Supporting Information

A theoretical study of oxidation of ascorbic acid and its antioxidant mechanism

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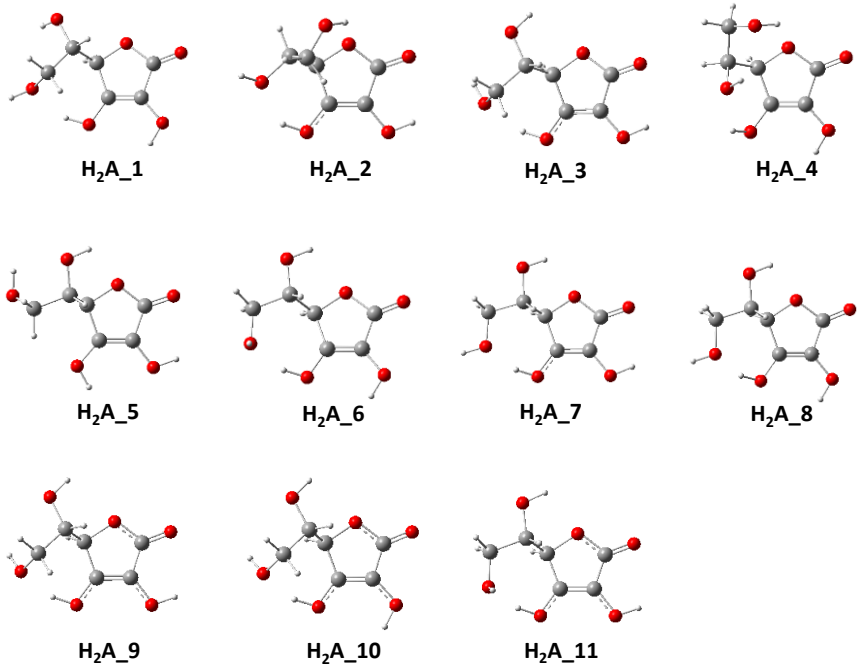
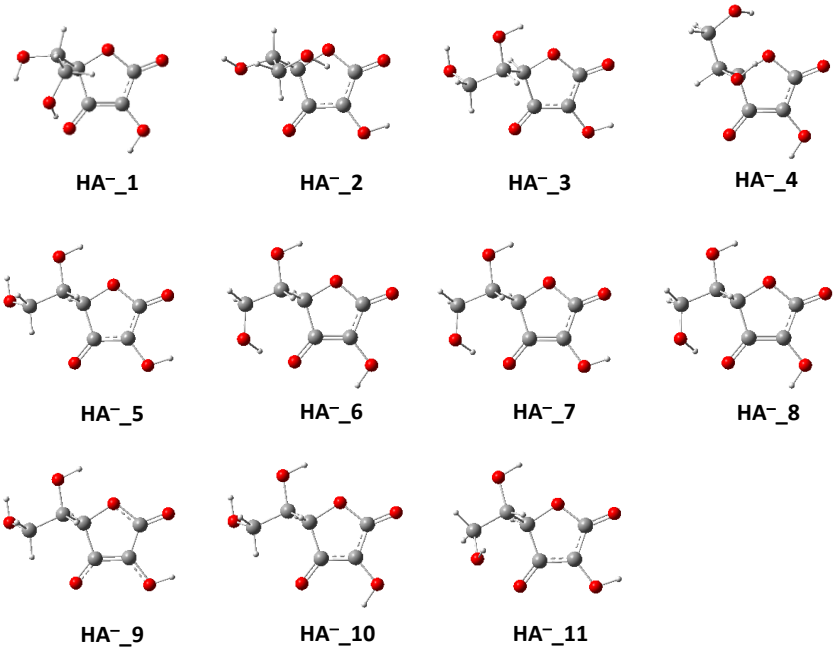
Table S1. The B3LYP/6-31+G(d,p) optimized structures of **H_2A**



	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	$\Delta G_{(aq)}$	population
H_2A_1	-5.0	176.6	73.8	70.1	-43.5	-169.3	1.39	3%
H_2A_2	180.0	168.2	-58.2	178.9	79.7	-68.8	3.26	0%
H_2A_3	176.5	178.1	74.1	-65.9	-34.6	-61.0	1.21	4%
H_2A_4	-3.2	-178.9	-64.5	80.5	-75.6	64.0	1.39	3%
H_2A_5	175.6	0.5	56.2	-61.8	-56.4	-64.1	0.56	12%
H_2A_6	-3.3	160.7	50.5	-63.9	65.3	76.1	0.00	30%
H_2A_7	-179.1	161.9	48.9	-64.2	66.9	-169.8	0.58	11%
H_2A_8	-3.7	161.0	49.4	-64.1	67.1	-170.1	0.55	12%
H_2A_9	177.5	178.5	74.2	-66.0	-34.7	-60.7	1.30	3%
H_2A_10	-3.2	178.3	74.6	-65.8	-34.7	-60.6	1.74	2%
H_2A_11	-179.5	161.5	50.2	-64.0	65.2	76.1	0.20	21%

ϕ_1: H2-O2-C2-C3; ϕ_2: H3-O3-C3-C2; ϕ_3: O5-C5-C4-O; ϕ_4: H5O-O5-C5-C4; ϕ_5: O6-C6-C5-C4; ϕ_6: H6O-O6-C6-C5

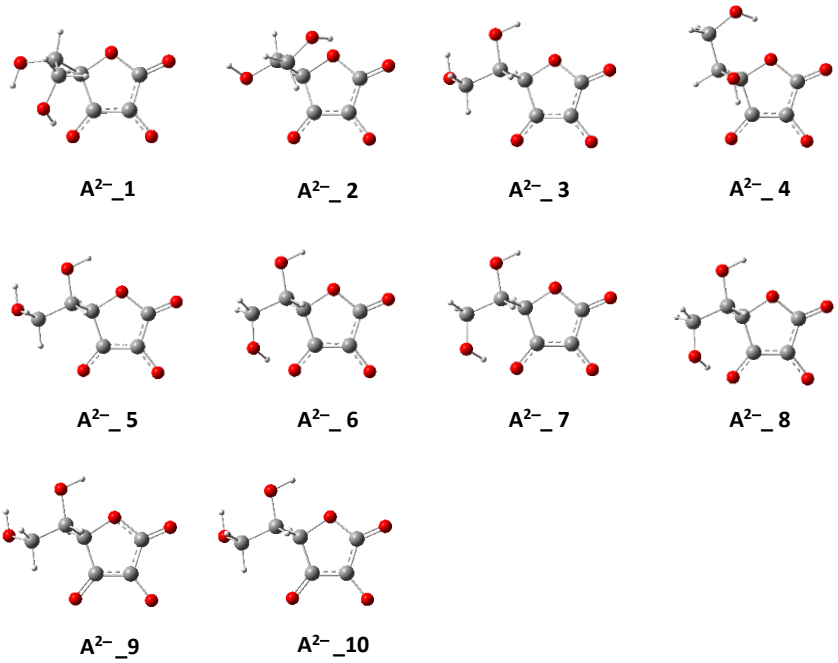
Table S2. The B3LYP/6-31+G(d,p) optimized structures of **HA⁻**



	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	$\Delta G_{(aq)}$	population
HA⁻_1	3.0		145.6	91.1	79.7	55.9	2.95	0%
HA⁻_2	175.9		160.3	-169.7	72.1	-77.7	4.63	0%
HA⁻_3	-179.9		54.4	-54.6	-57.4	-61.9	1.75	2%
HA⁻_4	-3.9		-64.4	74.0	-73.0	58.0	1.11	6%
HA⁻_5	174.2		54.7	-54.8	-57.5	-61.4	1.63	2%
HA⁻_6	-2.8		55.2	-56.2	74.6	-56.5	0.32	21%
HA⁻_7	176.3		54.5	-56.5	74.4	-55.8	0.45	17%
HA⁻_8	-2.9		55.1	-57.0	74.6	-56.4	0.00	36%
HA⁻_9	175.0		54.9	-54.7	-57.3	-61.8	1.90	1%
HA⁻_10	-2.9		55.3	-55.0	-57.2	-61.5	1.37	4%
HA⁻_11	170.0		61.5	-55.6	91.3	67.1	0.73	11%

ϕ_1: H2-O2-C2-C3; ϕ_2: H3-O3-C3-C2; ϕ_3: O5-C5-C4-O; ϕ_4: H5O-O5-C5-C4; ϕ_5: O6-C6-C5-C4; ϕ_6: H6O-O6-C6-C5

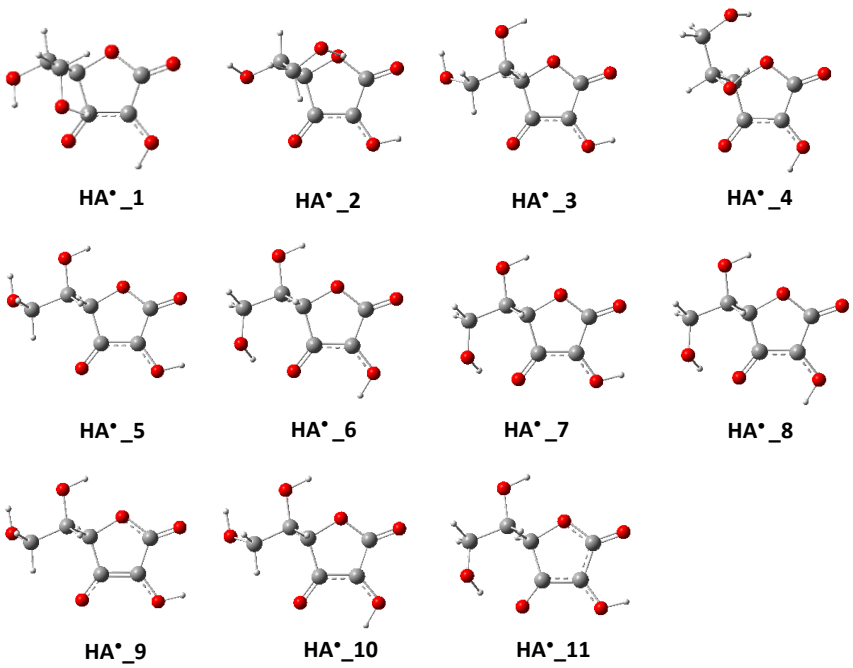
Table S3. The B3LYP/6-31+G(d,p) optimized structures of $\mathbf{A^{2-}}$



	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	$\Delta G_{(aq)}$	population
A^{2-}_1			144.3	88.3	-77.9	53.3	2.71	0%
A^{2-}_2			173.4	-167.3	76.7	-49.7	4.20	0%
A^{2-}_3			54.3	-51.9	-57.5	-60.7	1.93	1%
A^{2-}_4			-64.4	-59.8	-68.3	44.6	1.09	5%
A^{2-}_5			54.9	-52.4	-58.4	-60.4	1.94	1%
A^{2-}_6			54.8	-54.1	73.0	-54.2	0.00	32%
A^{2-}_7			54.9	-54.3	72.9	-54.1	0.07	28%
A^{2-}_8			55.0	-54.3	72.9	-54.2	0.04	30%
A^{2-}_9			55.0	-51.9	-57.8	-60.7	1.95	1%
A^{2-}_10			55.1	-52.1	-58.0	-60.6	1.96	1%

ϕ_1: H2-O2-C2-C3; ϕ_2: H3-O3-C3-C2; ϕ_3: O5-C5-C4-O; ϕ_4: H5O-O5-C5-C4; ϕ_5: O6-C6-C5-C4; ϕ_6: H6O-O6-C6-C5

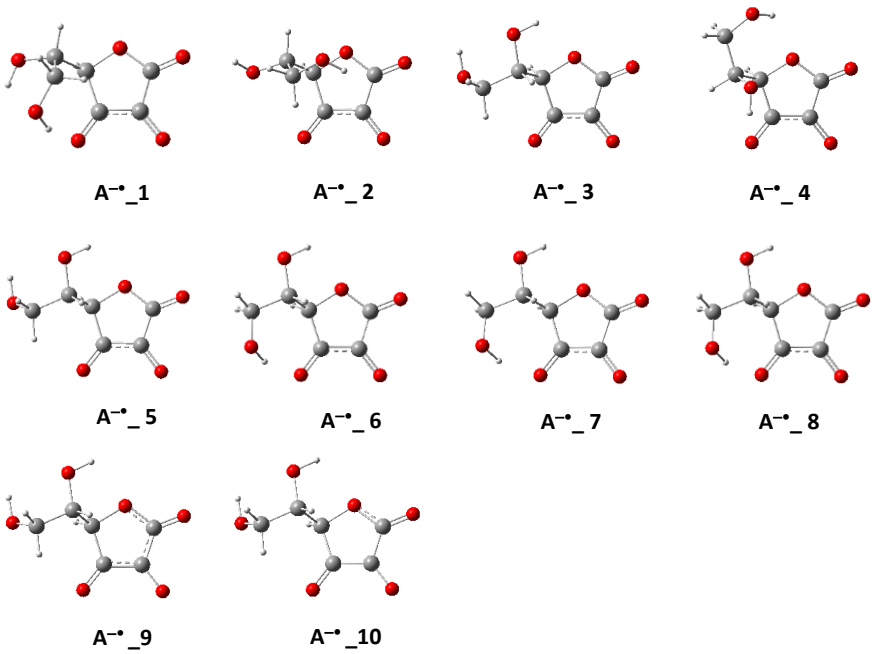
Table S4. The B3LYP/6-31+G(d,p) optimized structures of **HA•**



	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	$\Delta G_{(aq)}$	population
HA•_1	-1.0		174.5	78.2	-69.5	98.4	2.63	0%
HA•_2	179.0		168.0	-168.8	78.5	-75.8	4.54	0%
HA•_3	179.1		55.5	-66.4	-57.5	-65.8	0.83	7%
HA•_4	-0.3		-64.8	83.2	-76.2	66.5	0.00	29%
HA•_5	179.0		53.9	-64.6	-58.2	-64.2	0.63	10%
HA•_6	0.0		54.9	-62.9	79.2	-65.9	1.40	3%
HA•_7	-179.8		55.1	-64.1	78.0	-65.3	1.85	1%
HA•_8	0.0		55.8	-64.5	79.1	-66.0	1.57	2%
HA•_9	178.8		54.5	-64.6	-57.6	-64.1	0.35	16%
HA•_10	-0.8		55.6	-64.4	-57.5	-64.5	0.01	29%
HA•_11	-179.9		54.5	-63.0	79.0	-65.3	1.70	2%

ϕ_1: H2-O2-C2-C3; ϕ_2: H3-O3-C3-C2; ϕ_3: O5-C5-C4-O; ϕ_4: H5O-O5-C5-C4; ϕ_5: O6-C6-C5-C4; ϕ_6: H6O-O6-C6-C5

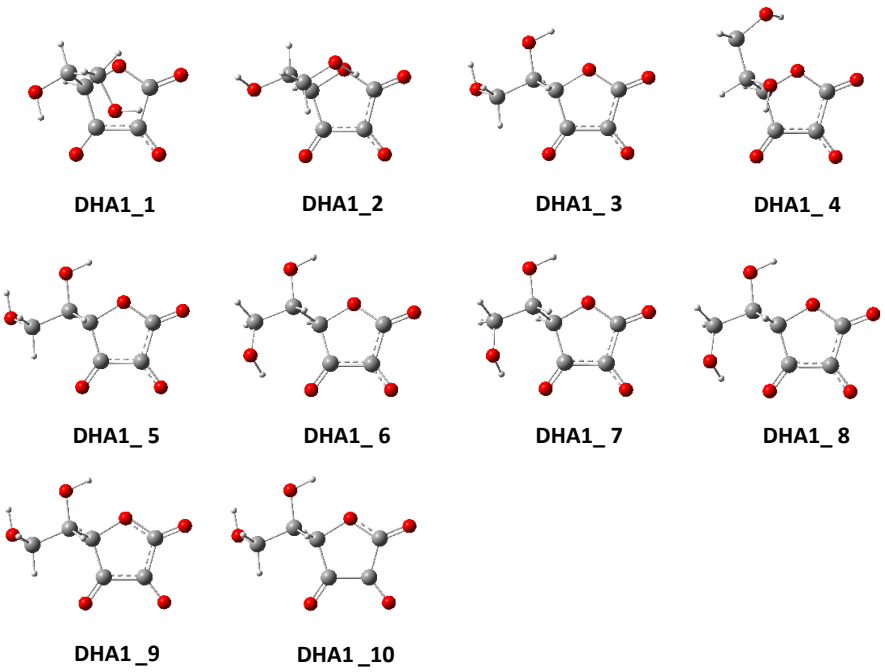
Table S5. The B3LYP/6-31+G(d,p) optimized structures of $\mathbf{A^{-\bullet}}$



	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	$\Delta G_{(aq)}$	population
$A^{-\bullet}$_1			146.1	93.9	-82.7	61.1	2.88	0%
$A^{-\bullet}$_2			161.2	-170.1	73.0	-79.1	3.45	0%
$A^{-\bullet}$_3			55.3	-59.1	-57.2	-63.8	0.18	17%
$A^{-\bullet}$_4			-63.7	-74.8	-70.8	55.3	1.21	3%
$A^{-\bullet}$_5			54.7	-58.4	-57.9	-62.9	0.46	10%
$A^{-\bullet}$_6			54.1	-57.9	75.8	-59.2	0.57	9%
$A^{-\bullet}$_7			54.5	-59.6	76.2	-59.8	0.48	10%
$A^{-\bullet}$_8			54.5	-60.0	76.4	-59.9	0.41	11%
$A^{-\bullet}$_9			55.3	-58.2	-57.4	-63.2	0.00	23%
$A^{-\bullet}$_10			54.7	-58.2	-57.8	-62.9	0.17	17%

