1.206	1.258	1.272
C1-O3	-	1.867	1.445	1.391	1.404
C2-C3	1.533	1.537	1.528	1.505	1.496
C1-C4	1.533	1.555	1.573	2.112	2.585
C2-C4	2.188	2.179	2.125	1.863	1.503
C2-C3-C4	90.4	89.8	87.2	76.6	59.6
C1-C2-C3-C4	0.0	-2.6	16.7	54.8	-109.8
	TS4	**Int4**	**TS5**	**P3a**	**TS3a**
C1-O1	1.396	1.429	1.531	1.337	1.224
C1-C2	1.484	1.483	1.853	2.317	1.545
C2-O2	1.261	1.309	1.233	1.367	1.222
C1-O3	1.383	1.369	1.383	1.210	1.314
C2-C3	1.535	1.541	1.531	1.527	1.486

C1-C4	1.536	1.522	1.520	1.518	2.975
C2-C4	2.162	2.177	2.306	2.399	2.259
C2-O1	1.747	1.504	1.385	1.469	-
C2-C3-C4	88.5	88.9	97.2	103.6	96.7
C1-C2-C3-C4	-8.3	-2.7	9.5	14.0	76.0

[a]M06-2X/6-31+G(d,p) results; distances in Å, angles in degrees.

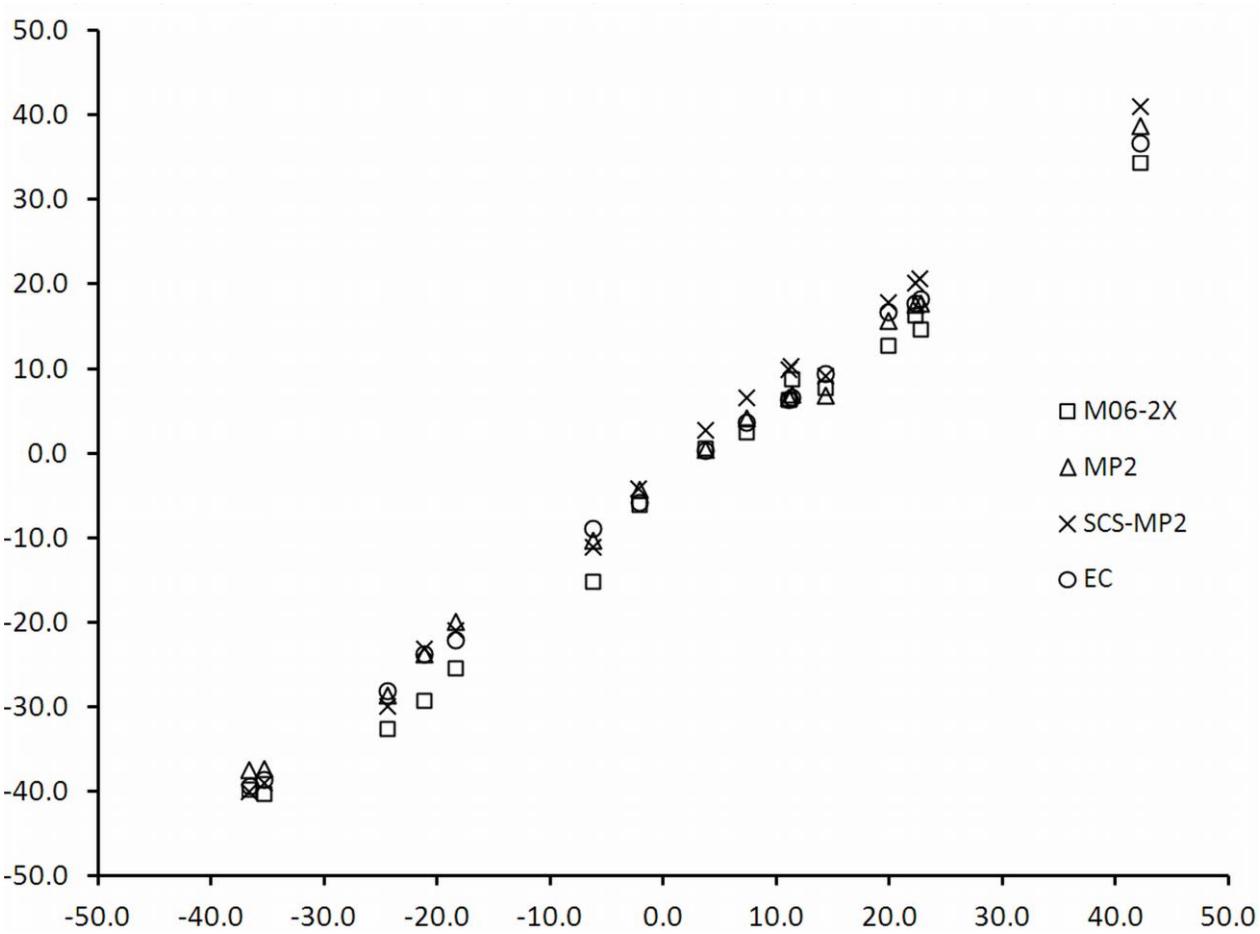

Figure S1: Plot of M06-2x, MP2, SCS-MP2, and E_C vs. LPNO-CEPA/1 relative Gibbs free energies.

cyclobutanedione + $2H_2O$: E(RM062X/6-31+G(d,p)) = -457.928387622

C	-0.77498	-1.01790	0.00042
C	0.77498	-1.01790	-0.00039
C	0.78605	0.51497	-0.00029
O	1.62517	1.37058	-0.00049
C	-0.78605	0.51497	0.00030
O	-1.62517	1.37058	0.00049
H	-1.26439	-1.43703	-0.88185
H	-1.26323	-1.43660	0.88356
H	1.26322	-1.43661	-0.88353
H	1.26439	-1.43702	0.88188