ϕ_1: H2-O2-C2-C3; ϕ_2: H3-O3-C3-C2; ϕ_3: O5-C5-C4-O; ϕ_4: H5O-O5-C5-C4; ϕ_5: O6-C6-C5-C4; ϕ_6: H6O-O6-C6-C5

Table S6. The B3LYP/6-31+G(d,p) optimized structures of **DHA1**

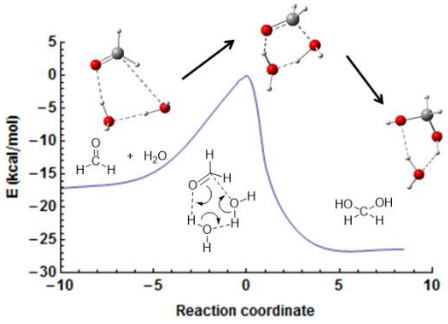


	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	$\Delta G_{(aq)}$	population
DHA1_1			179.6	73.7	-46.2	159.7	0.81	9%
DHA1_2			163.3	-169.2	72.8	-80.5	4.17	0%
DHA1_3			55.7	-69.7	-56.8	-67.3	0.99	7%
DHA1_4			-62.9	-88.1	-72.6	63.8	1.36	4%
DHA1_5			53.7	-70.8	-57.7	-65.8	0.41	18%
DHA1_6			54.8	-67.3	81.3	-73.1	2.52	1%
DHA1_7			54.8	-67.7	80.9	-73.7	2.16	1%
DHA1_8			54.3	-68.0	81.0	-73.0	1.80	2%
DHA1_9			53.2	-69.6	-57.9	-65.4	0.00	37%
DHA1_10			53.3	-70.7	-57.8	-65.7	0.31	22%

ϕ_1: H2-O2-C2-C3; ϕ_2: H3-O3-C3-C2; ϕ_3: O5-C5-C4-O; ϕ_4: H5O-O5-C5-C4; ϕ_5: O6-C6-C5-C4; ϕ_6: H6O-O6-C6-C5

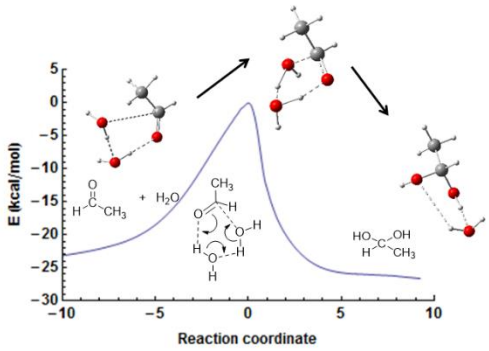
B. Reaction enthalpy and free energy for the hydration of a carbonyl group

Table S7. Reaction enthalpy and free energy for the hydration of formaldehyde



	Implicit		Inclusion of explicit water	
	ΔH (kcal/mol)	ΔG (kcal/mol)	ΔH (kcal/mol)	ΔG (kcal/mol)
B3LYP/6-31+G(d,p)	-8.1	3.11	-6.89	-2.28
B3LYP/CBSB7	-9.59	1.55		
B3LYP/CBSB7+	-6.64	4.55		
CBS-QB3	-9.04	2.09	-7.68	-4.41
Exp.	-7.5	-4.5		

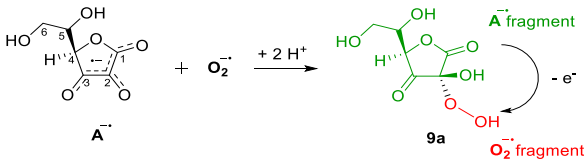
Table S8. Reaction enthalpy and free energy for the hydration of acetaldehyde



	Implicit		Inclusion of explicit water	
	ΔH (kcal/mol)	ΔG (kcal/mol)	ΔH (kcal/mol)	ΔG (kcal/mol)
B3LYP/6-31+G(d,p)	-1.82	10.00	-0.24	4.33
CBS-QB3	-5.49	6.62	-3.94	-1.38
Exp.		-0.21		

C. The change in bond distances for the reaction of ascorbic acid radical with superoxide

Table S9. Comparison of selected bond distances (Angstrom) of adduct **9a** with $\mathbf{O_2^{-\bullet}}$, $\mathbf{H_2O_2}$, $\mathbf{A^{-\bullet}}$, and **DHA**s



	$\mathbf{A^{-\bullet}}$ [a]	**9a** [a]	$\mathbf{O_2^{-\bullet}}$ [b] / $\mathbf{H_2O_2}$ [b]	**DHA2** [c] / $\mathbf{HA^-}$ [a]
O–O		1.451	1.336/1.453	
C1–C2	1.477	1.541		1.538 / 1.426
C2–C3	1.443	1.539		1.544 / 1.383
C1–O1	1.227	1.201		1.213 / 1.238
C3–O3	1.251	1.208		1.213 / 1.283

[a] The structures were optimized with SMD implicit solvation and inclusion of 2 explicit water molecules.

[b] The structures were optimized with SMD implicit solvation and inclusion of 5 explicit water molecules

[c] The structures were optimized with SMD implicit solvation and inclusion of 1 explicit water molecule.

D. Energy diagrams

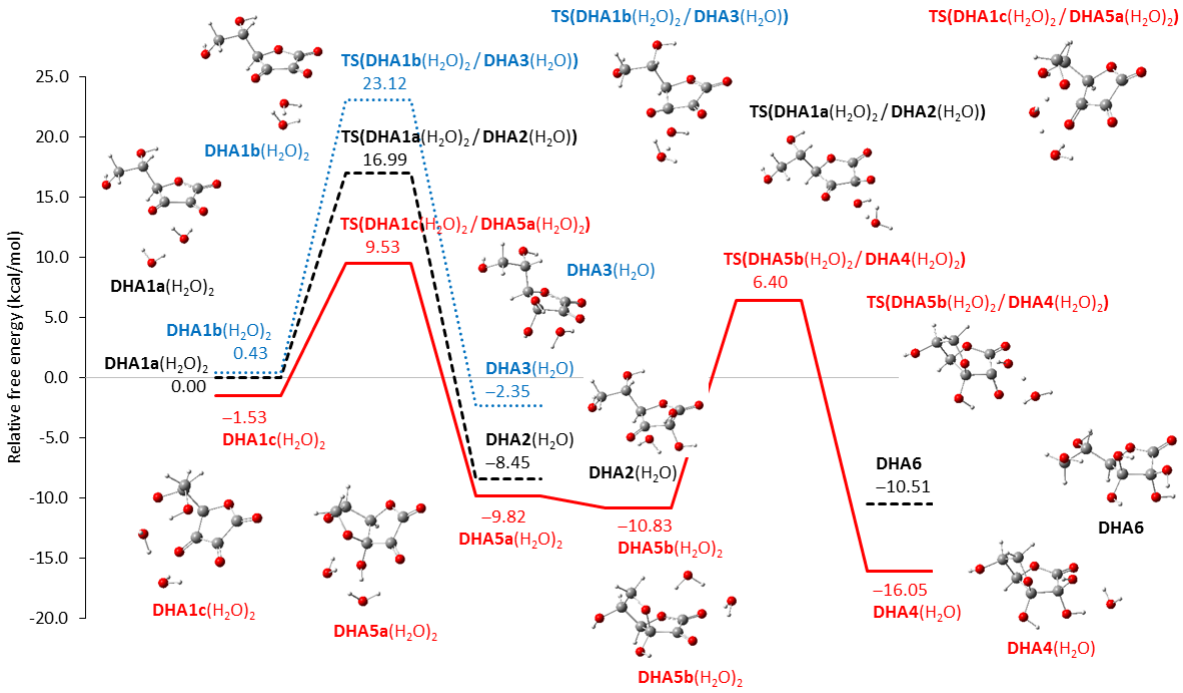


Figure S1. The energy diagram calculated at CBS-QB3 for hydration and cyclization of **DHA**s. Relative free energies of **DHA**s are with respect to **DHA1a**$(H_2O)_2$.

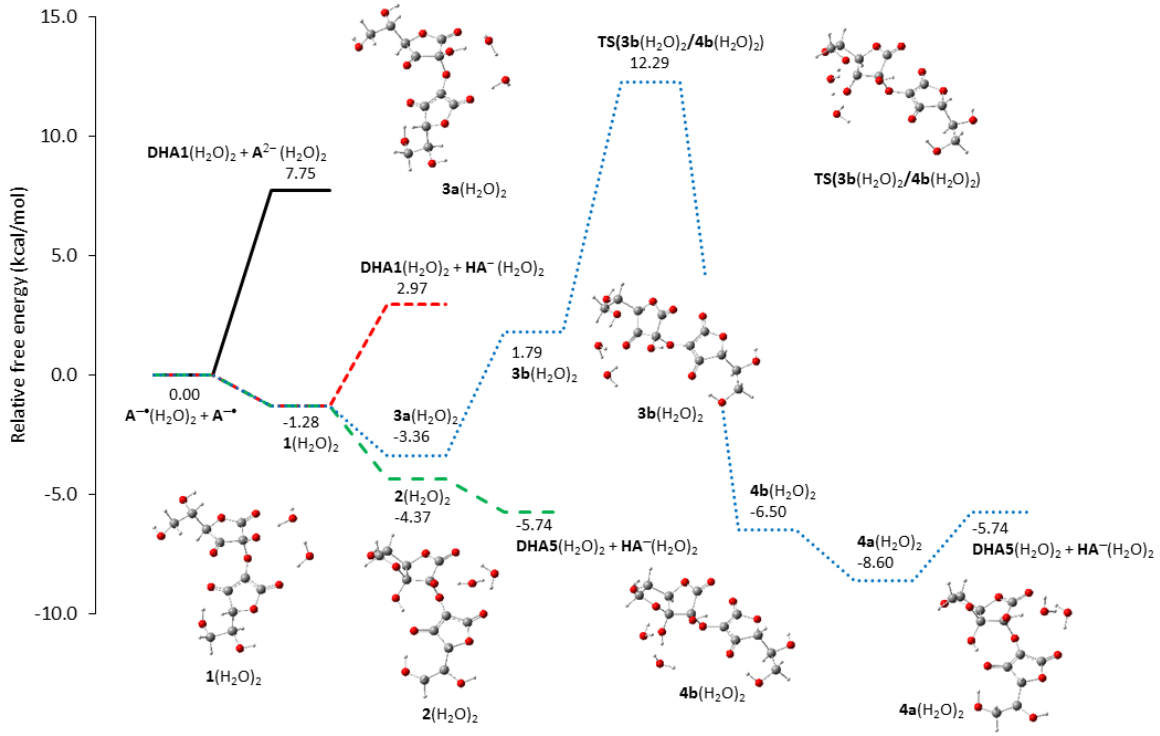


Figure S2. The energy diagram for the disproportionation of two ascorbic acid radicals (est. CBS-QB3 at pH 7).

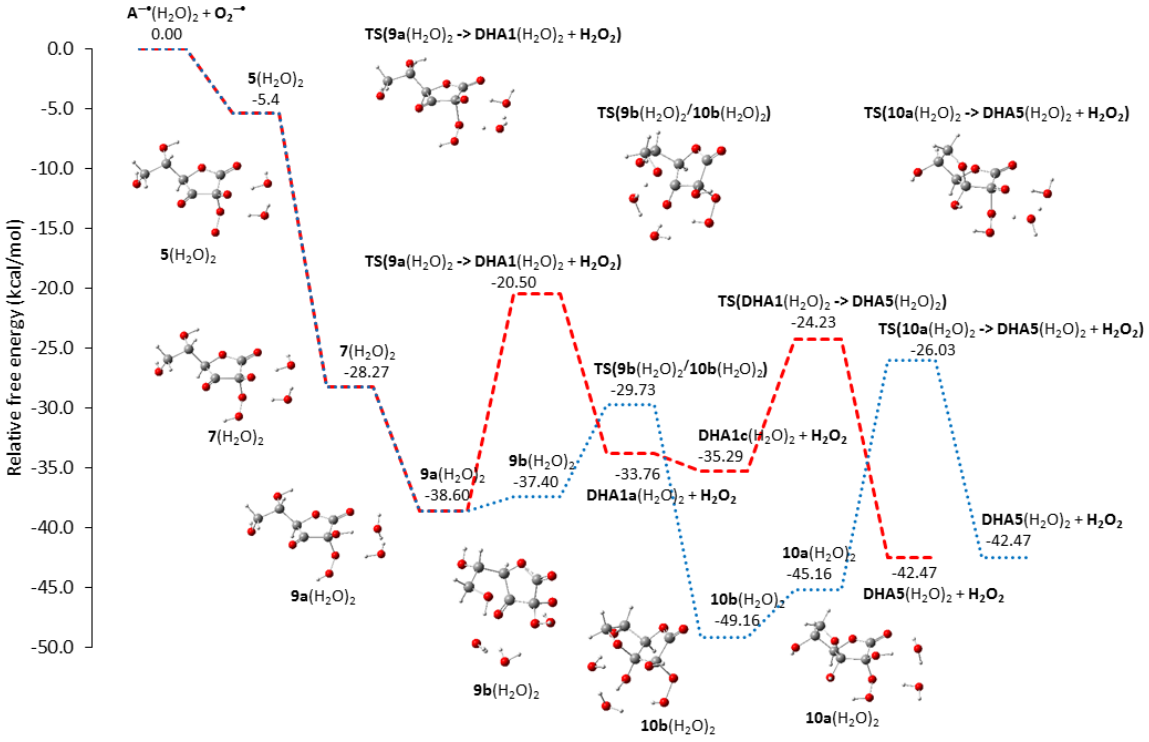


Figure S3. The energy diagram calculated at CBS-QB3 for the reaction of ascorbic acid radical with superoxide

E. Cartesian coordinates of optimized structures at SMD/B3LYP/6-31+G(d,p)

H_2A_1

charge: 0 multiplicity: 1

E(RB3LYP) = -684.853502 A.U.

C	-0.457751	0.698645	0.870908
C	1.013117	0.374127	0.913482
C	1.696206	1.310814	0.218968
C	0.748259	2.261060	-0.326182
O	-0.522296	1.888948	0.041172
O	0.943367	3.252054	-1.021304
O	3.031215	1.447532	-0.047010
O	1.523477	-0.715648	1.505037
H	-1.006324	-0.092931	0.348476
C	-1.162619	1.004197	2.214445
H	-0.885614	2.018277	2.515423
C	-0.757191	0.067120	3.345909
H	0.232289	0.349496	3.722910
O	-2.576819	1.037759	2.004671
H	-2.888215	0.136313	1.823642
H	0.797857	-1.192520	1.988173
H	3.531102	0.761214	0.423984
H	-1.482916	0.156375	4.158853
O	-0.720328	-1.292094	2.853550
H	-0.630104	-1.893503	3.608592

H_2A_2
charge: 0 multiplicity: 1
E(RB3LYP) = -684.850629 A.U.

C	-0.268804	0.802044	0.980515
C	1.197874	0.473062	0.889578
C	1.783458	1.298028	-0.004063
C	0.780609	2.226068	-0.486809
O	-0.422440	1.957617	0.123529
O	0.898352	3.136802	-1.298314
O	3.089282	1.310327	-0.406129
O	1.773228	-0.524010	1.581546
H	-0.863186	-0.010654	0.547961
C	-0.793338	1.078520	2.401397
H	-1.873245	1.259164	2.341967
C	-0.136051	2.255197	3.136264
H	-0.374552	2.160802	4.199952
O	-0.528936	-0.160544	3.082250
H	-0.809850	-0.087746	4.007542
H	1.149287	-0.813040	2.280522
H	3.212499	2.018996	-1.060339
H	0.955047	2.228271	3.026851
O	-0.658549	3.522461	2.725824
H	-0.379453	3.692653	1.814009

H_2A_3
charge: 0 multiplicity: 1
E(RB3LYP) = -684.854542 A.U.

C	-0.445240	0.723363	0.851531
C	1.030126	0.415769	0.866129
C	1.684701	1.351294	0.143575
C	0.711634	2.277347	-0.395976
O	-0.545598	1.898675	-0.000130
O	0.894203	3.256166	-1.113523
O	3.028697	1.428967	-0.097190
O	1.558602	-0.659134	1.465660
H	-1.003712	-0.081387	0.362330
C	-1.118194	1.058017	2.200938
H	-0.774296	2.051782	2.513576
C	-0.775478	0.077657	3.322356
H	0.181797	0.356050	3.766757
O	-2.539599	1.069255	2.027727
H	-2.775734	1.802767	1.439338
H	0.837337	-1.144617	1.946785
H	3.200308	2.176912	-0.694149
H	-1.549704	0.139300	4.092955
O	-0.606181	-1.288542	2.891444
H	-1.429508	-1.615803	2.496408

H_2A_4
charge: 0 multiplicity: 1
E(RB3LYP) = -684.852944 A.U.

C	-0.125764	1.144316	0.989388
C	1.179910	0.418115	0.820962
C	2.007732	1.150524	0.046355
C	1.313442	2.360699	-0.348788
O	0.052731	2.347089	0.192310
O	1.694454	3.290507	-1.049580
O	3.283870	0.923693	-0.387410
O	1.479244	-0.773334	1.370532
H	-0.953649	0.577221	0.549015
C	-0.488004	1.503977	2.444417
H	-0.615658	0.549973	2.969341
C	-1.809085	2.273503	2.560367
H	-2.588165	1.760806	1.983548
O	0.571981	2.196619	3.097016
H	0.528212	3.127301	2.821717
H	0.735919	-1.140311	1.878680
H	3.616049	0.095198	-0.005755
H	-2.108737	2.295695	3.610529
O	-1.688259	3.644516	2.160169
H	-1.462630	3.672945	1.217400

H_2A_5

charge: 0 multiplicity: 1

E(RB3LYP) = -684.852678 A.U.

C	-0.441871	0.780935	0.802470
C	1.023497	0.447573	0.831395
C	1.710992	1.365913	0.118715
C	0.767503	2.319596	-0.425863
O	-0.498326	1.969223	-0.040728
O	0.981525	3.297332	-1.135087
O	3.060439	1.410732	-0.090772
O	1.450168	-0.643839	1.486109
H	-1.022372	0.000790	0.301019
C	-1.093278	1.143461	2.152148
H	-0.484394	1.923617	2.628299
C	-1.202696	-0.029545	3.120529
H	-0.207471	-0.390524	3.383675
O	-2.421385	1.624341	1.922415
H	-2.372458	2.426615	1.380537
H	2.415453	-0.734631	1.405861
H	3.263318	2.142338	-0.698305
H	-1.691552	0.333087	4.032704
O	-1.915350	-1.149134	2.582104
H	-2.830574	-0.876072	2.418755

H_2A_6

charge: 0 multiplicity: 1

E(RB3LYP) = -684.856087 A.U.

C	-0.395457	0.731793	0.877933
C	1.091239	0.470989	0.927569
C	1.721520	1.343696	0.109568
C	0.738527	2.237450	-0.462914
O	-0.505209	1.889758	0.006446

O	0.883614	3.177579	-1.236199
O	3.045831	1.490950	-0.201981
O	1.665469	-0.514099	1.629556
H	-0.916516	-0.094749	0.379730
C	-1.106246	1.050914	2.210237
H	-0.517111	1.793983	2.763748
C	-1.331760	-0.195378	3.074305
H	-1.951859	0.080947	3.930895
O	-2.415601	1.553683	1.942473
H	-2.329898	2.391865	1.463007
H	1.046305	-0.790367	2.367973
H	3.573523	0.862133	0.316620
H	-1.850625	-0.962073	2.493221
O	-0.107413	-0.795011	3.534208
H	0.250362	-0.259208	4.260216

H_2A_7

charge: 0 multiplicity: 1

E(RB3LYP) = -684.855315 A.U.

C	-0.410698	0.749198	0.884631
C	1.076640	0.481040	0.926971
C	1.703639	1.345379	0.097910
C	0.718882	2.237680	-0.470443
O	-0.522440	1.904698	0.008913
O	0.876840	3.170085	-1.252679
O	3.044601	1.416532	-0.165286
O	1.643727	-0.500053	1.636677
H	-0.938992	-0.076439	0.392840
C	-1.113341	1.080166	2.220932
H	-0.502959	1.802585	2.777708
C	-1.380080	-0.158325	3.076912
H	-1.978680	0.142337	3.941575
O	-2.406983	1.621560	1.956351
H	-2.295334	2.462547	1.487575
H	1.013204	-0.776337	2.365432
H	3.206470	2.144657	-0.788591
H	-1.937094	-0.898923	2.492714
O	-0.131204	-0.717493	3.525604
H	-0.305419	-1.583275	3.924985

H_2A_8

charge: 0 multiplicity: 1

E(RB3LYP) = -684.855069 A.U.

C	-0.414185	0.740086	0.876921
C	1.068920	0.461831	0.942083
C	1.717942	1.324168	0.127555
C	0.751623	2.227854	-0.456749
O	-0.501054	1.896983	0.002254
O	0.914889	3.163794	-1.231486
O	3.047151	1.453894	-0.171691
O	1.622460	-0.525454	1.656120
H	-0.940196	-0.081398	0.375675
C	-1.134743	1.072854	2.202643

H	-0.531148	1.794667	2.767583
C	-1.414950	-0.164592	3.055882
H	-2.027902	0.136877	3.910106
O	-2.423863	1.616282	1.919844
H	-2.304187	2.455615	1.450055
H	0.985550	-0.791536	2.383751
H	3.562509	0.824089	0.358079
H	-1.961573	-0.906870	2.464026
O	-0.173142	-0.722265	3.526550
H	-0.354547	-1.585436	3.928484

H_2A_9

charge: 0 multiplicity: 1

E(RB3LYP) = -684.854590293 A.U.

C	-0.569894	0.936842	0.779687
C	0.825550	0.367113	0.779413
C	1.652874	1.222985	0.139648
C	0.874847	2.352321	-0.324405
O	-0.437876	2.178476	0.033417
O	1.244417	3.337449	-0.956057
O	2.992130	1.071865	-0.092096
O	1.137422	-0.830698	1.291142
H	-1.251260	0.290350	0.216653
C	-1.206870	1.267963	2.147654
H	-0.701452	2.153694	2.551951
C	-1.069678	0.146752	3.177049
H	-0.089890	0.208856	3.653942
O	-2.600081	1.544656	1.965452
H	-2.691310	2.357186	1.444681
H	0.327705	-1.217208	1.721380
H	3.308792	1.831295	-0.609808
H	-1.839364	0.275988	3.943773
O	-1.135279	-1.183702	2.623270
H	-1.992157	-1.320037	2.189057

H_2A_10

charge: 0 multiplicity: 1

E(RB3LYP) = -684.854268761 A.U.

C	-0.556004	0.930007	0.786195
C	0.839778	0.363969	0.807613
C	1.675280	1.215719	0.172461
C	0.904557	2.343254	-0.310416
O	-0.413979	2.165858	0.034226
O	1.267730	3.329113	-0.942296
O	3.016491	1.143391	-0.088365
O	1.153045	-0.829545	1.330864
H	-1.227876	0.277894	0.218039
C	-1.212204	1.266943	2.143446
H	-0.717832	2.158941	2.547685
C	-1.080402	0.154739	3.183367
H	-0.106706	0.227158	3.671192
O	-2.604964	1.532837	1.942290
H	-2.695445	2.339370	1.412145
H	0.341482	-1.215950	1.758533

H	3.384111	0.339469	0.313071
H	-1.859962	0.284968	3.939877
O	-1.130574	-1.180794	2.640299
H	-1.980881	-1.326017	2.196216

H_2A_11

charge: 0 multiplicity: 1

E(RB3LYP) = -684.856340326 A.U.

C	-0.399034	0.737568	0.875684
C	1.091070	0.487643	0.918869
C	1.708267	1.363097	0.094206
C	0.713051	2.246105	-0.471624
O	-0.524411	1.895351	0.003950
O	0.860999	3.183819	-1.249509
O	3.048436	1.451088	-0.167013
O	1.670815	-0.491716	1.622001
H	-0.915770	-0.092661	0.379251
C	-1.107281	1.051417	2.210820
H	-0.519850	1.795881	2.764204
C	-1.326036	-0.197385	3.073091
H	-1.943827	0.075775	3.932371
O	-2.419494	1.548774	1.947510
H	-2.339220	2.389041	1.470810
H	1.050799	-0.777540	2.355549
H	3.202818	2.179674	-0.791647
H	-1.845225	-0.963969	2.492166
O	-0.098950	-0.795171	3.527343
H	0.260496	-0.259622	4.252741

HA^-_1

charge: -1 multiplicity: 1

E(RB3LYP) = -684.399486 A.U.

C	-0.668086	0.892877	0.754318
C	0.647383	0.119361	0.699910
C	1.615793	1.018039	0.300672
C	1.065719	2.319086	0.182632
O	-0.289390	2.272062	0.483673
O	1.587571	3.403746	-0.117628
O	2.968196	0.783851	0.094031
O	0.758851	-1.125702	0.990699
H	-1.323575	0.572248	-0.063070
C	-1.490386	0.845178	2.066825
H	-2.017412	1.802602	2.127760
C	-0.660197	0.666106	3.343048
H	0.218641	1.323044	3.308298
O	-2.496939	-0.169754	1.986523
H	-2.107059	-0.987873	2.338311
H	3.131789	-0.162997	0.234470
H	-1.264133	0.943457	4.210629
O	-0.277002	-0.702675	3.546782
H	0.203377	-1.009837	2.745431

HA^-_2

charge: -1 multiplicity: 1
E(RB3LYP) = -684.395503 A.U.

C	-0.207979	0.704675	1.029827
C	1.315595	0.565579	0.951313
C	1.725058	1.457251	-0.030339
C	0.616459	2.138866	-0.578539
O	-0.550300	1.723441	0.051238
O	0.558600	2.994303	-1.480767
O	3.041032	1.645578	-0.438993
O	1.987371	-0.246273	1.664637
H	-0.681811	-0.228971	0.706538
C	-0.812218	1.085165	2.393388
H	-1.833936	1.438949	2.202869
C	-0.063211	2.157803	3.199310
H	-0.513968	2.199542	4.195593
O	-0.849974	-0.133025	3.153755
H	-1.370440	0.024784	3.955898
H	3.045054	2.274399	-1.178565
H	0.992503	1.887516	3.313624
O	-0.192301	3.477620	2.654219
H	0.399074	3.559568	1.892028

HA^{-}_3
charge: -1 multiplicity: 1
E(RB3LYP) = -684.399737 A.U.

C	-0.271359	0.599786	0.910938
C	1.258762	0.527731	0.948388
C	1.704273	1.527085	0.094414
C	0.616796	2.199081	-0.502313
O	-0.577613	1.662379	-0.039774
O	0.594936	3.128316	-1.330807
O	3.039572	1.808359	-0.173782
O	1.912445	-0.319083	1.636932
H	-0.695505	-0.325162	0.508308
C	-0.951432	0.963963	2.238730
H	-0.480223	1.876738	2.629704
C	-0.847322	-0.112751	3.312574
H	0.200344	-0.287292	3.560193
O	-2.352896	1.198125	2.021500
H	-2.443719	1.870421	1.328848
H	3.074154	2.550150	-0.798951
H	-1.362861	0.250359	4.210317
O	-1.387984	-1.377796	2.908825
H	-2.331999	-1.257046	2.727047

HA^{-}_4
charge: -1 multiplicity: 1
E(RB3LYP) = -684.401747 A.U.

C	-0.181942	1.162251	0.909471
C	1.091088	0.341943	0.725976
C	1.958976	1.135530	-0.007139
C	1.364721	2.381129	-0.309500
O	0.077564	2.418424	0.219414

O	1.790968	3.366792	-0.935338
O	3.246483	0.824687	-0.430606
O	1.247556	-0.833102	1.192437
H	-1.025213	0.676465	0.405684
C	-0.561636	1.419142	2.373782
H	-0.737085	0.434270	2.820352
C	-1.848609	2.234019	2.535279
H	-2.646488	1.778119	1.935508
O	0.516275	2.006184	3.108711
H	0.591249	2.933520	2.832449
H	3.474404	-0.046007	-0.066675
H	-2.150701	2.218982	3.585331
O	-1.684280	3.619713	2.197892
H	-1.371806	3.675935	1.280900

HA¯_5
charge: -1 multiplicity: 1
E(RB3LYP) = -684.399716 A.U.

C	-0.451611	0.770584	0.804360
C	1.032445	0.391786	0.845219
C	1.691355	1.370419	0.113838
C	0.775458	2.305989	-0.411576
O	-0.515637	1.964280	-0.031442
O	0.963137	3.308813	-1.125075
O	3.064369	1.417357	-0.102109
O	1.484462	-0.638374	1.439055
H	-1.038313	-0.006476	0.305002
C	-1.084598	1.129260	2.157008
H	-0.457357	1.891805	2.639814
C	-1.218424	-0.043745	3.120155
H	-0.230942	-0.441031	3.358032
O	-2.408086	1.651138	1.951561
H	-2.345622	2.394030	1.331663
H	3.249961	2.145002	-0.717369
H	-1.678396	0.325524	4.045223
O	-1.981767	-1.134970	2.588747
H	-2.877115	-0.812980	2.405836

HA¯_6
charge: -1 multiplicity: 1
E(RB3LYP) = -684.404034 A.U.

C	-0.438769	0.740764	0.916403
C	1.051684	0.418876	1.001054
C	1.694920	1.326955	0.185558
C	0.762921	2.219539	-0.401251
O	-0.517338	1.888812	0.024317
O	0.921211	3.171477	-1.179511
O	3.053511	1.427562	-0.077352
O	1.542267	-0.539521	1.699602
H	-0.979093	-0.082233	0.433195
C	-1.146371	1.106145	2.230710
H	-0.590056	1.914655	2.723831
C	-1.290843	-0.079341	3.194997

H	-1.996083	0.210881	3.978270
O	-2.485208	1.536218	1.944980
H	-2.436999	2.272727	1.316294
H	3.510357	0.758528	0.457796
H	-1.714353	-0.938878	2.655849
O	-0.069203	-0.432827	3.839287
H	0.593146	-0.621520	3.126934

HA^-_7

charge: -1 multiplicity: 1

E(RB3LYP) = -684.403627 A.U.

C	-0.474391	0.733699	0.880955
C	1.006761	0.364630	0.984904
C	1.692318	1.311138	0.249986
C	0.794188	2.260193	-0.298121
O	-0.504181	1.938647	0.062565
O	1.013413	3.255087	-1.007367
O	3.067544	1.351027	0.068878
O	1.435897	-0.655079	1.632699
H	-1.021555	-0.042703	0.332865
C	-1.206678	1.036701	2.197900
H	-0.637037	1.790023	2.758594
C	-1.422463	-0.202423	3.076903
H	-2.137131	0.064019	3.860116
O	-2.520631	1.534636	1.905896
H	-2.427107	2.312046	1.334118
H	3.273487	2.082917	-0.535146
H	-1.864735	-1.006258	2.471057
O	-0.234271	-0.648289	3.726500
H	0.442819	-0.804752	3.019872

HA^-_8

charge: -1 multiplicity: 1

E(RB3LYP) = -684.404031 A.U.

C	-0.473880	0.738912	0.871533
C	0.999668	0.356726	0.994244
C	1.709639	1.305939	0.287864
C	0.835081	2.275209	-0.264878
O	-0.473940	1.954868	0.070459
O	1.060658	3.281932	-0.952322
O	3.081525	1.384234	0.094733
O	1.423967	-0.674151	1.630008
H	-1.020459	-0.023573	0.303632
C	-1.224814	1.029625	2.180751
H	-0.661437	1.775009	2.758012
C	-1.453756	-0.219045	3.042805
H	-2.181444	0.037993	3.817123
O	-2.533260	1.533973	1.875865
H	-2.430081	2.322420	1.321139
H	3.496450	0.660821	0.591713
H	-1.884456	-1.017685	2.422059
O	-0.275342	-0.669236	3.707315
H	0.410407	-0.827439	3.010301

HA⁻_9
charge: -1 multiplicity: 1
E(RB3LYP) = -684.399727813 A.U.

C	-0.420731	0.768254	0.818973
C	1.071133	0.423383	0.874722
C	1.712002	1.400761	0.126011
C	0.778515	2.305491	-0.422117
O	-0.506542	1.943877	-0.040323
O	0.948225	3.297820	-1.154568
O	3.084545	1.472298	-0.085998
O	1.542972	-0.583905	1.492085
H	-0.987107	-0.031237	0.331693
C	-1.069878	1.138980	2.160408
H	-0.465128	1.927712	2.629692
C	-1.178026	-0.016032	3.148119
H	-0.181584	-0.379927	3.401410
O	-2.405223	1.621603	1.937316
H	-2.358738	2.351409	1.300725
H	3.258392	2.199065	-0.705715
H	-1.655081	0.360173	4.061629
O	-1.906189	-1.140214	2.635939
H	-2.810637	-0.850157	2.444423

HA⁻_10
charge: -1 multiplicity: 1
E(RB3LYP) = -684.400205927 A.U.

C	-0.448245	0.769057	0.809020
C	1.033295	0.393013	0.857669
C	1.698879	1.363253	0.123366
C	0.791621	2.301792	-0.412934
O	-0.502473	1.958694	-0.031948
O	0.968316	3.304717	-1.126506
O	3.064834	1.447136	-0.121948
O	1.501510	-0.628280	1.457362
H	-1.033843	-0.009192	0.310010
C	-1.087663	1.134002	2.156748
H	-0.465967	1.903326	2.635950
C	-1.216415	-0.033149	3.127569
H	-0.226447	-0.419492	3.373403
O	-2.413165	1.647108	1.943535
H	-2.352532	2.387773	1.320799
H	3.493752	0.719305	0.356840
H	-1.684473	0.338382	4.047642
O	-1.966267	-1.135773	2.600280
H	-2.864119	-0.824684	2.410919

HA⁻_11
charge: -1 multiplicity: 1
E(RB3LYP) = -684.403662318 A.U.

C	-0.438718	0.744852	0.915419
C	1.056501	0.431440	0.996597
C	1.687155	1.345505	0.176413
C	0.741645	2.226974	-0.404031

O	-0.533403	1.892754	0.023467
O	0.905295	3.177385	-1.185638
O	3.054012	1.411871	-0.053064
O	1.540215	-0.527349	1.696962
H	-0.973561	-0.082603	0.433901
C	-1.145922	1.105702	2.231393
H	-0.591718	1.915233	2.725231
C	-1.287641	-0.081070	3.194388
H	-1.991926	0.207713	3.979079
O	-2.486221	1.532238	1.946919
H	-2.440360	2.267840	1.316986
H	3.223378	2.132179	-0.681751
H	-1.711610	-0.939905	2.654439
O	-0.064771	-0.434797	3.835856
H	0.596703	-0.616520	3.120228

A^{2-}_1

charge: -2 multiplicity: 1

E(RB3LYP) = -683.917994 A.U.

C	-0.583277	0.891235	0.830166
C	0.781187	0.255733	0.889204
C	1.744214	1.054567	0.288106
C	1.013811	2.334369	-0.005086
O	-0.323031	2.244859	0.373487
O	1.413515	3.388211	-0.494812
O	2.993898	0.883632	0.031028
O	0.924548	-1.018173	1.362264
H	-1.214127	0.419226	0.056903
C	-1.473775	0.922593	2.112237
H	-1.890967	1.937147	2.189983
C	-0.736564	0.490523	3.412120
H	0.250589	0.994776	3.444310
O	-2.564232	-0.003282	1.979466
H	-2.162850	-0.775291	2.468327
H	-1.326014	0.887158	4.276172
O	-0.653689	-0.895426	3.429979
H	0.327359	-1.107617	2.193782

A^{2-}_2

charge: -2 multiplicity: 1

E(RB3LYP) = -683.912559 A.U.

C	-0.206630	0.749341	1.033841
C	1.282373	0.446603	0.902559
C	1.834445	1.344316	-0.021113
C	0.784771	2.210257	-0.452233
O	-0.427882	1.907181	0.183435
O	0.784348	3.152741	-1.276491
O	3.099928	1.408020	-0.468968
O	1.855454	-0.526325	1.527304
H	-0.796646	-0.079657	0.622990
C	-0.767893	1.079148	2.428349
H	-1.822337	1.358852	2.297810
C	-0.056223	2.230446	3.150971
H	-0.356830	2.220349	4.202724

O	-0.681238	-0.125509	3.203268
H	-1.206930	-0.002302	4.007817
H	1.032778	2.103631	3.102080
O	-0.438013	3.518116	2.640225
H	-0.357168	3.489573	1.673288

A^{2-}_3

charge: -2 multiplicity: 1

E(RB3LYP) = -683.916891 A.U.

C	-0.252735	0.592927	0.917822
C	1.268145	0.508374	0.952207
C	1.782888	1.501498	0.109532
C	0.671095	2.181834	-0.476111
O	-0.545135	1.661612	-0.024948
O	0.631487	3.119444	-1.306228
O	3.069763	1.779300	-0.159018
O	1.905283	-0.375182	1.645929
H	-0.696321	-0.323888	0.513271
C	-0.940661	0.961447	2.240309
H	-0.464366	1.870641	2.634274
C	-0.861082	-0.110852	3.319729
H	0.181512	-0.297312	3.579335
O	-2.341600	1.212613	2.014564
H	-2.414958	1.856843	1.293574
H	-1.382256	0.259727	4.211461
O	-1.412945	-1.372617	2.916242
H	-2.348843	-1.236284	2.705776

A^{2-}_4

charge: -2 multiplicity: 1

E(RB3LYP) = -683.917573 A.U.