O	-3.67859	-0.60460	-0.00040
H	-4.63743	-0.53620	0.00001
H	-3.33272	0.29957	0.00010
H	3.33272	0.29957	-0.00008
O	3.67859	-0.60460	0.00035
H	4.63743	-0.53619	0.00003

[$OH(H_2O)4$]-: E(RM062X/6-31+G(d,p)) = -381.497273531

O	-0.06850	-0.69264	2.04151
O	-1.50909	-0.34609	0.00000
H	1.35811	-0.57488	0.77137
H	-0.06284	0.20017	2.40277
O	1.88015	-0.28094	0.00000
H	1.35811	-0.57488	-0.77137
O	-0.06850	-0.69264	-2.04151
H	-0.06284	0.20017	-2.40277

H	-0.73170	-0.63228	-1.25021
O	-0.06850	1.99353	0.00000
H	0.74908	1.46976	0.00000
H	-0.76781	1.30269	0.00000
H	-0.73170	-0.63228	1.25021
H	-2.43295	-0.60830	0.00000

IDCa: E(RM062X/6-31+G(d,p)) = -839.479243669

H	3.43390	0.01694	0.59990
O	3.36539	0.69255	1.29692
H	2.76683	1.34320	0.89476
O	1.59417	2.13122	-0.47223
H	2.24169	2.35414	-1.14876
O	0.38802	0.07173	-1.12609
H	0.19178	-0.06305	-2.06149
H	-1.10211	1.14844	-0.92430
O	-1.86653	1.75043	-0.79974
H	-1.48959	2.59314	-0.49571
H	0.49451	3.33384	-0.01401
O	-0.26931	3.90418	0.25102
H	-0.29537	3.87439	1.21171
H	-1.07977	0.33017	1.11501
H	-1.70008	-1.01393	2.10311
C	-1.01090	-0.74217	1.29876
C	0.42455	-1.31897	1.40747
H	0.60467	-1.95399	2.28037
H	1.24063	-0.59867	1.31140

C	0.18911	-2.16003	0.14375
O	0.80427	-3.01623	-0.43302
C	-1.25761	-1.58108	0.03408
O	-2.20878	-1.82224	-0.65876
H	1.07520	1.26706	-0.81477
O	2.88209	-0.98331	-0.96511
H	2.73390	-1.92716	-0.83151
H	1.96634	-0.61279	-1.06765
O	-3.95413	0.30979	0.46087
H	-3.70638	-0.52640	0.04460
H	-3.32855	0.94324	0.06219

TS1: E(RM062X/6-31+G(d,p)) = -839.473374959

H	3.100064	0.719273	1.252814
O	2.926497	1.675043	1.300951
H	2.840287	1.900668	0.362548
O	1.820094	1.464806	-1.371798
H	1.876373	1.824700	-2.262100
O	-0.106392	-0.132378	-1.238091
H	-0.263459	-0.637566	-2.046976
H	-1.393226	1.089227	-0.925841
O	-2.021298	1.769106	-0.601626
H	-1.482264	2.305004	0.001800
H	0.788720	2.581957	-0.162992
O	0.336360	2.899857	0.637671

H	0.918950	2.593425	1.347946
H	-1.728899	0.216558	1.307053
H	-1.566399	-1.237514	2.323335
C	-1.209548	-0.737528	1.418399
C	0.326988	-0.697494	1.227719
H	0.890358	-1.241849	1.990982
H	0.760135	0.291967	1.085315
C	0.202382	-1.551699	-0.065792
O	0.996167	-2.356171	-0.561458
C	-1.335415	-1.638802	0.180180
O	-2.262876	-2.188283	-0.358315
H	1.032245	0.779047	-1.364991
O	3.266166	-0.772521	-0.144923
H	2.613192	-1.495038	-0.244641
H	2.982148	-0.117836	-0.801145
O	-4.252908	0.098772	0.141848
H	-3.826459	-0.749465	-0.040853
H	-3.593162	0.769907	-0.107977

IDC: E(RM062X/6-31+G(d,p)) = -839.483915125

H	-3.46174	0.31211	-1.31075
O	-3.21337	1.24597	-1.25999
H	-2.93364	1.32037	-0.32308
O	-2.00989	1.00450	1.22257
H	-2.38838	1.43497	1.99568
O	0.27695	0.09147	1.55402
H	0.33692	-0.46473	2.33720

H	1.45953	1.48467	1.22338
O	1.93021	2.20738	0.76425
H	1.23050	2.59604	0.21199
H	-1.10818	2.10411	0.24253
O	-0.60276	2.58150	-0.46287
H	-1.12722	2.42703	-1.25891
H	1.25359	0.67753	-0.97634
H	1.60316	-0.52624	-2.24609
C	1.08664	-0.35162	-1.29822
C	-0.38783	-0.81712	-1.22149
H	-0.79938	-1.27609	-2.12529
H	-1.08833	-0.06397	-0.85543
C	-0.01359	-1.86292	-0.16486
O	-0.59662	-2.74730	0.40304
C	1.47863	-1.38451	-0.23523
O	2.50740	-1.74621	0.26753
H	-0.70802	0.46480	1.49570
O	-3.24186	-1.25246	0.28481
H	-2.60028	-1.97230	0.34403
H	-2.83095	-0.49652	0.76843
O	4.06923	0.76671	-0.48990
H	3.80203	-0.11113	-0.18734
H	3.42299	1.37391	-0.08444