C	-0.185086	1.205664	0.915193
C	1.145803	0.488211	0.759293
C	1.996113	1.292362	-0.006029
C	1.261833	2.472322	-0.353735
O	-0.036610	2.440922	0.164293
O	1.595378	3.471341	-1.027967
O	3.264562	1.056306	-0.378912
O	1.362266	-0.665692	1.301939
H	-0.999360	0.635129	0.451123
C	-0.584509	1.496425	2.370535
H	-0.756351	0.516163	2.837635
C	-1.887919	2.279666	2.500689
H	-2.674715	1.731265	1.966008
O	0.432096	2.209820	3.086882
H	1.240893	1.676068	3.089345
H	-2.169242	2.340736	3.555513
O	-1.808254	3.634029	2.030830
H	-1.335614	3.624741	1.181274

A^{2-}_5

charge: -2 multiplicity: 1
E(RB3LYP) = -683.916806 A.U.

C	-0.439417	0.749988	0.799607
C	1.033073	0.360047	0.836543
C	1.760314	1.323848	0.127001
C	0.821891	2.271157	-0.387996
O	-0.488324	1.945991	-0.027787
O	0.996361	3.293478	-1.090687
O	3.085865	1.382603	-0.086884
O	1.457065	-0.707404	1.427382
H	-1.047099	-0.014335	0.302451
C	-1.072440	1.121399	2.148923
H	-0.437138	1.881319	2.626068
C	-1.224046	-0.037026	3.125774
H	-0.243464	-0.453695	3.358929
O	-2.392402	1.660436	1.941227
H	-2.319422	2.374763	1.289538
H	-1.669296	0.349374	4.051380
O	-2.016486	-1.117510	2.612191
H	-2.900247	-0.771183	2.417655

A^{2-}_6
charge: -2 multiplicity: 1
E(RB3LYP) = -683.922896 A.U.

C	-0.434033	0.742308	0.913288
C	1.052161	0.431775	0.988660
C	1.741769	1.331174	0.179903
C	0.761479	2.214405	-0.393308
O	-0.527133	1.889287	0.025441
O	0.900038	3.175810	-1.176242
O	3.055438	1.419240	-0.059239
O	1.520248	-0.556053	1.702173
H	-0.986591	-0.079083	0.437480
C	-1.138569	1.109204	2.228650
H	-0.581099	1.920691	2.716626
C	-1.276311	-0.071590	3.198047
H	-1.963379	0.223867	3.996248
O	-2.482011	1.540927	1.951804
H	-2.433320	2.254868	1.297561
H	-1.721322	-0.925970	2.666532
O	-0.042964	-0.437948	3.810442
H	0.611136	-0.598902	3.069289

A^{2-}_7
charge: -2 multiplicity: 1
E(RB3LYP) = -683.922867 A.U.

C	-0.469675	0.727962	0.882125
C	0.999306	0.350816	0.984885
C	1.752709	1.274141	0.265082
C	0.829313	2.234147	-0.278591
O	-0.485740	1.933160	0.069293
O	1.035196	3.242761	-0.983351
O	3.076858	1.324220	0.077265

O	1.400771	-0.702171	1.643659
H	-1.038496	-0.037085	0.336689
C	-1.202671	1.040836	2.196143
H	-0.628923	1.795327	2.751989
C	-1.421457	-0.190914	3.083446
H	-2.120993	0.084360	3.878033
O	-2.517432	1.546686	1.906770
H	-2.418167	2.300277	1.304815
H	-1.885221	-0.989499	2.485497
O	-0.226186	-0.650676	3.708387
H	0.444893	-0.793327	2.979373

A^{2-}_8

charge: -2 multiplicity: 1

E(RB3LYP) = -683.922868 A.U.

C	-0.468144	0.743671	0.870067
C	1.001738	0.372838	0.983669
C	1.757824	1.310018	0.284908
C	0.835262	2.273102	-0.254676
O	-0.481889	1.960404	0.074531
O	1.042974	3.291650	-0.944470
O	3.083407	1.368608	0.110403
O	1.401474	-0.688091	1.630557
H	-1.026078	-0.016571	0.306942
C	-1.218543	1.033147	2.179525
H	-0.657368	1.784543	2.752106
C	-1.437622	-0.211913	3.047878
H	-2.148167	0.047307	3.838099
O	-2.533917	1.532636	1.881600
H	-2.433702	2.295394	1.291464
H	-1.888313	-1.006244	2.434469
O	-0.245687	-0.670241	3.680180
H	0.433645	-0.799595	2.956227

A^{2-}_9

charge: -2 multiplicity: 1

E(RB3LYP) = -683.916816308 A.U.

C	-0.419634	0.761849	0.813792
C	1.065445	0.423958	0.858303
C	1.759244	1.397385	0.128562
C	0.789071	2.302481	-0.403071
O	-0.509285	1.940379	-0.035024
O	0.928642	3.316918	-1.124820
O	3.081597	1.495829	-0.088809
O	1.526526	-0.615091	1.471364
H	-0.999517	-0.031962	0.329799
C	-1.067827	1.134786	2.155198
H	-0.462192	1.927037	2.618249
C	-1.176759	-0.009367	3.154086
H	-0.180800	-0.376945	3.403896
O	-2.406581	1.619988	1.935933
H	-2.359716	2.318940	1.265421
H	-1.647029	0.375431	4.067890
O	-1.915049	-1.135282	2.657002

H	-2.813610	-0.836046	2.452368

A^{2-}_10

charge: -2 multiplicity: 1

E(RB3LYP) = -683.916808599 A.U.

C	-0.445650	0.764431	0.800582
C	1.032786	0.397846	0.836324
C	1.743670	1.370801	0.122713
C	0.789641	2.302062	-0.393028
O	-0.514633	1.957422	-0.029884
O	0.947168	3.325513	-1.098112
O	3.067681	1.449086	-0.094373
O	1.474590	-0.661041	1.429576
H	-1.041949	-0.010621	0.306236
C	-1.083372	1.129698	2.149252
H	-0.462268	1.904361	2.621431
C	-1.210428	-0.026299	3.132269
H	-0.220917	-0.417700	3.371361
O	-2.413913	1.641863	1.940931
H	-2.356327	2.351830	1.282959
H	-1.668026	0.354750	4.054069
O	-1.974426	-1.129146	2.622817
H	-2.866785	-0.807172	2.425812

HA˙_1

charge: 0 multiplicity: 2

E(UB3LYP) = -684.220152 A.U.

C	-0.751890	0.945596	0.707728
C	0.400069	-0.011595	0.429174
C	1.581406	0.806757	0.361523
C	1.213554	2.207085	0.558787
O	-0.133991	2.270584	0.746426
O	1.924740	3.198318	0.561861
O	2.826028	0.443270	0.134463
O	0.329196	-1.234654	0.255905
H	-1.443772	0.934173	-0.139386
C	-1.567558	0.733611	2.007567
H	-2.325939	1.523334	2.017278
C	-0.786364	0.842909	3.316182
H	-0.264972	1.803361	3.367311
O	-2.273650	-0.500870	1.915322
H	-1.649381	-1.222560	2.095082
H	2.892425	-0.525457	0.017748
H	-1.510853	0.799490	4.134729
O	0.128706	-0.245813	3.506295
H	1.015386	0.035277	3.239319

HA˙_2

charge: 0 multiplicity: 2

E(UB3LYP) = -684.216874 A.U.

C	-0.199031	0.723117	1.033206
C	1.309659	0.491363	0.953076
C	1.787427	1.396436	-0.055640
C	0.667629	2.185066	-0.566413

O	-0.462021	1.807033	0.087177
O	0.679971	3.051181	-1.426916
O	3.037570	1.480623	-0.459219
O	1.962278	-0.332718	1.602916
H	-0.717365	-0.163918	0.655375
C	-0.793061	1.081005	2.407305
H	-1.835815	1.373647	2.229459
C	-0.099009	2.207899	3.190309
H	-0.458683	2.152670	4.221818
O	-0.735950	-0.138485	3.154556
H	-1.256100	-0.023433	3.964457
H	3.145596	2.149877	-1.164650
H	0.988518	2.069921	3.203794
O	-0.442852	3.517969	2.726877
H	0.025848	3.697517	1.899550

HA˙_3

charge: 0 multiplicity: 2

E(UB3LYP) = -684.221448 A.U.

C	-0.269207	0.587698	0.909529
C	1.254110	0.511533	0.972102
C	1.733109	1.533437	0.083212
C	0.595789	2.208280	-0.537096
O	-0.547334	1.648247	-0.068039
O	0.608124	3.119194	-1.350866
O	3.000883	1.804141	-0.143613
O	1.921644	-0.280816	1.646357
H	-0.686458	-0.335905	0.500751
C	-0.965459	0.965235	2.230205
H	-0.502161	1.881030	2.620386
C	-0.848000	-0.117370	3.299100
H	0.201910	-0.280787	3.547220
O	-2.358947	1.180677	1.992693
H	-2.465692	1.963827	1.431959
H	3.096204	2.528691	-0.793929
H	-1.365793	0.240601	4.196778
O	-1.373769	-1.383355	2.887729
H	-2.330582	-1.290995	2.766613

HA˙_4

charge: 0 multiplicity: 2

E(UB3LYP) = -684.223409 A.U.

C	-0.192658	1.123380	0.906909
C	1.084614	0.309295	0.752491
C	1.988521	1.129260	-0.003994
C	1.335572	2.395577	-0.331095
O	0.076934	2.369798	0.184207
O	1.770600	3.348414	-0.956536
O	3.218235	0.862589	-0.390620
O	1.290089	-0.826544	1.196025
H	-1.025003	0.627230	0.398874
C	-0.563831	1.406617	2.369630
H	-0.755085	0.426027	2.819326

C	-1.833143	2.251665	2.527450
H	-2.633104	1.842230	1.899533
O	0.531163	1.984374	3.077373
H	0.525112	2.938740	2.894866
H	3.494162	-0.025241	-0.086964
H	-2.150720	2.210193	3.571753
O	-1.610018	3.638862	2.243190
H	-1.399913	3.735526	1.301510

HA˙_5

charge: 0 multiplicity: 2

E(UB3LYP) = -684.221466 A.U.

C	-0.440875	0.750644	0.813116
C	1.039175	0.383163	0.874450
C	1.720884	1.376405	0.091189
C	0.743731	2.309185	-0.464656
O	-0.494062	1.932865	-0.056942
O	0.945897	3.274237	-1.185450
O	3.021302	1.425045	-0.105858
O	1.530250	-0.582280	1.470180
H	-1.014237	-0.034979	0.314582
C	-1.084770	1.126321	2.161291
H	-0.452846	1.877363	2.653379
C	-1.233329	-0.061609	3.106907
H	-0.251522	-0.478070	3.337839
O	-2.392735	1.656202	1.933544
H	-2.312117	2.484282	1.436139
H	3.262410	2.177195	-0.683215
H	-1.682685	0.305015	4.037509
O	-2.014100	-1.128563	2.559377
H	-2.917055	-0.804011	2.424560

HA˙_6

charge: 0 multiplicity: 2

E(UB3LYP) = -684.221245 A.U.

C	-0.421252	0.732361	0.925000
C	1.065132	0.406549	1.011507
C	1.729364	1.340574	0.150010
C	0.741850	2.245925	-0.437029
O	-0.486492	1.885305	0.021466
O	0.911906	3.176606	-1.205713
O	3.011315	1.445049	-0.121041
O	1.591040	-0.496964	1.678588
H	-0.952120	-0.088097	0.430358
C	-1.140836	1.102401	2.235992
H	-0.583710	1.901416	2.740765
C	-1.312656	-0.090946	3.190116
H	-2.072087	0.190917	3.922793
O	-2.465427	1.538388	1.923311
H	-2.410708	2.339303	1.379725
H	3.529476	0.768619	0.359343
H	-1.677266	-0.964478	2.634093
O	-0.134921	-0.411395	3.929172

H	0.543095	-0.722715	3.302504

HA˙_7

charge: 0 multiplicity: 2

E(UB3LYP) = -684.220943 A.U.

C	-0.470953	0.714947	0.870692
C	1.004381	0.334702	0.969402
C	1.718471	1.322191	0.214453
C	0.768369	2.289712	-0.334417
O	-0.482790	1.925791	0.041425
O	1.003295	3.269348	-1.022785
O	3.021953	1.351905	0.048025
O	1.470182	-0.642069	1.573659
H	-1.019559	-0.053884	0.316740
C	-1.200689	1.033857	2.190794
H	-0.625127	1.785254	2.745704
C	-1.425522	-0.200837	3.077450
H	-2.173415	0.072116	3.825242
O	-2.504482	1.531904	1.884405
H	-2.412691	2.369667	1.405151
H	3.290944	2.115927	-0.500995
H	-1.826475	-1.025787	2.474141
O	-0.263106	-0.611669	3.795417
H	0.403461	-0.907819	3.148671

HA˙_8

charge: 0 multiplicity: 2

E(UB3LYP) = -684.221258 A.U.

C	-0.462176	0.732042	0.875767
C	1.004720	0.337357	0.999976
C	1.745609	1.316736	0.260263
C	0.822450	2.308625	-0.290799
O	-0.440125	1.956803	0.069911
O	1.065526	3.295445	-0.963996
O	3.042510	1.394990	0.059996
O	1.462467	-0.644218	1.604078
H	-1.001138	-0.022046	0.292253
C	-1.226480	1.025869	2.180986
H	-0.669259	1.768379	2.765498
C	-1.467206	-0.227022	3.037348
H	-2.247624	0.022275	3.759744
O	-2.523736	1.525120	1.849396
H	-2.422737	2.374100	1.392238
H	3.514360	0.658992	0.499148
H	-1.831146	-1.048518	2.406704
O	-0.326702	-0.631369	3.793771
H	0.365212	-0.917031	3.170070

HA˙_9

charge: 0 multiplicity: 2

E(UB3LYP) = -684.221492337 A.U.

C	-0.409460	0.755371	0.832473

C	1.077321	0.419622	0.908470
C	1.742380	1.406286	0.103054
C	0.749865	2.309521	-0.474038
O	-0.481739	1.920035	-0.059505
O	0.935635	3.263026	-1.214309
O	3.042355	1.472980	-0.091917
O	1.585375	-0.522020	1.527604
H	-0.961193	-0.051653	0.343662
C	-1.074088	1.139126	2.167593
H	-0.469971	1.919975	2.648009
C	-1.192348	-0.032950	3.136880
H	-0.199271	-0.407308	3.390415
O	-2.396707	1.622025	1.919768
H	-2.340068	2.441194	1.404639
H	3.272482	2.212997	-0.689018
H	-1.668849	0.336267	4.052781
O	-1.924176	-1.140697	2.602056
H	-2.836624	-0.854442	2.445807

HA˙_10

charge: 0 multiplicity: 2

E(UB3LYP) = -684.221849587 A.U.

C	-0.449903	0.752283	0.813147
C	1.021325	0.361777	0.876072
C	1.726032	1.349183	0.106153
C	0.772516	2.308568	-0.445110
O	-0.475406	1.941027	-0.047193
O	0.977875	3.282091	-1.151406
O	3.017223	1.438280	-0.132112
O	1.509419	-0.613741	1.459411
H	-1.033683	-0.020628	0.306670
C	-1.096415	1.130183	2.159287
H	-0.469808	1.889399	2.645645
C	-1.234854	-0.051060	3.114350
H	-0.248335	-0.449051	3.357763
O	-2.407942	1.649225	1.926899
H	-2.333444	2.473585	1.422346
H	3.504452	0.714375	0.309900
H	-1.697374	0.317338	4.037768
O	-1.993224	-1.136501	2.571433
H	-2.901613	-0.830479	2.430128

HA˙_11

charge: 0 multiplicity: 2

E(UB3LYP) = -684.220987483 A.U.

C	-0.425679	0.733612	0.916421
C	1.065655	0.416851	0.995011
C	1.715681	1.361371	0.134466
C	0.713017	2.253711	-0.446971
O	-0.509162	1.885095	0.010783
O	0.887454	3.183760	-1.217349
O	3.010929	1.421471	-0.083009
O	1.587520	-0.488426	1.661401
H	-0.955121	-0.090841	0.427329
C	-1.136982	1.102682	2.232658

H	-0.577282	1.902370	2.733574
C	-1.301669	-0.090687	3.188034
H	-2.053687	0.192449	3.927862
O	-2.464163	1.537149	1.929311
H	-2.414344	2.339151	1.386855
H	3.232266	2.144747	-0.703964
H	-1.673473	-0.962931	2.634665
O	-0.117829	-0.414188	3.915593
H	0.555920	-0.717903	3.280125

$A^{-\bullet}$_1

charge: -1 multiplicity: 2

E(UB3LYP) = -683.782497 A.U.

C	-0.657622	0.881232	0.735847
C	0.649566	0.104180	0.667974
C	1.688198	1.021500	0.274419
C	1.061506	2.357338	0.185451
O	-0.268936	2.269798	0.486336
O	1.574049	3.436849	-0.093343
O	2.919836	0.784972	0.065783
O	0.763250	-1.119315	0.929412
H	-1.313640	0.582617	-0.088669
C	-1.483275	0.832081	2.047202
H	-2.002662	1.794207	2.101777
C	-0.660694	0.653919	3.330938
H	0.242873	1.274989	3.287370
O	-2.488575	-0.178174	1.959907
H	-2.116024	-0.987053	2.350948
H	-1.257969	0.972560	4.188167
O	-0.333442	-0.722610	3.575623
H	0.204158	-1.054849	2.832492

$A^{-\bullet}$_2

charge: -1 multiplicity: 2

E(UB3LYP) = -683.780704 A.U.

C	-0.187973	0.702877	1.035637
C	1.327152	0.556447	0.964353
C	1.799093	1.447701	-0.069198
C	0.613961	2.142865	-0.607602
O	-0.513478	1.728942	0.050302
O	0.544561	2.982940	-1.500777
O	2.991324	1.627903	-0.477330
O	2.000350	-0.226078	1.670510
H	-0.665973	-0.224341	0.701352
C	-0.807871	1.083425	2.392646
H	-1.830643	1.425096	2.186461
C	-0.082609	2.167322	3.205452
H	-0.539131	2.191764	4.199584
O	-0.835844	-0.135861	3.147370
H	-1.359809	0.013470	3.948983
H	0.978223	1.919738	3.324306
O	-0.239781	3.485832	2.666918
H	0.364757	3.594737	1.918890

$A^{-\bullet}$_3

charge: -1 multiplicity: 2

E(UB3LYP) = -683.785134 A.U.

C	-0.250455	0.584018	0.920314
C	1.268368	0.485002	0.978885
C	1.804509	1.499647	0.102533
C	0.654369	2.194841	-0.503854
O	-0.515672	1.655528	-0.043344
O	0.642405	3.116286	-1.316260
O	3.024880	1.765948	-0.143324
O	1.902420	-0.349961	1.660658
H	-0.688559	-0.329107	0.507284
C	-0.948174	0.963918	2.236530
H	-0.474221	1.872785	2.632028
C	-0.861267	-0.115024	3.310387
H	0.182838	-0.290661	3.573035
O	-2.340944	1.206487	1.994602
H	-2.421440	1.923906	1.347652
H	-1.387751	0.250183	4.200520
O	-1.397104	-1.378175	2.898092
H	-2.344934	-1.265496	2.731982

$A^{-\bullet}$_4

charge: -1 multiplicity: 2

E(UB3LYP) = -683.784863 A.U.

C	-0.167271	1.204549	0.921132
C	1.153700	0.464119	0.769897
C	2.019526	1.277504	-0.047779
C	1.258635	2.494576	-0.395408
O	0.007498	2.438823	0.155613
O	1.602113	3.458688	-1.073088
O	3.212817	1.039030	-0.421136
O	1.395971	-0.646448	1.292916
H	-0.976521	0.641891	0.443217
C	-0.567635	1.506334	2.373285
H	-0.740915	0.527052	2.839761
C	-1.876890	2.285748	2.495642
H	-2.656220	1.748699	1.939946
O	0.451553	2.219504	3.080338
H	1.170099	1.606766	3.295218
H	-2.165815	2.319774	3.548932
O	-1.796517	3.651130	2.067965
H	-1.462844	3.667740	1.157461

$A^{-\bullet}$_5

charge: -1 multiplicity: 2

E(UB3LYP) = -683.785134 A.U.

C	-0.433076	0.739753	0.810094
C	1.036705	0.343960	0.867457
C	1.780959	1.326496	0.114870
C	0.800859	2.286805	-0.424523

O	-0.463993	1.929644	-0.044096
O	0.987681	3.277124	-1.126823
O	3.036770	1.385664	-0.085136
O	1.480322	-0.665461	1.457569
H	-1.029978	-0.027623	0.309128
C	-1.072981	1.123913	2.155143
H	-0.434379	1.874339	2.641079
C	-1.234194	-0.047774	3.116797
H	-0.255638	-0.465383	3.357916
O	-2.380391	1.668720	1.931438
H	-2.295734	2.439531	1.349562
H	-1.687596	0.332060	4.040502
O	-2.017921	-1.121141	2.582110
H	-2.912628	-0.787377	2.418227

$A^{-\bullet}$_6

charge: -1 multiplicity: 2

E(UB3LYP) = -683.786513 A.U.

C	-0.416392	0.735211	0.922335
C	1.071337	0.419888	0.996436
C	1.761343	1.346672	0.138194
C	0.734608	2.240720	-0.437462
O	-0.503863	1.883354	0.019182
O	0.871384	3.180080	-1.213696
O	3.006564	1.428052	-0.102540
O	1.570039	-0.506471	1.683348
H	-0.955626	-0.088582	0.440566
C	-1.125622	1.108098	2.236486
H	-0.562186	1.907210	2.735590
C	-1.294940	-0.080735	3.194215
H	-2.011421	0.216372	3.963870
O	-2.455478	1.551716	1.941073
H	-2.398941	2.306812	1.335554
H	-1.714201	-0.936130	2.646706
O	-0.092561	-0.447144	3.868643
H	0.571492	-0.681114	3.184855

$A^{-\bullet}$_7

charge: -1 multiplicity: 2

E(UB3LYP) = -683.786523 A.U.

C	-0.457420	0.716703	0.884954
C	1.011856	0.330676	0.987720
C	1.773070	1.288607	0.229567
C	0.807087	2.265734	-0.315598
O	-0.462736	1.925777	0.059975
O	1.013846	3.254574	-1.010882
O	3.029168	1.334324	0.042355
O	1.444295	-0.664858	1.620703
H	-1.015324	-0.047797	0.332077
C	-1.192689	1.037015	2.198644
H	-0.613676	1.780463	2.761834
C	-1.435781	-0.198013	3.077874
H	-2.167824	0.079825	3.840070

O	-2.493739	1.553758	1.894081
H	-2.386354	2.353912	1.357187
H	-1.864734	-1.005550	2.468808
O	-0.270322	-0.644983	3.768671
H	0.405363	-0.869148	3.093470

$A^{-\bullet}$_8

charge: -1 multiplicity: 2

E(UB3LYP) = -683.786516 A.U.

C	-0.454652	0.734644	0.875291
C	1.015536	0.355620	0.989003
C	1.778624	1.324220	0.246535
C	0.812817	2.302971	-0.296072
O	-0.458323	1.954707	0.066885
O	1.020900	3.299677	-0.979675
O	3.035907	1.377065	0.069523
O	1.447193	-0.644175	1.615831
H	-1.000497	-0.025595	0.304656
C	-1.208727	1.029566	2.183921
H	-0.642914	1.767994	2.766687
C	-1.453380	-0.221520	3.039571
H	-2.199241	0.037255	3.795062
O	-2.509490	1.541789	1.870482
H	-2.400695	2.353771	1.351956
H	-1.865599	-1.023239	2.411569
O	-0.294015	-0.668460	3.740543
H	0.393449	-0.875626	3.071713

$A^{-\bullet}$_9

charge: -1 multiplicity: 2

E(UB3LYP) = -683.785124247 A.U.

C	-0.414935	0.753106	0.821692
C	1.066538	0.405357	0.887187
C	1.780419	1.398077	0.118667
C	0.771284	2.318636	-0.436443
O	-0.482418	1.927774	-0.051334
O	0.927806	3.303456	-1.153605
O	3.033990	1.493063	-0.081758
O	1.541068	-0.579776	1.494108
H	-0.985350	-0.041208	0.332019
C	-1.070928	1.138004	2.158378
H	-0.464700	1.925084	2.627589
C	-1.182751	-0.017867	3.145529
H	-0.187162	-0.383122	3.401357
O	-2.400165	1.622206	1.923348
H	-2.348389	2.382426	1.323954
H	-1.659514	0.360751	4.057850
O	-1.910979	-1.139833	2.631633
H	-2.821289	-0.855842	2.459967

$A^{-\bullet}$_10

charge: -1 multiplicity: 2

E(UB3LYP) = -683.785121873 A.U.

C	-0.447104	0.749893	0.808800
C	1.026849	0.368904	0.859601
C	1.757957	1.359500	0.104829
C	0.765974	2.310510	-0.429494
O	-0.493617	1.940280	-0.044134
O	0.939991	3.303378	-1.131435
O	3.012267	1.431570	-0.100403
O	1.482964	-0.636583	1.446999
H	-1.038460	-0.022958	0.309737
C	-1.084713	1.126408	2.157121
H	-0.451791	1.883287	2.640485
C	-1.229201	-0.047539	3.118660
H	-0.245299	-0.454817	3.355674
O	-2.398912	1.657383	1.939995
H	-2.325461	2.428981	1.357629
H	-1.683009	0.326718	4.044442
O	-2.003554	-1.128860	2.586220
H	-2.902493	-0.804576	2.426526

DHA1_1

charge: 0 multiplicity: 1

E(RB3LYP) = -683.611004716 A.U.

C	-0.843449	0.938949	0.641907
C	0.224528	-0.100480	0.366612
C	1.568015	0.614883	0.494186
C	1.217886	2.084757	0.740493
O	-0.122344	2.218674	0.731754
O	1.983376	3.011835	0.881099
O	2.678166	0.157450	0.364230
O	0.065562	-1.259641	0.043167
H	-1.533569	1.012421	-0.200881
C	-1.629434	0.733063	1.966022
H	-2.383700	1.521748	2.026231
C	-0.694508	0.856399	3.161883
H	-0.428262	1.905054	3.320604
O	-2.347720	-0.492799	1.913511
H	-1.736188	-1.240023	2.009231
H	-1.195032	0.475028	4.058523
O	0.484810	0.082532	2.876602
H	1.212459	0.384390	3.442460

DHA1_2

charge: 0 multiplicity: 1

E(RB3LYP) = -683.603812553 A.U.

C	-0.177282	0.703796	1.050176
C	1.326306	0.514538	0.997762
C	1.839669	1.434994	-0.117718
C	0.601436	2.169048	-0.637483
O	-0.468966	1.752701	0.061210
O	0.552263	3.000502	-1.515422
O	2.970449	1.559928	-0.516557
O	2.013782	-0.222204	1.668268
H	-0.661935	-0.210660	0.692199
C	-0.805814	1.082723	2.405823

H	-1.829258	1.408925	2.181445
C	-0.102104	2.181097	3.219042
H	-0.572083	2.197202	4.206712
O	-0.813371	-0.138065	3.148172
H	-1.350358	-0.008647	3.945012
H	0.960661	1.949115	3.353312
O	-0.274699	3.492094	2.673308
H	0.347611	3.617691	1.942595

DHA1_3

charge: 0 multiplicity: 1

E(RB3LYP) = -683.608503887 A.U.

C	-0.237616	0.571934	0.931536
C	1.268920	0.455876	1.017548
C	1.846477	1.511739	0.066461
C	0.633991	2.216167	-0.542761
O	-0.479846	1.643361	-0.058444
O	0.634586	3.126928	-1.340276
O	3.006543	1.742237	-0.167427
O	1.925180	-0.311654	1.685687
H	-0.666763	-0.342109	0.512594
C	-0.959182	0.963832	2.239307
H	-0.492156	1.872748	2.639173
C	-0.875050	-0.124547	3.306126
H	0.166982	-0.291897	3.584305
O	-2.338254	1.195757	1.960452
H	-2.425010	2.006936	1.437269
H	-1.415331	0.235368	4.189421
O	-1.393755	-1.385624	2.875863
H	-2.350442	-1.296926	2.750888

DHA1_4

charge: 0 multiplicity: 1

E(RB3LYP) = -683.607498046 A.U.

C	-0.166791	1.182031	0.924088
C	1.135376	0.419620	0.784830
C	2.060898	1.281499	-0.080043
C	1.246778	2.530585	-0.422857
O	0.030568	2.414028	0.135090
O	1.597356	3.477877	-1.089516
O	3.191069	1.042448	-0.425650
O	1.415872	-0.656334	1.262927
H	-0.975491	0.625223	0.440380
C	-0.554161	1.508213	2.376899
H	-0.730777	0.534095	2.850787
C	-1.861652	2.296998	2.491776
H	-2.642758	1.770624	1.929381
O	0.485178	2.217224	3.049759
H	1.097646	1.581375	3.448102
H	-2.148376	2.319389	3.545624
O	-1.767846	3.664328	2.083180
H	-1.551605	3.696256	1.139155

DHA1_5

charge: 0 multiplicity: 1

E(RB3LYP) = -683.608596513 A.U.

C	-0.414047	0.727753	0.832285
C	1.042851	0.328136	0.916180
C	1.826988	1.344029	0.076511
C	0.777594	2.301736	-0.487634
O	-0.432586	1.907325	-0.059092
O	0.962046	3.256628	-1.208431
O	3.016732	1.385240	-0.114545
O	1.530891	-0.608159	1.509214
H	-0.994781	-0.050231	0.329364
C	-1.079977	1.124579	2.169083
H	-0.446443	1.865342	2.672644
C	-1.260637	-0.066017	3.107397
H	-0.287667	-0.489334	3.363154
O	-2.369362	1.671737	1.905368
H	-2.265534	2.541112	1.489714
H	-1.729384	0.304484	4.026469
O	-2.033530	-1.125606	2.538196
H	-2.938366	-0.805507	2.405438

DHA1_6

charge: 0 multiplicity: 1

E(RB3LYP) = -683.606621648 A.U.

C	-0.407865	0.722938	0.915264
C	1.064730	0.378420	0.991496
C	1.799609	1.369475	0.081820
C	0.713853	2.289114	-0.476313
O	-0.473452	1.886892	0.007043
O	0.855857	3.226362	-1.228325
O	2.980573	1.419461	-0.153829
O	1.595856	-0.509598	1.622476
H	-0.947746	-0.090068	0.417945
C	-1.124978	1.101686	2.230459
H	-0.562134	1.898868	2.730257
C	-1.297451	-0.087923	3.190753
H	-2.079147	0.192789	3.899905
O	-2.442527	1.542597	1.910578
H	-2.385758	2.377386	1.420653
H	-1.632070	-0.975844	2.640325
O	-0.133238	-0.373967	3.964600
H	0.531425	-0.784577	3.388248

DHA1_7

charge: 0 multiplicity: 1

E(RB3LYP) = -683.606595631 A.U.

C	-0.446801	0.702020	0.880222
C	1.008338	0.292024	0.981371
C	1.814010	1.318519	0.177206
C	0.785623	2.315438	-0.354368
O	-0.434724	1.921843	0.046344
O	0.991963	3.298843	-1.028635
O	3.004981	1.342528	-0.006492
O	1.481100	-0.660478	1.562723
H	-1.003632	-0.054512	0.317026
C	-1.188745	1.032888	2.195429

H	-0.607890	1.773027	2.758446
C	-1.441652	-0.200945	3.077871
H	-2.226678	0.074422	3.785374
O	-2.475027	1.551269	1.865550
H	-2.365658	2.412729	1.434258
H	-1.803761	-1.037672	2.467883
O	-0.311204	-0.588374	3.857851
H	0.343845	-1.002547	3.273452

DHA1_8

charge: 0 multiplicity: 1

E(RB3LYP) = -683.606555662 A.U.

C	-0.438174	0.724685	0.876975
C	1.019397	0.326912	0.989675
C	1.822133	1.356293	0.186614
C	0.791119	2.351933	-0.342139
O	-0.427759	1.956550	0.061056
O	0.995111	3.338311	-1.012759
O	3.012719	1.382145	0.000804
O	1.495631	-0.621167	1.575618
H	-0.977283	-0.029444	0.293209
C	-1.204846	1.024335	2.185165
H	-0.639457	1.756114	2.774127
C	-1.465689	-0.229534	3.036888
H	-2.265568	0.026109	3.735055
O	-2.488652	1.541376	1.843474
H	-2.377666	2.414677	1.437206
H	-1.810743	-1.055203	2.402478
O	-0.348239	-0.626957	3.830497
H	0.324858	-1.016472	3.249538

DHA1_9

charge: 0 multiplicity: 1

E(RB3LYP) = -683.608566987 A.U.

C	-0.388752	0.735631	0.849352
C	1.083378	0.399813	0.942880
C	1.825443	1.427184	0.078580
C	0.736987	2.327225	-0.507019
O	-0.455828	1.893655	-0.067525
O	0.881703	3.271943	-1.249862
O	3.012428	1.512260	-0.114889
O	1.609684	-0.500484	1.558534
H	-0.935800	-0.076764	0.363404
C	-1.070953	1.133651	2.177628
H	-0.463487	1.903669	2.669465
C	-1.215227	-0.046220	3.135387
H	-0.229911	-0.436298	3.396806
O	-2.377047	1.632683	1.901995
H	-2.300774	2.488948	1.454215
H	-1.694547	0.324539	4.048926
O	-1.956296	-1.137201	2.583368
H	-2.868474	-0.843946	2.438895

DHA1_10

charge: 0 multiplicity: 1

E(RB3LYP) = -683.608577033 A.U.

C	-0.424568	0.736502	0.833813
C	1.038054	0.358060	0.912602
C	1.804031	1.381371	0.065049
C	0.738804	2.322502	-0.497207
O	-0.463524	1.914214	-0.059494
O	0.906373	3.276830	-1.222846
O	2.992128	1.437856	-0.132262
O	1.542163	-0.568319	1.507803
H	-0.996153	-0.050481	0.334385
C	-1.089953	1.125344	2.173345
H	-0.460592	1.869383	2.677320
C	-1.259464	-0.069559	3.108302
H	-0.282938	-0.488201	3.358229
O	-2.383966	1.663469	1.914588
H	-2.287559	2.534222	1.499984
H	-1.726443	0.294818	4.030734
O	-2.028692	-1.131386	2.538395
H	-2.935313	-0.815144	2.408511

1$(H_2O)_2$

Charge = -2 Multiplicity = 1

E(RB3LYP) = -1520.47910259 A.U.

C	-2.565621	1.168653	0.171362
C	-1.328593	0.785813	0.969205
C	-0.147280	1.668177	0.516370
C	-0.856474	2.676877	-0.416485
O	-2.153190	2.339186	-0.606908
O	-0.384600	3.667367	-0.939884
O	0.591545	2.162372	1.479917
O	-1.285475	-0.055445	1.848509
H	-2.817874	0.377016	-0.540132
C	-3.801535	1.566666	1.000145
H	-3.500238	2.315325	1.744487
C	-4.436490	0.393520	1.740573
H	-3.721331	-0.029198	2.447265
O	-4.802620	2.112669	0.135330
H	-4.449709	2.911141	-0.285628
H	-5.296662	0.777722	2.301717
O	-4.839938	-0.673786	0.876153
H	-5.549270	-0.348376	0.301788
O	0.603722	0.860957	-0.535387
C	1.121891	-0.362511	-0.152277
C	0.535840	-1.596577	-0.417098
C	2.416399	-0.551145	0.408995
C	1.504001	-2.660549	0.095584
O	-0.584291	-1.865169	-0.959008
O	2.649903	-1.906830	0.580705
O	3.311679	0.243535	0.735194
H	1.067185	-3.183153	0.955013
C	2.008301	-3.696808	-0.922533
H	2.411331	-3.173311	-1.799732
C	0.926227	-4.688942	-1.369550
O	3.033161	-4.496363	-0.314927

H	1.424650	-5.515671	-1.882514
H	0.414412	-5.095068	-0.485403
O	-0.009990	-4.129584	-2.288274
H	3.741802	-3.905623	-0.017287
H	-0.397697	-3.329464	-1.855075
O	4.054636	2.868983	-0.036355
H	3.735161	1.969850	0.180624
H	3.388290	3.464041	0.372218
O	2.028895	4.387036	1.213967
H	1.622491	4.948003	0.537854
H	1.439578	3.577202	1.265681

2$(H_2O)_2$
Charge = -2 Multiplicity = 1
E(RB3LYP) = -1520.48898530 A.U.