TS1a: E(RM062X/6-31+G(d,p)) = -839.473184876

C	2.39124	-1.91915	0.03815
C	2.17884	-0.50976	-0.54820

O	2.48857	0.02200	-1.58940
C	1.83786	-1.42887	1.40262
C	1.60530	-0.02402	0.80129
O	1.39920	1.06079	1.30189
O	0.10758	3.47735	0.49336
O	0.20045	1.83895	-1.79453
O	-0.03004	-0.79210	-0.30526
O	-1.69179	-2.65326	-0.97310
O	-2.15685	1.71991	-0.01142
O	-3.77518	-0.84310	-0.30023
O	-1.73180	-0.45556	1.74473
H	3.44837	-2.20120	0.04573
H	1.79781	-2.67964	-0.46919
H	0.92690	-1.90994	1.75765
H	2.58278	-1.39288	2.20298
H	-2.55348	-0.81168	1.37033
H	-1.04361	-0.63600	1.05320
H	-1.49355	1.55224	-0.70062
H	-1.94275	1.10990	0.72492
H	-0.96689	-1.97698	-0.77027
H	-1.71009	-3.24206	-0.21221
H	-3.46930	0.05752	-0.48676
H	-3.13971	-1.44843	-0.72849
H	-0.19280	-0.05684	-0.91478
H	-0.82021	3.19809	0.55950
H	0.60642	2.76853	0.93458
H	0.35061	2.56226	-1.15635

H	1.05890	1.39809	-1.90167

Int1: E(RM062X/6-31+G(d,p)) = -839.500175556

C	-2.19657	-1.04298	-1.51195
C	-1.22543	-0.07515	-0.74019
O	0.08136	-0.26771	-0.79607
C	-3.18639	-1.03482	-0.31650
C	-2.04360	-0.47798	0.53060
O	-1.77721	-0.56345	1.70324
O	0.98344	-0.41934	2.60461
O	1.38794	-2.31773	0.47650
O	-1.60761	1.29164	-1.00954
O	-0.56328	3.15610	1.03309
O	3.62818	-0.77638	-0.20227
O	2.27378	0.58396	-2.36779
O	1.64220	1.35550	0.44542
H	-1.71833	-2.01566	-1.64813
H	-2.57316	-0.65649	-2.46039
H	-3.97341	-0.28429	-0.43685
H	-3.61375	-1.97997	0.02394
H	2.08703	1.75900	-0.31379
H	0.98166	0.71816	0.00412
H	3.01392	-1.52046	-0.04103
H	3.22687	-0.06137	0.31512
H	-1.13974	2.61295	0.47626
H	0.27890	2.67310	1.00953
H	2.92756	0.05892	-1.87470

H	1.42395	0.20575	-2.07760
H	-0.97969	1.58970	-1.68342
H	1.40727	0.31327	2.13215
H	0.03606	-0.31928	2.41377
H	1.30228	-1.92760	1.36413
H	0.83412	-1.72086	-0.07238

TS2: E(RM062X/6-31+G(d,p)) = -839.468667489

C	-3.08007	-1.02966	-1.15601
C	-1.44060	0.19019	-0.62137
O	-0.24497	-0.01946	-0.93551
C	-3.67837	-0.44841	0.09249
C	-2.20836	-0.51649	0.40829
O	-1.70806	-1.38866	1.16402
O	0.84654	-1.35056	2.10263
O	1.56013	-2.06902	-0.42001
O	-1.99534	1.39064	-1.05231
O	-0.51465	3.41380	0.64836
O	3.93614	-1.22810	-1.01952
O	3.93858	1.35737	-0.26174
O	1.37068	1.25771	0.93377
H	-2.92049	-2.10187	-1.18204
H	-3.20614	-0.51371	-2.10161
H	-4.11294	0.54053	-0.03056
H	-4.25717	-1.10572	0.73606
H	2.29485	1.37312	0.64414
H	0.92303	0.78423	0.20293

H	3.00280	-1.55855	-0.82069
H	4.53070	-1.83648	-0.57213
H	-1.24098	2.85368	0.34663
H	0.20070	2.78882	0.86398
H	4.00396	0.40987	-0.53260
H	3.83984	1.85633	-1.07778
H	-1.37313	1.71265	-1.72040
H	1.09841	-0.41625	2.01824
H	-0.10397	-1.37593	1.83712
H	1.41249	-1.97962	0.55122
H	0.83999	-1.51483	-0.78034