C	-2.067145	2.317714	-0.779590
C	-1.964454	1.237341	0.309145
C	-0.497072	0.696732	0.221098
C	0.209500	1.897575	-0.471221
O	-0.685342	2.742591	-1.019590
O	1.405891	2.128783	-0.540269
O	0.056353	0.229580	1.300915
O	-2.998295	0.304554	0.206208
H	-2.481240	1.968799	-1.725046
C	-2.860217	3.480419	-0.155282
H	-2.289745	4.408381	-0.261732
C	-3.003201	3.059986	1.319260
H	-2.757803	3.853196	2.026454
O	-4.162732	3.636045	-0.716953
H	-4.072345	4.056344	-1.585733
H	-4.024543	2.706932	1.504209
O	-2.054223	1.992762	1.521973
O	-0.527408	-0.290396	-0.980814
C	-0.311893	-1.609759	-0.670619
C	-1.123503	-2.449239	0.074263
C	0.809018	-2.345123	-1.154036
C	-0.460453	-3.819241	0.094881
O	-2.220785	-2.192604	0.689440
O	0.723060	-3.660697	-0.736930
O	1.770112	-2.006697	-1.864870
H	-0.114987	-4.057282	1.108043
C	-1.275500	-5.003001	-0.452014
H	-1.644037	-4.753034	-1.455711
C	-2.457596	-5.397724	0.443364
O	-0.435440	-6.164169	-0.512711
H	-2.802805	-6.383681	0.121797
H	-2.119176	-5.477053	1.485974
O	-3.569648	-4.511004	0.334703
H	0.329410	-5.956443	-1.070928
H	-3.244795	-3.609873	0.568953
H	-2.682919	-0.612005	0.456328
H	2.844385	-0.603623	-1.398247
O	3.410454	0.123786	-1.062722
H	3.072897	-0.421139	0.806043

O	2.625688	-0.580820	1.659143
H	1.696342	-0.274925	1.488910
H	2.779550	0.850015	-0.898054

3a$(H_2O)_2$
Charge = -1 Multiplicity = 1
E(RB3LYP) = -1520.94322365 A.U.

C	-2.624991	1.204423	0.214858
C	-1.387047	0.786106	0.991276
C	-0.203439	1.644345	0.509615
C	-0.902787	2.696682	-0.371552
O	-2.199829	2.384385	-0.541158
O	-0.405236	3.679670	-0.880825
O	0.481459	2.148137	1.593172
O	-1.326814	-0.067118	1.850060
H	-2.894210	0.432883	-0.512385
C	-3.848120	1.596744	1.068792
H	-3.529987	2.321053	1.829296
C	-4.482848	0.406306	1.782635
H	-3.763889	-0.040724	2.470408
O	-4.847765	2.173494	0.227186
H	-4.521131	3.019083	-0.115278
H	-5.333841	0.781618	2.363040
O	-4.901185	-0.632818	0.892705
H	-5.626221	-0.293708	0.346713
O	0.618829	0.928398	-0.431668
C	1.113206	-0.317358	-0.052862
C	0.553602	-1.535524	-0.424714
C	2.352921	-0.519256	0.609531
C	1.488602	-2.615521	0.118871
O	-0.516822	-1.777709	-1.060837
O	2.582556	-1.876629	0.734167
O	3.200659	0.269338	1.056201
H	0.986746	-3.178249	0.914597
C	2.087484	-3.599631	-0.900416
H	2.557531	-3.032342	-1.714549
C	1.055824	-4.574262	-1.484540
O	3.064228	-4.420101	-0.245978
H	1.603878	-5.373679	-1.989726
H	0.471654	-5.022849	-0.668803
O	0.199545	-3.976449	-2.455959
H	3.750198	-3.842089	0.121567
H	-0.240996	-3.207796	-2.020677
O	4.195352	2.615048	-0.033642
H	3.819348	1.759038	0.273096
H	2.849537	3.661880	0.396936
H	4.263028	2.537133	-0.996398
O	2.052798	4.136618	0.742391
H	1.494455	4.310672	-0.034293
H	1.108124	2.877957	1.300848

4a$(H_2O)_2$
Charge = -1 Multiplicity = 1

E(RB3LYP) = -1520.95448202 A.U.

C	-2.042432	2.355301	-0.788355
C	-1.946433	1.188632	0.214286
C	-0.473426	0.686861	0.095323
C	0.233117	1.938926	-0.491230
O	-0.664687	2.812868	-0.967954
O	1.428606	2.155130	-0.540096
O	0.031736	0.267120	1.296624
O	-2.944055	0.250822	-0.028056
H	-2.434386	2.076445	-1.765778
C	-2.867046	3.447620	-0.082500
H	-2.302956	4.385253	-0.088555
C	-3.045659	2.895286	1.343394
H	-2.833384	3.623515	2.126394
O	-4.153812	3.638639	-0.663483
H	-4.048417	4.138772	-1.487077
H	-4.063667	2.508609	1.464357
O	-2.081931	1.828148	1.479927
O	-0.374291	-0.289592	-0.969281
C	-0.228823	-1.625278	-0.622562
C	-1.080608	-2.432191	0.110900
C	0.870097	-2.390763	-1.106153
C	-0.453681	-3.820636	0.136704
O	-2.171447	-2.148590	0.718771
O	0.740595	-3.697794	-0.686516
O	1.840165	-2.076753	-1.812433
H	-0.123066	-4.064278	1.153237
C	-1.297322	-4.982553	-0.414904
H	-1.646239	-4.726630	-1.423892
C	-2.500846	-5.340516	0.467991
O	-0.489065	-6.165864	-0.458767
H	-2.862669	-6.321520	0.150081
H	-2.179987	-5.417145	1.516197
O	-3.592355	-4.432017	0.334237
H	0.279191	-5.990162	-1.023152
H	-3.257265	-3.539640	0.579177
H	-2.684169	-0.645720	0.341788
H	2.868145	-0.637304	-1.399277
O	3.418812	0.094231	-1.043868
H	3.043727	-0.251897	0.690456
O	2.614024	-0.408211	1.565182
H	1.014485	0.081128	1.271700
H	3.032157	0.217383	2.175143
H	2.814880	0.858832	-1.021777

3b$(H_2O)_2$

Charge = -1 Multiplicity = 1

E(RB3LYP) = -1520.93496153 A.U.

C	-1.838592	2.388369	-0.581778
C	-1.973093	1.078111	0.169559
C	-0.557920	0.521114	0.396179
C	0.315828	1.747194	0.087493
O	-0.407832	2.687127	-0.549797
O	1.493162	1.888129	0.341116

O	-0.388627	0.005574	1.667508
O	-3.010726	0.518637	0.461600
H	-2.121606	2.246482	-1.629422
C	-2.615332	3.600760	-0.000289
H	-1.996347	4.476941	-0.223771
C	-2.846511	3.479445	1.506088
H	-3.070964	4.468892	1.921231
O	-3.895658	3.732255	-0.606618
H	-3.785881	4.117852	-1.489173
H	-3.708361	2.825961	1.682731
O	-1.670361	2.926776	2.097068
H	-1.929130	2.449599	2.922989
O	-0.427329	-0.459394	-0.645242
C	0.853289	-0.927484	-0.946533
C	1.515302	-1.991642	-0.347498
C	1.579722	-0.445754	-2.071262
C	2.818524	-2.165215	-1.134338
O	1.201006	-2.714796	0.648172
O	2.756225	-1.165259	-2.191843
O	1.322906	0.450033	-2.883416
H	3.674522	-1.912840	-0.497494
C	3.056767	-3.536561	-1.788750
H	2.176818	-3.806241	-2.387806
C	3.353148	-4.654344	-0.780068
O	4.217315	-3.461010	-2.628329
H	3.747425	-5.508190	-1.337090
H	4.128597	-4.317038	-0.077740
O	2.195830	-5.109250	-0.082179
H	4.072060	-2.761425	-3.283695
H	1.793908	-4.320370	0.355926
O	-2.469455	1.545058	4.333432
H	-1.687478	1.287522	4.843304
H	-2.815814	0.707604	3.942973
O	-3.525005	-0.688348	3.060204
H	-3.029925	-1.491330	3.280160
H	-3.265251	-0.472713	2.144915
H	0.560101	-0.105280	1.856107

4b$(H_2O)_2$
Charge = -1 Multiplicity = 1
E(RB3LYP) = -1520.94830948 A.U.

C	-1.807552	2.493810	-0.586156
C	-1.788790	1.465585	0.559639
C	-0.349401	0.891911	0.522822
C	0.430162	2.074615	-0.090572
O	-0.410977	2.897315	-0.743613
O	1.625149	2.273736	-0.022666
O	0.125203	0.525237	1.773971
O	-2.831107	0.559438	0.424410
H	-2.163780	2.103143	-1.538499
C	-2.629799	3.684463	-0.056608
H	-2.069669	4.609789	-0.219499
C	-2.800489	3.373104	1.441661
H	-2.516081	4.196719	2.096083

O	-3.919363	3.773674	-0.654858
H	-3.821202	4.160726	-1.538293
H	-3.832774	3.072658	1.646640
O	-1.894832	2.277011	1.727897
H	-2.197193	1.455893	3.401089
O	-0.384133	-0.191123	-0.408758
C	0.831913	-0.761290	-0.782655
C	1.467120	-1.837360	-0.175992
C	1.482435	-0.413786	-2.000218
C	2.685135	-2.151305	-1.049787
O	1.184871	-2.481406	0.883044
O	2.595928	-1.220436	-2.166109
O	1.209638	0.434628	-2.857112
H	3.606985	-1.918780	-0.503567
C	2.780737	-3.574725	-1.624608
H	1.839259	-3.819958	-2.134045
C	3.087331	-4.645190	-0.568807
O	3.870669	-3.632534	-2.555394
H	3.378357	-5.557491	-1.095939
H	3.938605	-4.319525	0.045941
O	1.964688	-4.972977	0.246887
H	3.720473	-2.962805	-3.240198
H	1.647942	-4.129889	0.654602
O	-2.461130	0.931947	4.185882
H	-1.651465	0.830182	4.707417
H	-2.747154	-0.556953	3.210317
O	-2.951416	-1.202141	2.492444
H	-2.183611	-1.791261	2.448961
H	-2.823910	-0.094548	1.175862
H	1.096455	0.473665	1.753223

TS(3b$(H_2O)_2$ / **4b**$(H_2O)_2$**)**
Charge = -1 Multiplicity = 1
E(RB3LYP) = -1520.91917179 A.U.

C	-0.712356	1.538235	0.841610
C	-0.744864	0.439207	1.927527
C	0.724328	-0.079262	1.957654
C	1.505667	1.142296	1.447345
O	0.686820	1.971767	0.774089
O	2.688029	1.375523	1.603794
O	1.140974	-0.514570	3.207737
O	-1.732726	-0.393855	1.947299
H	-1.007648	1.174024	-0.142335
C	-1.564577	2.719136	1.331425
H	-1.078390	3.658037	1.049509
C	-1.638417	2.550432	2.858140
H	-1.286806	3.426546	3.403590
O	-2.892310	2.674635	0.811882
H	-2.865209	2.932135	-0.122389
H	-2.659736	2.303972	3.161219
O	-0.747739	1.450945	3.184703
H	-1.029383	0.908646	4.239905
O	0.748400	-1.114020	0.966437
C	1.984475	-1.658062	0.622448

C	2.581479	-2.779018	1.185202
C	2.699470	-1.235774	-0.534113
C	3.840319	-3.045770	0.355115
O	2.239562	-3.491824	2.181071
O	3.816623	-2.038691	-0.696407
O	2.475491	-0.330372	-1.345825
H	4.735728	-2.864099	0.961135
C	3.949457	-4.427292	-0.311562
H	3.030208	-4.626287	-0.878517
C	4.196292	-5.570095	0.682059
O	5.080566	-4.434826	-1.193687
H	4.506502	-6.447571	0.108707
H	5.018375	-5.295793	1.358384
O	3.032388	-5.940930	1.417607
H	4.967633	-3.716748	-1.835356
H	2.700287	-5.123381	1.863924
O	-1.342559	0.356411	5.258111
H	-0.570122	0.288774	5.843310
H	-1.594868	-0.587498	4.964668
O	-2.040966	-1.851891	4.121841
H	-1.377906	-2.555433	4.184753
H	-1.879581	-1.395495	3.238232
H	2.111136	-0.584644	3.224148

F. Cartesian coordinates of optimized structures at CBS-QB3

H_2A

charge: 0 multiplicity: 1

CBS-QB3 Free Energy= -683.929637 A.U.

C	-0.398437	0.729848	0.880564
C	1.084240	0.461268	0.921993
C	1.713439	1.341478	0.118864
C	0.734772	2.250521	-0.442084
O	-0.511505	1.891991	0.020384
O	0.881910	3.194258	-1.190586
O	3.036630	1.490423	-0.188373
O	1.656434	-0.535432	1.607512
H	-0.925906	-0.091383	0.384999
C	-1.101477	1.050388	2.213032
H	-0.502489	1.789135	2.760454
C	-1.326583	-0.188498	3.081419
H	-1.950479	0.094688	3.931372
O	-2.407218	1.555953	1.948592
H	-2.308882	2.339485	1.393057
H	1.043024	-0.810729	2.341524
H	3.548787	0.857412	0.333887
H	-1.847342	-0.953624	2.503589
O	-0.106530	-0.788638	3.544857
H	0.276309	-0.213691	4.221554

HA^-

charge: -1 multiplicity: 1

CBS-QB3 Free Energy= -683.489850 A.U.

C	-0.475914	0.740647	0.871356

C	0.995058	0.354245	0.988659
C	1.699110	1.305349	0.284083
C	0.829621	2.283280	-0.261705
O	-0.483394	1.954639	0.074743
O	1.049185	3.286856	-0.932831
O	3.074589	1.375989	0.102954
O	1.421424	-0.668840	1.619746
H	-1.025748	-0.021847	0.309882
C	-1.218700	1.029004	2.181368
H	-0.641858	1.761863	2.759960
C	-1.444089	-0.217468	3.041676
H	-2.174435	0.042070	3.811051
O	-2.520492	1.545290	1.881939
H	-2.396874	2.294171	1.284921
H	3.457030	0.650770	0.616383
H	-1.879844	-1.011592	2.419462
O	-0.267057	-0.659922	3.705042
H	0.406915	-0.817973	3.003666

A^{2-}

charge: -2 multiplicity: 1

CBS-QB3 Free Energy= -683.029138

C	-0.441613	0.746454	0.905231
C	1.037549	0.414698	0.976636
C	1.742184	1.322090	0.191440
C	0.771922	2.224319	-0.372481
O	-0.522370	1.903434	0.029837
O	0.924609	3.191802	-1.131908
O	3.049813	1.395555	-0.049294
O	1.492140	-0.593839	1.663495
H	-1.001693	-0.063618	0.423434
C	-1.147833	1.106005	2.217531
H	-0.597980	1.924923	2.697950
C	-1.257689	-0.064032	3.197707
H	-1.958927	0.225376	3.983687
O	-2.499799	1.511458	1.943822
H	-2.457860	2.228722	1.297967
H	-1.675915	-0.934800	2.674142
O	-0.017994	-0.382423	3.822482
H	0.616994	-0.572115	3.081677

HA$^{\bullet}$

charge: 0 multiplicity: 2

CBS-QB3 Free Energy= -683.304633

C	-0.423430	0.742418	0.857765
C	1.057404	0.400031	0.920731
C	1.714558	1.361667	0.085763
C	0.731548	2.278284	-0.481938
O	-0.499381	1.900464	-0.033573
O	0.895801	3.219522	-1.223210
O	2.998956	1.466250	-0.172180
O	1.585727	-0.512311	1.554231
H	-0.986011	-0.064630	0.386525

C	-1.064425	1.120805	2.201471
H	-0.416745	1.845034	2.710271
C	-1.259293	-0.089445	3.106866
H	-0.300020	-0.562795	3.313158
O	-2.359148	1.676659	1.975928
H	-2.261175	2.433818	1.384741
H	3.489416	0.768614	0.300513
H	-1.685359	0.262632	4.052967
O	-2.094790	-1.083721	2.512623
H	-2.936792	-0.657440	2.308500

$A^{-\bullet}$

charge: -1 multiplicity: 2

CBS-QB3 Free Energy= -682.878970

C	-0.422582	0.739373	0.846470
C	1.061732	0.408160	0.900081
C	1.749134	1.383311	0.089918
C	0.723645	2.287582	-0.461138
O	-0.523951	1.898848	-0.034121
O	0.852964	3.251216	-1.194336
O	2.991294	1.488603	-0.135425
O	1.551124	-0.540353	1.540216
H	-0.991901	-0.069263	0.383737
C	-1.054228	1.115379	2.193118
H	-0.402916	1.842779	2.694302
C	-1.247957	-0.083587	3.111735
H	-0.290889	-0.566921	3.302273
O	-2.354591	1.677434	1.982817
H	-2.265288	2.375424	1.321210
H	-1.654911	0.277175	4.063558
O	-2.107998	-1.072096	2.539040
H	-2.930292	-0.621586	2.307796

DHA1

Charge = 0 Multiplicity = 1

CBS-QB3 Free Energy= -682.709727

C	-0.397499	0.720337	0.866234
C	1.066445	0.357818	0.948524
C	1.813220	1.361466	0.063725
C	0.737360	2.285980	-0.503597
O	-0.459558	1.880441	-0.042378
O	0.889631	3.220570	-1.241819
O	2.991177	1.420017	-0.149819
O	1.580735	-0.531563	1.576360
H	-0.966595	-0.082108	0.394735
C	-1.051028	1.117378	2.204035
H	-0.398004	1.830415	2.720381
C	-1.273233	-0.093321	3.103597
H	-0.322222	-0.575723	3.327315
O	-2.328337	1.691273	1.952722
H	-2.206280	2.480207	1.409504
H	-1.710506	0.264640	4.042000
O	-2.106678	-1.078548	2.494823

H	-2.953840	-0.656030	2.304973

$H_2A(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -836.648798

C	0.920221	0.160777	0.438987
C	-0.207242	-0.411207	-0.381422
C	-1.169568	0.521101	-0.533212
C	-0.721373	1.747889	0.105967
O	0.515380	1.533780	0.666766
O	-1.268683	2.828308	0.182926
O	-2.377962	0.503317	-1.149541
O	-0.240118	-1.681455	-0.815609
H	0.972425	-0.327141	1.417794
C	2.326767	0.176942	-0.189312
H	2.251953	0.560787	-1.214581
C	2.996104	-1.198324	-0.193427
H	4.033135	-1.075735	-0.511674
O	3.185880	0.999160	0.596278
H	2.796912	1.882318	0.626106
H	2.985442	-1.617793	0.813769
O	2.331804	-2.151332	-1.038526
H	2.497144	-1.907506	-1.959558
O	-3.139950	-1.774935	-2.395882
H	-2.551415	-0.364590	-1.587664
H	-3.968368	-1.635439	-2.872648
O	-2.667975	-3.023529	0.097797
H	-1.742796	-2.745689	0.039945
H	-3.016385	-2.705346	-0.752145
H	-2.515501	-2.100997	-3.056552
H	0.693099	-2.027080	-0.873364