P1a: E(RM062X/6-31+G(d,p)) = -839.509427431

C	1.15567	2.37550	1.24643
C	-0.49995	1.10389	-0.21594
O	-0.83275	0.03496	-0.71594
C	1.27961	2.91997	-0.14711
C	0.92995	1.44730	0.05601
O	1.82054	0.48994	-0.23135
O	3.12732	-1.27698	-1.83320
O	2.83835	-1.18316	1.34160
O	-1.39915	2.03027	0.12518
O	-3.91174	1.02184	-0.15473
O	0.74650	-2.26848	-0.11198
O	-1.51106	-3.01200	1.14701
O	-3.13415	-1.48777	-0.52690
H	2.06939	2.15339	1.78713

H	0.30478	2.69326	1.83943
H	0.51255	3.60591	-0.49191
H	2.27683	3.06190	-0.54893
H	-2.80603	-2.12737	0.13577
H	-2.30907	-1.06146	-0.82488
H	1.48666	-2.09137	0.50967
H	0.52312	-1.37208	-0.43562
H	-4.30257	1.23492	-1.00752
H	-3.76958	0.03944	-0.16400
H	-0.66471	-2.81461	0.66449
H	-1.37895	-2.64187	2.02503
H	-2.31501	1.66268	0.02315
H	2.45903	-1.94406	-1.62918
H	2.72346	-0.46089	-1.46853
H	3.61731	-1.40987	0.81951
H	2.43015	-0.39683	0.81256

P1b = 2: E(RM062X/6-31+G(d,p)) = -839.54451899

C	2.76019	-1.80292	-0.04742
C	2.63687	-0.65933	0.92652
H	3.46711	0.03708	0.98753
H	2.06986	-0.81577	1.83731
H	1.54747	0.36007	-1.93722
C	1.86874	-0.63234	-0.35638
O	2.29784	0.29120	-1.32242
H	3.66940	-1.86228	-0.63601
H	2.27388	-2.73867	0.20536

C	0.37205	-0.85604	-0.33163
O	-0.26460	-0.30631	-1.28617
O	-0.10426	-1.54488	0.59125
H	-1.68407	-2.69072	0.53140
O	-2.57294	-3.04115	0.35464
H	-3.00433	-2.28652	-0.07075
H	-3.29110	-0.20581	-1.74777
O	-2.90055	-0.43597	-0.89953
H	-1.91621	-0.46685	-1.05353
H	-2.89520	1.00922	0.40287
O	-2.58179	1.82417	0.83201
H	-2.07825	2.27117	0.12446
O	-0.74876	2.52631	-1.19987
H	0.02171	2.76659	-0.64955
H	-0.61396	1.57451	-1.35271
H	1.98310	1.85103	-0.05757
O	1.48880	2.46599	0.50556
H	1.00026	1.90708	1.14692
O	-0.23996	0.93495	2.10643
H	-0.26040	-0.00358	1.85800
H	-1.10645	1.28280	1.80930

P2: E(RM062X/6-31+G(d,p)) = -839.555289901

C	1.03668	-3.25686	-0.60922
C	2.06469	-2.14316	-0.40310
C	1.51109	-0.75873	-0.64358
O	2.20148	0.15290	-1.06201

C	0.02441	-0.51880	-0.32021
O	-0.29512	-0.55836	0.89440
O	-0.71385	-0.30653	-1.30956
H	2.41710	-2.13624	0.63756
H	2.93828	-2.25721	-1.05178
H	1.48921	-4.23272	-0.41471
H	0.19182	-3.13502	0.07489
H	0.64581	-3.25644	-1.63107
O	-1.43750	2.40927	-0.94380
H	-1.13851	1.55277	-1.29591
H	-1.86650	2.15858	-0.10201
O	1.32941	2.80577	-0.29227
H	1.65192	2.01080	-0.74787
H	0.38661	2.88080	-0.52682
O	-3.49182	0.09652	-1.51796
H	-2.58178	-0.25878	-1.48567
H	-3.36617	1.01107	-1.80135
O	1.91136	-1.10833	2.69596
H	1.05387	-1.15533	2.24306
H	2.07106	-0.15044	2.71449
O	1.19542	1.64239	2.27716
H	0.42100	1.12614	2.01033
H	1.38408	2.18285	1.48677
O	-2.68806	0.92318	1.13077
H	-1.92981	0.30922	1.18564
H	-3.26334	0.52999	0.45515

Int4: E(RM062X/6-31+G(d,p)) = -839.468068741

C	-2.830678	-1.321073	0.321440
C	-1.924857	-0.098541	0.333066
O	-1.894578	0.409656	-1.001658
C	-0.964913	-0.708837	-0.618031
C	-1.866099	-1.953199	-0.741087
O	-1.828613	0.791445	1.369273
O	0.323633	-0.602772	-0.819501
H	-2.291633	-2.111883	-1.735716
H	-1.370873	-2.861250	-0.385546
H	-2.823342	-1.859952	1.272684
H	-3.858444	-1.131261	-0.004720
H	-1.612636	1.681922	0.989699
O	1.590635	-2.683830	0.594394
O	1.058610	2.121007	-1.005232
O	0.986332	-0.086449	1.726119
O	3.137186	-0.914591	-1.085695
O	3.217278	1.330096	0.667360
O	-1.308594	3.030756	-0.063008
H	1.863370	2.055272	-0.457350
H	0.747406	1.196781	-1.100702
H	2.580092	0.954690	1.299768
H	3.426897	0.585526	0.073336
H	2.240674	-0.704957	-1.398007
H	2.981088	-1.673036	-0.498815
H	0.158833	0.277325	2.074484
H	0.794531	-0.192583	0.755616

H	1.027832	-2.185174	-0.031183
H	1.529611	-2.139395	1.393850
H	-0.363878	2.888835	-0.308844
H	-1.765371	2.546484	-0.767312

TS5: E(RM062X/6-31+G(d,p)) = -839.443477678

C	-2.64240200	0.63808500	0.69785300
C	-1.15405000	0.33027300	0.70984200
O	-0.79826500	0.72882800	-0.72517500
C	-1.45125000	-0.47483200	-0.93282800
C	-2.91241300	-0.24867100	-0.53576700
O	-0.31705000	1.00233500	1.58223900
O	-0.97921600	-1.40401900	-1.59186300
H	-3.44816500	0.25340500	-1.35045700
H	-3.40064900	-1.19811000	-0.30372600
H	-3.14340900	0.29367700	1.60616800
H	-2.88398200	1.70227000	0.52663600
H	-0.26470100	1.94404000	1.30751400
O	-0.81362400	-2.86535500	0.88315700
O	1.79800100	1.74136100	-1.19974000
O	2.01920400	-0.49636400	1.80078500
O	1.53871000	-2.10516600	-0.58957100
O	3.74404400	-0.15618200	-0.35768200
O	-0.08250500	3.36616900	0.04439500
H	2.58940400	1.21819500	-0.97580900
H	1.04865600	1.12579200	-1.12395000
H	3.41122500	-0.08594700	0.55713000

H	3.28245000	-0.94557900	-0.68139100
H	0.82827600	-1.70707800	-1.13186700
H	1.03921100	-2.72528300	-0.03221000
H	1.27840300	0.13457200	1.86778800
H	1.71772600	-1.11579900	1.11641300
H	-1.18149600	-2.92110800	-0.01029900
H	-0.86969100	-1.89813600	1.05437600
H	0.78292800	3.05199500	-0.28614400
H	-0.69988900	2.91111100	-0.54712300

P3a: E(RM062X/6-31+G(d,p)) = -839.543187140

C	-1.518598	-0.924722	1.583360
C	-1.227184	0.372347	0.832915
O	-1.784152	0.154442	-0.508987
C	-1.922217	-1.149882	-0.769419
C	-1.618475	-1.967358	0.472613
O	-1.834497	1.450690	1.412734
O	-2.231262	-1.567110	-1.862433
H	-2.397178	-2.720147	0.610958
H	-0.667219	-2.485481	0.316443
H	-0.728979	-1.144727	2.302813
H	-2.471969	-0.793067	2.104336
H	-1.508817	2.241071	0.908781
O	1.496742	-1.761385	1.046617
O	1.297301	1.809640	-0.835776