$HA^-(H_2O)_2$
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -836.208380

C	-1.078811	0.148627	-0.572523
C	0.373739	-0.165530	-0.252476
C	1.001818	1.032625	-0.023326
C	0.074623	2.111138	-0.167354
O	-1.166616	1.596793	-0.516602
O	0.222433	3.319340	-0.046882
O	2.329408	1.273478	0.282688
O	0.843281	-1.368369	-0.236044
H	-1.316639	-0.154267	-1.597257
C	-2.137675	-0.426948	0.378482
H	-1.873062	-0.151591	1.407269
C	-2.278680	-1.949419	0.291026
H	-3.204433	-2.220603	0.802527
O	-3.419905	0.106544	0.032287
H	-3.339370	1.068776	0.031811
H	-2.376842	-2.244778	-0.762496
O	-1.220254	-2.649491	0.933211
H	-0.390854	-2.364664	0.491598

O	2.878558	-1.070212	1.616483
H	2.647413	0.519018	0.830948
H	2.417998	-1.000150	2.461989
O	3.277433	-0.985386	-1.648561
H	2.440290	-1.272277	-1.238339
H	3.388385	-0.102067	-1.272966
H	2.189933	-1.390770	0.993656

$\mathbf{A}^{2-}(H_2O)_2$
Charge = -2 Multiplicity = 1
CBS-QB3 Free Energy= -835.746865

C	1.280257	0.403062	0.623748
C	-0.150108	0.027815	0.958101
C	-0.983237	1.063340	0.569260
C	-0.149543	2.093211	-0.003388
O	1.197313	1.731628	0.047853
O	-0.448390	3.183707	-0.490949
O	-2.313756	1.161688	0.648929
O	-0.440471	-1.107331	1.527826
H	1.898035	0.474170	1.526530
C	2.001204	-0.491852	-0.392266
H	1.386565	-0.547493	-1.300393
C	2.263591	-1.914564	0.107307
H	2.991099	-2.372052	-0.567195
O	3.285665	0.069905	-0.696722
H	3.136038	0.990838	-0.946157
H	2.715033	-1.873025	1.108613
O	1.097295	-2.728623	0.095078
H	0.444228	-2.267058	0.678342
O	-3.298698	-0.164369	-1.327471
H	-2.925519	0.399838	-0.562126
O	-2.631852	-2.320573	0.374173
H	-1.916331	-1.859678	0.864775
H	-2.918119	-1.646470	-0.272573
H	-2.563048	-0.224854	-1.947883

$\mathbf{A}^{2-}(H_2O)_2$
(solvation cavity scaled by 0.9)
Charge = -2 Multiplicity = 1
CBS-QB3 Free Energy= -835.754811

C	-1.205160	0.267800	-0.580224
C	0.253428	-0.076225	-0.343896
C	0.935990	1.081378	-0.009504
C	-0.022958	2.158184	-0.020187
O	-1.286261	1.703275	-0.369396
O	0.129302	3.360654	0.216264
O	2.225404	1.272465	0.284136
O	0.701353	-1.294129	-0.487292
H	-1.488279	0.076693	-1.621380
C	-2.243131	-0.392722	0.336455
H	-1.966394	-0.192513	1.379055
C	-2.376231	-1.904247	0.137268
H	-3.283633	-2.226624	0.652383

O	-3.544055	0.149122	0.055289
H	-3.474298	1.110620	0.118505
H	-2.497099	-2.120164	-0.932656
O	-1.287433	-2.637577	0.693658
H	-0.473135	-2.290538	0.254566
O	3.350465	-0.763184	1.519816
H	2.902204	0.017934	1.067000
O	3.334878	-1.413931	-1.349326
H	2.375185	-1.379747	-1.138786
H	3.714427	-1.161633	-0.493214
H	2.731883	-1.484729	1.348395

HA$^{\bullet}(H_2O)_2$
Charge = 0 Multiplicity = 2
CBS-QB3 Free Energy= -836.024532

C	1.102831	0.234421	0.385746
C	-0.239794	-0.343120	-0.036310
C	-1.116015	0.779913	-0.211233
C	-0.382392	2.010318	0.092490
O	0.889901	1.678503	0.450903
O	-0.769944	3.156216	0.062415
O	-2.369021	0.816203	-0.570344
O	-0.492097	-1.541250	-0.186757
H	1.367143	-0.100534	1.389735
C	2.262606	-0.034889	-0.585103
H	1.937008	0.223224	-1.600328
C	2.714514	-1.489745	-0.570711
H	1.889080	-2.141050	-0.855055
O	3.393397	0.750541	-0.207645
H	3.121417	1.676863	-0.190874
H	3.516429	-1.599696	-1.309426
O	3.153375	-1.914233	0.720841
H	3.877115	-1.329721	0.979497
O	-3.552272	-1.412821	-1.103924
H	-2.769533	-0.099925	-0.768922
H	-4.401350	-1.260155	-1.540671
O	-2.825390	-2.523363	1.418161
H	-1.898760	-2.418211	1.165592
H	-3.282340	-2.200409	0.624702
H	-3.035381	-1.955042	-1.715094

A$^{-\bullet}(H_2O)_2$
Charge = -1 Multiplicity = 2
CBS-QB3 Free Energy= -835.596412

C	1.190542	0.213059	0.477958
C	-0.257602	-0.203842	0.279906
C	-1.041104	0.999753	0.184094
C	-0.111662	2.135929	0.350129
O	1.163723	1.670611	0.536211
O	-0.346695	3.328258	0.343376
O	-2.286546	1.142784	-0.007795
O	-0.635505	-1.390640	0.222258
H	1.573999	-0.142553	1.436069

C	2.146580	-0.194538	-0.652467
H	1.686478	0.073414	-1.612047
C	2.458416	-1.685243	-0.658658
H	1.539295	-2.259646	-0.764321
O	3.398509	0.480540	-0.496325
H	3.213023	1.424459	-0.411031
H	3.102923	-1.893998	-1.520367
O	3.082559	-2.115738	0.553247
H	3.871196	-1.570289	0.666888
O	-3.963314	-0.700296	-1.192974
H	-3.347504	-0.063892	-0.767131
O	-3.230489	-2.267046	1.051259
H	-2.313960	-2.006794	0.854394
H	-3.711995	-1.812900	0.337048
H	-3.381101	-1.252238	-1.729308

DHA1a$(H_2O)_2$
charge: 0 multiplicity: 1
CBS-QB3 Free Energy= -835.425431 A.U.

C	-0.962394	-0.295439	0.954328
C	-0.427291	0.856454	0.128863
C	0.780899	0.317657	-0.636209
C	0.932809	-1.131021	-0.175986
O	-0.068764	-1.431124	0.664844
O	1.783329	-1.919837	-0.502354
O	-0.874839	1.971256	0.038806
H	-0.871615	-0.085091	2.020132
O	1.419951	0.865863	-1.493094
O	1.894186	0.797828	1.563754
H	1.756556	0.143188	2.261337
H	2.750065	0.543784	1.151553
O	4.110198	-0.045327	0.089559
H	3.623608	-0.803633	-0.267193
H	4.048938	0.610981	-0.616928
C	-2.402926	-0.721108	0.618356
H	-2.507444	-0.804445	-0.469655
C	-3.427903	0.280486	1.138125
H	-3.258379	1.259863	0.692015
H	-4.420332	-0.072020	0.836439
O	-3.355596	0.449328	2.553692
H	-3.506656	-0.417873	2.950540
O	-2.687539	-1.966799	1.247980
H	-2.074552	-2.628514	0.903671

DHA1b$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.424974

C	0.720084	-0.458053	-0.131230
C	-0.049849	0.767203	0.307723
C	-1.514594	0.345665	0.422423
C	-1.547979	-1.109704	-0.040749
O	-0.292990	-1.507143	-0.321341
O	-2.508153	-1.826039	-0.136470

O	-2.431107	0.965953	0.891425
O	0.390058	1.862861	0.557910
H	1.191322	-0.289781	-1.099318
C	1.759894	-0.968981	0.883230
H	1.301274	-1.005643	1.878306
C	2.989862	-0.070395	0.936861
H	2.707979	0.939624	1.232725
O	2.210863	-2.260815	0.487837
H	1.445812	-2.847909	0.438849
H	3.667962	-0.477920	1.694788
O	3.643013	0.033137	-0.327950
H	3.880881	-0.863228	-0.597079
O	-1.693517	3.462658	-1.028108
H	-1.029273	3.328656	-0.336061
H	-2.529842	3.319122	-0.566106
O	-1.283127	0.893242	-2.015230
H	-2.136562	0.532091	-2.289738
H	-1.471006	1.835008	-1.801053

DHA1c$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.428090

C	1.176680	0.757605	-0.977711
C	0.038314	-0.234907	-1.051204
C	0.459177	-1.434566	-0.211245
C	1.899788	-1.138101	0.212071
O	2.270555	0.055982	-0.296082
O	2.630598	-1.841257	0.854912
O	-0.146959	-2.446974	0.018207
O	-0.972760	-0.138222	-1.708652
H	1.524655	1.016106	-1.977922
C	0.819320	2.031567	-0.171552
H	1.670209	2.718917	-0.217079
C	0.548595	1.652976	1.282116
H	1.494601	1.537063	1.810602
O	-0.347512	2.629187	-0.718707
H	-0.132602	2.982467	-1.591277
H	-0.021979	2.456607	1.754990
O	-0.150442	0.409548	1.384326
H	-1.130760	0.556874	1.294148
O	-2.801152	0.694632	1.168267
H	-3.002891	-0.111497	0.642059
H	-3.152725	0.507410	2.047574
O	-3.105095	-1.576412	-0.412853
H	-2.539899	-2.201707	0.060612
H	-2.496249	-1.208469	-1.075862

DHA2(H_2O)
charge: 0 multiplicity: 1
CBS-QB3 Free Energy= -835.439119 A.U.

C	-0.917288	0.387887	-0.487851
C	0.299533	-0.511602	-0.520652
C	1.530124	0.338717	-0.154755

C	0.942132	1.753094	-0.057728
O	-0.389218	1.732490	-0.278080
O	1.547024	2.771687	0.147600
O	2.038221	0.003823	1.102217
O	0.302360	-1.696152	-0.755213
H	-1.428121	0.383072	-1.451248
C	-1.915870	0.070239	0.644482
H	-1.359292	-0.042931	1.582228
C	-2.702793	-1.206508	0.377189
H	-2.025337	-2.054767	0.284829
O	-2.864277	1.127774	0.745442
H	-2.387985	1.944716	0.940937
H	-3.360779	-1.379506	1.235881
O	-3.454515	-1.139708	-0.834675
H	-4.057162	-0.389797	-0.752556
O	2.674763	-2.615167	0.754656
H	2.313975	-0.949838	1.066850
H	3.489335	-2.573527	0.236927
O	2.458231	0.234398	-1.200243
H	3.147695	0.899973	-1.051760
H	1.975689	-2.706678	0.088027

DHA3(H_2O)
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.429401 A.U.

C	0.632838	-0.591937	-0.372272
C	-0.252119	0.672913	-0.516767
C	-1.613487	0.194695	0.023373
C	-1.568004	-1.336069	0.035818
O	-0.317290	-1.719362	-0.255015
O	-2.476616	-2.093564	0.248250
O	-2.566781	0.844532	0.364355
O	0.266831	1.755175	0.164743
H	1.191186	-0.778452	-1.286843
C	1.575485	-0.635175	0.838056
H	1.066889	-0.223458	1.716589
C	2.860761	0.150107	0.584776
H	2.634449	1.189411	0.357328
O	1.990775	-1.980832	1.083614
H	1.202415	-2.534072	1.150570
H	3.463855	0.113530	1.499019
O	3.593955	-0.371173	-0.525259
H	3.738672	-1.309231	-0.345976
O	-1.704854	3.619824	-0.013755
H	-0.385284	2.500951	0.113018
H	-2.338462	2.909240	0.173905
O	-0.445784	1.037564	-1.878094
H	-0.545753	0.248940	-2.430904
H	-1.775507	3.745174	-0.969315

DHA4(H_2O)
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.451234 A.U.

C	-0.989352	-0.560800	-0.879946
C	0.482845	-0.812056	-0.469307
C	0.903403	0.478901	0.318976
C	-0.375544	1.336345	0.332566
O	-1.397524	0.684597	-0.249512
O	-0.509195	2.439591	0.806043
O	1.944038	1.105618	-0.366281
O	1.323111	-1.084319	-1.544983
H	-1.106668	-0.440895	-1.954397
C	-1.772446	-1.751093	-0.319384
H	-2.774340	-1.460770	0.006042
C	-0.892460	-2.202803	0.835700
H	-1.112300	-1.633671	1.742342
O	-1.809029	-2.800494	-1.282626
H	-2.342256	-2.499203	-2.029005
H	-0.976250	-3.269412	1.035419
O	0.466195	-1.935998	0.403582
H	1.332939	-0.758933	1.725795
O	1.225135	0.205937	1.658460
H	2.170216	1.949722	0.102757
H	2.611015	3.109935	1.874304
O	2.254971	3.411555	1.028424
H	1.293064	3.405547	1.162898
H	2.080138	-0.479928	-1.480108

DHA5a$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.441309 A.U.

C	-1.039353	1.004057	-0.659448
C	-0.205263	-0.249279	-0.349303
C	1.233274	0.219443	-0.564605
C	1.176483	1.755732	-0.573294
O	-0.113467	2.136345	-0.571046
O	2.104582	2.517231	-0.579988
O	2.242536	-0.418485	-0.706143
O	-0.607453	-1.352149	-1.067980
H	-1.473877	0.999297	-1.655856
C	-2.064564	1.080483	0.472139
H	-2.376178	2.110643	0.660349
C	-1.306005	0.484132	1.647942
H	-0.780837	1.251980	2.217066
O	-3.170579	0.236831	0.171810
H	-3.641740	0.619018	-0.579416
H	-1.957813	-0.089146	2.306061
O	-0.318162	-0.421299	1.075024
H	0.289496	-2.021008	1.885940
O	0.670874	-2.883516	2.130598
H	1.107669	-3.247406	0.424334
H	1.517226	-2.659912	2.537628
O	1.267307	-3.238240	-0.546223
H	1.959861	-2.569717	-0.655866
H	0.037230	-2.093339	-0.912559

DHA5b$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.442913 A.U.

C	-1.167596	-0.563621	-0.896253
C	0.363902	-0.655368	-0.918020
C	0.812277	0.767338	-0.611192
C	-0.410924	1.458248	0.014332
O	-1.474431	0.658478	-0.141741
O	-0.455757	2.535418	0.550024
O	1.878114	1.280771	-0.812234
O	0.857111	-1.190778	-2.096870
H	-1.618530	-0.474817	-1.881105
C	-1.615818	-1.790336	-0.102048
H	-2.568409	-1.616155	0.403437
C	-0.469587	-1.982480	0.878350
H	-0.640669	-1.441594	1.809194
O	-1.669349	-2.920005	-0.965561
H	-2.415328	-2.800775	-1.567055
H	-0.279651	-3.035043	1.084374
O	0.716196	-1.419350	0.237617
H	1.517258	-0.323794	1.885012
O	1.427206	0.233651	2.669515
H	2.730202	2.633159	1.103183
H	1.693553	1.123543	2.369863
O	2.145784	2.878610	1.831795
H	1.289112	2.999696	1.390968
H	1.817499	-1.060783	-2.110966

DHA6
charge: 0 multiplicity: 1
CBS-QB3 Free Energy= -835.442408 A.U.

C	-0.481267	1.001215	1.007827
C	1.022868	0.781031	0.777746
C	1.284456	1.622998	-0.502989
C	0.257486	2.757159	-0.341249
O	-0.734395	2.343488	0.467459
O	0.268059	3.838206	-0.869231
O	2.570623	2.166264	-0.590522
O	1.272903	-0.589272	0.645931
H	-1.041762	0.293925	0.396127
C	-1.015383	0.975987	2.440110
H	-0.586428	1.813930	2.998220
C	-0.690493	-0.324606	3.187833
H	-1.458324	-0.452043	3.951907
H	-0.741431	-1.182941	2.507586
O	0.560832	-0.282774	3.872738
O	-2.442127	1.083095	2.400385
H	-2.666499	1.933607	2.002507
H	1.235416	0.031810	3.252994
O	1.740807	1.354402	1.846797
H	2.610161	1.629808	1.514707
H	2.210933	-0.709115	0.438785
O	0.946298	0.834334	-1.612924
H	0.961006	1.399987	-2.399623

H	3.173384	1.451340	-0.847358

TS(DHA1a(H_2O)$_2$ / **DHA2**(H_2O)**)**
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.398577 A.U.

C	0.308007	-0.307712	-0.452936
C	-0.749264	0.758702	-0.244100
C	-2.126141	0.064088	-0.225435
C	-1.753915	-1.428553	-0.263823
O	-0.421840	-1.577933	-0.431092
O	-2.497142	-2.370018	-0.159228
O	-3.035603	0.462949	0.580059
O	-0.559294	1.938459	-0.072265
H	0.759097	-0.207903	-1.441888
C	1.403579	-0.366183	0.624863
H	0.931228	-0.328574	1.613643
C	2.390976	0.787722	0.505292
H	1.870404	1.738714	0.609061
O	2.158494	-1.567282	0.476431
H	1.550928	-2.314913	0.540559
H	3.116050	0.694731	1.321552
O	3.051664	0.808693	-0.760769
H	3.496955	-0.042463	-0.860224
O	-3.808706	2.236757	-1.131225
H	-3.710695	1.844043	-0.211401
H	-4.748753	2.182111	-1.366279
O	-2.518558	0.319918	-1.804916
H	-3.151992	-0.376979	-2.042671
H	-3.238382	1.391337	-1.645743

TS(DHA1b(H_2O)$_2$ / **DHA3**(H_2O)**)**
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.388817 A.U.