O	2.781482	0.910417	1.214943
O	1.066668	-0.590482	-1.392778
O	3.823366	-1.028454	-0.604852
O	-0.839058	3.097626	-0.418481
H	1.898376	2.267953	-1.432224
H	1.128759	0.458491	-1.228890
H	3.711081	-0.265145	-0.006575
H	3.044588	-0.975351	-1.182625
H	0.359567	-0.754434	-2.026339
H	1.227453	-1.399149	0.172362
H	2.227827	1.360467	0.523426
H	2.224995	0.190791	1.547326
H	2.424493	-1.987584	0.885656
H	-0.156978	0.542192	0.662682
H	0.064565	2.627537	-0.593044
H	-1.411051	2.773687	-1.123725

TS4: E(RM062X/6-31+G(d,p)) = -839.474534165

C	2.456452	-1.424898	-0.864228
C	1.921303	-2.482084	0.155263
C	0.676624	-1.600303	0.331892
O	-0.015715	-1.596053	-0.880862
C	1.289368	-0.510745	-0.467043
O	-0.069807	-1.576456	1.495796
O	1.105624	0.728596	-0.611482
O	-0.269568	1.309039	1.645676
O	-2.361203	-2.653083	0.331580

O	-2.485726	-0.205270	-0.886114
O	1.894039	3.033863	0.850906
O	-2.386840	2.436457	0.143837
O	-0.062058	3.198572	-1.311504
H	2.451740	-1.732778	-1.911324
H	3.425062	-0.990124	-0.599224
H	2.531816	-2.540601	1.060865
H	1.716264	-3.480208	-0.242692
H	-0.943295	-1.977222	1.284736
H	-2.552675	0.719196	-0.580185
H	-1.536132	-0.410135	-0.984160
H	-1.836710	2.141881	0.891162
H	-1.744846	2.869308	-0.448488
H	0.220427	2.280425	-1.461055
H	0.558478	3.501451	-0.628030
H	-0.367259	0.413996	2.007116
H	0.123288	1.127992	0.756365
H	2.039268	2.233429	0.318339
H	1.271173	2.724074	1.526824
H	-2.727382	-1.785094	0.061315
H	-1.726692	-2.816716	-0.384421

TS3a: E(RM062X/6-31+G(d,p)) = -839.463877139

C	2.61233	-0.26168	1.60627
C	0.95138	0.69300	-0.66989
O	-0.02724	0.26108	-1.26469
C	3.29870	0.32027	0.36259

C	2.27060	-0.10982	-0.62110
O	2.33545	-1.11360	-1.31436
O	-0.16356	-2.56386	-1.34690
O	-1.61878	-1.91931	1.05205
O	1.00857	1.88408	-0.11776
O	-1.33800	2.99164	0.03701
O	-3.89378	-0.85899	0.55081
O	-0.02144	-0.15910	2.07100
O	-2.71920	1.05806	-0.92979
H	2.86083	-1.32446	1.70372
H	2.90722	0.27921	2.51312
H	3.34785	1.41026	0.42271
H	4.27863	-0.08673	0.08229
H	-3.24403	0.42659	-0.37998
H	-1.90281	0.58486	-1.16784
H	-3.01474	-1.31607	0.78664
H	-4.41915	-1.51445	0.08412
H	-1.50444	3.75926	-0.51754
H	-1.99004	2.27828	-0.25839
H	-0.30491	0.76178	2.06634
H	1.07302	-0.18310	1.80140
H	0.10045	2.32703	-0.11224
H	-0.09118	-1.61442	-1.55442
H	0.75949	-2.78897	-1.17631
H	-1.14864	-2.25286	0.26741
H	-1.00188	-1.23676	1.47274