C	0.336520	-0.083900	-0.564338
C	-0.562420	1.160619	-0.360145
C	-1.892064	0.548420	0.123503
C	-1.816159	-0.957606	-0.154533
O	-0.593057	-1.236557	-0.630965
O	-2.689186	-1.775367	-0.023969
O	-2.815601	1.101168	0.659618
O	-0.112018	2.187795	0.276337
H	0.853619	-0.066846	-1.519267
C	1.319912	-0.344133	0.583693
H	0.815645	-0.158676	1.540140
C	2.555569	0.545860	0.495186
H	2.260581	1.592686	0.510818
O	1.800493	-1.690024	0.525347
H	1.037624	-2.278621	0.463668
H	3.183903	0.340246	1.369466
O	3.286635	0.331841	-0.713840
H	3.492783	-0.610954	-0.749560
O	-1.630567	3.766337	-1.018972
H	-1.082388	3.431848	-0.231355

H	-2.557048	3.793709	-0.732446
O	-0.945707	1.639814	-1.870003
H	-1.563897	1.047360	-2.326833
H	-1.451633	2.801246	-1.609598

TS(DHA1c$(H_2O)_2$ / **DHA5a**(H_2O)**)**
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.410476 A.U.

C	-0.651645	0.972788	0.723083
C	0.247886	-0.272617	0.800463
C	1.664611	0.276518	0.721729
C	1.539771	1.797892	0.883379
O	0.237449	2.134342	0.880122
O	2.432739	2.598252	0.984204
O	2.704576	-0.303523	0.537170
O	-0.089884	-1.376027	0.281081
H	-1.147714	1.060500	-0.241623
C	-1.616939	0.940516	1.907674
H	-2.055246	1.926660	2.085422
C	-0.745857	0.485866	3.076082
H	-0.324353	1.348356	3.597901
O	-2.625316	-0.040750	1.677414
H	-3.169705	0.255264	0.936480
H	-1.329266	-0.112746	3.779795
O	0.316836	-0.305268	2.525168
H	0.597608	-1.558440	3.021681
O	0.853346	-2.571782	3.298969
H	1.190325	-2.999852	2.408786
H	1.596964	-2.542428	3.920499
O	1.519495	-3.355452	0.998735
H	2.431334	-3.075417	0.842938
H	0.963972	-2.630906	0.590107

TS(DHA5b$(H_2O)_2$ / **DHA4**(H_2O)**)**
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -835.415467 A.U.

C	-1.360642	0.590010	-0.603091
C	-0.361874	-0.570093	-0.412610
C	1.034218	0.142301	-0.223237
C	0.663722	1.622831	-0.020854
O	-0.663341	1.809415	-0.212045
O	1.403421	2.540041	0.232828
O	1.882400	-0.090773	-1.195992
O	-0.269817	-1.468316	-1.468009
H	-1.683764	0.704818	-1.635383
C	-2.508976	0.294588	0.364444
H	-2.965448	1.210181	0.748464
C	-1.813346	-0.507562	1.451625
H	-1.359431	0.151936	2.195386
O	-3.466884	-0.551359	-0.267485
H	-3.880386	-0.048998	-0.980936
H	-2.478800	-1.217155	1.940180
O	-0.778245	-1.261756	0.767966

H	0.936565	-0.960512	1.480554
O	1.575224	-0.295011	1.149501
H	3.294197	-0.827919	-0.533794
H	2.669125	-0.786098	0.918528
O	3.644359	-1.167136	0.340702
H	4.402109	-0.610511	0.577625
H	0.653416	-1.340534	-1.786288

DHA2^{-}(H_2O)
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -834.991200 A.U.

C	-0.929329	0.420856	-0.543496
C	0.310452	-0.440680	-0.716767
C	1.494704	0.365172	-0.176841
C	0.935687	1.795595	-0.187768
O	-0.419577	1.774459	-0.338193
O	1.526706	2.837529	-0.034586
O	1.692765	-0.003956	1.107502
O	0.316938	-1.584486	-1.123259
H	-1.522288	0.431988	-1.458260
C	-1.814039	0.040241	0.656406
H	-1.173369	-0.064804	1.539246
C	-2.567965	-1.263812	0.432059
H	-1.867339	-2.078589	0.250624
O	-2.798960	1.052415	0.868477
H	-2.339605	1.894493	0.979756
H	-3.133668	-1.489248	1.343070
O	-3.436731	-1.201656	-0.700966
H	-4.033123	-0.456569	-0.554076
O	2.465678	-2.594802	0.851129
H	2.212591	-1.652689	1.020877
O	2.614003	0.233439	-1.044427
H	3.355784	0.648823	-0.581395
H	2.016005	-2.766290	0.014736

DHA3^{-}(H_2O)$_2$
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -834.980044 A.U.

C	0.613941	-0.626723	-0.406913
C	-0.283050	0.656796	-0.532847
C	-1.570916	0.159363	0.164483
C	-1.545589	-1.372108	0.103994
O	-0.328200	-1.765152	-0.296657
O	-2.453929	-2.132631	0.328294
O	-2.452341	0.787517	0.696276
O	0.246556	1.779071	-0.095578
H	1.183812	-0.811730	-1.315535
C	1.534596	-0.659997	0.816386
H	1.002620	-0.248352	1.683097
C	2.812266	0.143485	0.596508
H	2.559608	1.167705	0.332586
O	1.964896	-2.000712	1.090056
H	1.188670	-2.574041	1.057626

H	3.384131	0.144190	1.532023
O	3.599518	-0.389676	-0.472113
H	3.719426	-1.328651	-0.278982
O	-1.679386	3.657007	-0.084388
H	-0.928545	3.007159	-0.109048
H	-2.389985	3.110800	0.271678
O	-0.770143	0.694498	-1.924305
H	0.016658	0.756732	-2.483743

DHA4^{-}$(H_2O)_2$
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -835.001238 A.U.

C	-1.023549	-0.650163	-0.955807
C	0.330687	-0.288980	-0.308049
C	0.109756	1.137980	0.363698
C	-1.370204	1.433488	0.061427
O	-1.960564	0.402170	-0.597055
O	-1.996675	2.429798	0.335654
O	0.946682	2.053275	-0.141245
O	1.403143	-0.194718	-1.188096
H	-0.971897	-0.688127	-2.042254
C	-1.426711	-1.994423	-0.340771
H	-2.504733	-2.061404	-0.173916
C	-0.631812	-2.006873	0.957017
H	-1.172952	-1.481358	1.748692
O	-0.950764	-3.068204	-1.153135
H	-1.428795	-3.042370	-1.991392
H	-0.381193	-3.014464	1.285254
O	0.599735	-1.314213	0.652565
H	0.678185	0.209972	1.979046
O	0.160867	1.011321	1.802374
H	2.489670	1.734686	0.630194
H	3.400220	0.518215	0.629628
O	3.345592	1.407048	0.999336
H	1.644538	0.764294	-1.090995

5$(H_2O)_2$
Charge = -2 Multiplicity = 1
CBS-QB3 Free Energy= -985.934281 A.U.

C	1.381433	-0.118952	-0.288882
C	0.474605	0.797645	0.518785
C	-0.972870	0.312205	0.354992
C	-0.746817	-1.099896	-0.245592
O	0.550893	-1.277049	-0.606222
O	-1.546439	-1.994573	-0.391152
O	-1.762062	0.402243	1.401372
O	0.843266	1.761959	1.155161
H	1.663591	0.354950	-1.231274
C	2.631976	-0.615361	0.447676
H	2.351885	-0.916981	1.464400
C	3.715858	0.452540	0.531682
H	3.335438	1.330673	1.051071
O	3.207732	-1.718636	-0.256604

H	2.514199	-2.376103	-0.395946
H	4.553767	0.040513	1.105631
O	4.151984	0.884155	-0.758831
H	4.435780	0.093034	-1.234615
O	-1.389394	1.027368	-0.877746
O	-4.080930	0.344086	-1.285264
H	-4.199092	-0.153933	-0.455353
H	-3.148818	0.628889	-1.214451
O	-3.932459	-1.082736	1.175754
H	-3.547020	-1.826622	0.694559
H	-3.125510	-0.495355	1.297564
O	-1.543671	2.473756	-0.616403

6$(H_2O)_2$
Charge = -2 Multiplicity = 1
CBS-QB3 Free Energy= -985.950563 A.U.

C	-1.272395	1.031198	-0.751401
C	-1.015985	0.010858	0.372229
C	0.506555	-0.307918	0.284567
C	1.029976	0.981324	-0.414143
O	0.013876	1.692075	-0.964486
O	2.168255	1.385945	-0.465740
O	1.122645	-0.666653	1.383197
O	-1.846028	-1.106837	0.326927
H	-1.591515	0.583132	-1.690035
C	-2.285250	2.035990	-0.184932
H	-1.912568	3.052915	-0.335744
C	-2.351825	1.662577	1.308053
H	-2.251054	2.517185	1.975761
O	-3.589068	1.888703	-0.742463
H	-3.562213	2.226047	-1.646174
H	-3.304080	1.157756	1.503445
O	-1.245933	0.780484	1.558124
O	0.626099	-1.261079	-0.869244
O	3.779715	-1.005720	1.043939
H	3.750176	-1.513714	0.215534
O	3.043502	-2.501619	-1.291532
H	2.210978	-1.988829	-1.181133
H	-1.204516	-1.867910	-0.028331
O	-0.040562	-2.543399	-0.523625
H	2.814584	-0.833049	1.200775
H	2.873689	-3.297186	-0.772408

7$(H_2O)_2$
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -986.401476 A.U.

C	1.407909	-0.157495	-0.293037
C	0.519360	0.774167	0.512497
C	-0.935974	0.280214	0.387922
C	-0.734134	-1.125029	-0.247329
O	0.556792	-1.303088	-0.612240
O	-1.548151	-2.003577	-0.386736
O	-1.713306	0.403402	1.405812

O	0.886228	1.736688	1.145560
H	1.690658	0.315356	-1.236010
C	2.659045	-0.675347	0.429508
H	2.379140	-1.007255	1.436542
C	3.740073	0.392550	0.545620
H	3.369137	1.238153	1.122627
O	3.230371	-1.754329	-0.311697
H	2.549944	-2.428950	-0.431894
H	4.591321	-0.047686	1.076923
O	4.144222	0.901526	-0.726581
H	4.452083	0.148684	-1.246955
O	-1.399199	1.003660	-0.908057
O	-4.185357	0.206598	-1.233612
H	-4.246070	-0.258253	-0.378188
H	-3.261295	0.503517	-1.238018
O	-3.917537	-1.137661	1.263867
H	-3.536141	-1.892181	0.796202
H	-3.123618	-0.548638	1.366668
O	-1.544480	2.418168	-0.628799
H	-0.740486	2.783169	-1.030184

8$(H_2O)_2$
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -986.411136 A.U.

C	-1.242425	0.970906	-0.779530
C	-1.071181	-0.025370	0.364938
C	0.433728	-0.419602	0.346552
C	1.038056	0.872976	-0.294037
O	0.069506	1.597951	-0.908417
O	2.180585	1.253316	-0.254539
O	0.971974	-0.893957	1.414029
O	-1.995144	-1.085648	0.251367
H	-1.517486	0.528032	-1.733802
C	-2.259563	2.001008	-0.269630
H	-1.930707	3.008996	-0.533766
C	-2.269786	1.772000	1.252126
H	-1.978804	2.652386	1.822642
O	-3.568215	1.744674	-0.770324
H	-3.580955	1.999328	-1.701322
H	-3.265164	1.444615	1.562741
O	-1.291634	0.742351	1.531742
O	0.580431	-1.312556	-0.920080
O	3.691350	-1.221123	1.199976
H	3.737332	-1.478979	0.263475
O	3.263707	-2.062295	-1.519624
H	2.361540	-1.719846	-1.370365
H	-1.939994	-1.594528	1.074097
O	0.133719	-2.662326	-0.629641
H	-0.830963	-2.534668	-0.597074
H	2.724779	-1.071685	1.320439
H	3.187661	-2.994504	-1.281444

9a$(H_2O)_2$

Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -986.848688 A.U.

C	1.446132	-0.198438	-0.295473
C	0.573076	0.835384	0.394470
C	-0.881319	0.343495	0.293741
C	-0.699180	-1.139386	-0.101558
O	0.578624	-1.365348	-0.455625
O	-1.535863	-2.001208	-0.098797
O	-1.584345	0.586137	1.433250
O	0.932891	1.854967	0.920754
H	1.720706	0.148840	-1.293876
C	2.700452	-0.637607	0.475446
H	2.418876	-0.868307	1.509478
C	3.780675	0.438012	0.486318
H	3.409924	1.338002	0.974274
O	3.268246	-1.780737	-0.159893
H	2.607016	-2.484263	-0.170207
H	4.627740	0.051413	1.063664
O	4.190245	0.813755	-0.828709
H	4.525986	0.017145	-1.258713
O	-1.469885	0.890089	-0.906468
O	-4.124909	-0.268051	-1.348569
H	-3.928216	-1.169198	-1.635046
H	-4.162789	-0.480664	0.430610
H	-3.254607	0.163807	-1.334284
O	-3.974929	-0.569414	1.392715
H	-3.769179	-1.506398	1.504657
H	-2.477295	0.128005	1.404663
O	-1.568110	2.330210	-0.778976
H	-0.867889	2.621865	-1.385935

10a$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -986.859135 A.U.

C	1.581590	-0.133370	-0.910643
C	0.951858	0.520879	0.327454
C	-0.545177	0.123434	0.231782
C	-0.451886	-1.207379	-0.567807
O	0.737804	-1.287422	-1.188824
O	-1.280338	-2.076196	-0.640099
O	-1.167479	0.043768	1.443679
O	1.198573	1.906769	0.334239
H	1.611942	0.503809	-1.791162
C	2.955070	-0.603785	-0.426738
H	3.281458	-1.493574	-0.970052
C	2.707577	-0.889580	1.050099
H	2.488984	-1.942997	1.227324
O	3.901610	0.454395	-0.533903
H	4.071364	0.609994	-1.471691
H	3.552790	-0.578135	1.663399
O	1.532982	-0.118072	1.437544
H	-3.047891	-1.908007	0.572217
O	-1.224730	0.968176	-0.726316
O	-3.508432	-1.240181	1.102074

H	-3.877759	-0.635759	0.420428
O	-4.118283	0.520631	-0.947382
H	-3.158503	0.632332	-1.047797
H	1.103178	2.209931	1.249365
O	-1.443230	2.292836	-0.172837
H	-0.533509	2.649385	-0.182817
H	-2.055797	-0.399449	1.345192
H	-4.400513	1.343561	-0.528267

9b$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -986.846767 A.U.

C	1.118059	-1.198098	-0.524399
C	-0.026061	-0.225827	-0.751382
C	-1.174369	-0.659130	0.176914
C	-0.468198	-1.641774	1.131074
O	0.737150	-1.975492	0.650247
O	-0.917952	-2.070199	2.159133
O	-1.818771	0.382246	0.805637
O	-0.053063	0.638218	-1.594581
H	1.195213	-1.887707	-1.367058
C	2.500179	-0.547601	-0.260451
H	3.008212	-1.225294	0.432517
C	2.360731	0.844068	0.353842
H	3.283579	1.105772	0.881226
O	3.244589	-0.398753	-1.458916
H	3.600633	-1.262655	-1.700265
H	2.210449	1.562333	-0.457669
O	1.241198	0.842557	1.236887
H	0.858674	1.752445	1.230407
O	-2.052923	-1.526823	-0.541736
O	0.258619	3.366656	1.051577
H	-0.182033	3.576719	1.884226
H	-0.474700	3.249406	0.408942
O	-1.815512	2.802059	-0.745225
H	-2.159292	2.128199	-0.137835
H	-1.275436	2.257608	-1.339842
O	-2.712024	-0.774821	-1.592712
H	-2.254042	-1.106197	-2.382873
H	-2.378697	0.023227	1.513097

10b$(H_2O)_2$
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -986.865509 A.U.

C	-1.631313	0.314263	-0.543832
C	-0.198022	-0.199371	-0.324667
C	0.568596	1.078663	0.107600
C	-0.563163	1.912092	0.756581
O	-1.760974	1.463428	0.344212
O	-0.420065	2.819904	1.529025
O	1.633122	0.834693	0.946767
O	0.280870	-0.845490	-1.461745
H	-1.840538	0.629882	-1.562932

C	-2.525699	-0.820559	-0.040545
H	-3.469250	-0.431578	0.349018
C	-1.676635	-1.462663	1.051540
H	-1.946819	-1.100517	2.043345
O	-2.740377	-1.774703	-1.074798
H	-3.303885	-1.366667	-1.744840
H	-1.746447	-2.549667	1.019783
O	-0.297731	-1.065531	0.795615
H	1.220193	-1.859727	1.552336
O	0.900844	1.897568	-1.015839
O	2.087838	-2.254755	1.757284
H	2.573188	-1.534337	2.178570
H	2.590057	-2.076893	0.046324
O	2.692147	-1.872223	-0.910900
H	3.173259	-1.034532	-0.923668
H	1.149776	-1.286503	-1.242435
O	1.967714	1.294969	-1.795087
H	1.490487	0.567250	-2.237526
H	1.893238	1.673380	1.359408

11$(H_2O)_2$
Charge = -1 Multiplicity = 1
CBS-QB3 Free Energy= -986.392669 A.U.

C	-1.417377	-0.317291	0.007362
C	-0.186398	-0.602217	0.855142
C	0.978635	0.152939	0.208846
C	0.243530	1.204378	-0.639205
O	-1.061081	0.875936	-0.759296
O	0.703917	2.190006	-1.155252
O	1.847308	0.663969	1.154800
O	-0.133511	-1.308424	1.830300
H	-1.582287	-1.130559	-0.702646
C	-2.704381	-0.024208	0.789652
H	-2.476170	0.671318	1.605928
C	-3.319883	-1.290595	1.373902
H	-2.615077	-1.775038	2.047934
O	-3.685760	0.533408	-0.084327
H	-3.310309	1.321737	-0.496223
H	-4.208334	-0.999557	1.945590
O	-3.656198	-2.242027	0.363260
H	-4.249455	-1.795423	-0.254344
O	1.551264	-0.699135	-0.762653
O	3.530523	0.530652	-2.264209
H	3.011970	1.105054	-2.841516
H	3.797682	1.632404	-0.880342
H	2.849415	0.023444	-1.774171
O	3.753272	2.171746	-0.057901
H	3.211149	2.929567	-0.311573
H	2.542609	1.212178	0.704005
O	2.145663	-1.896308	-0.126051

TS(9b$(H_2O)_2$ **/ 10b**$(H_2O)_2$**)**
Charge = 0 Multiplicity = 1

CBS-QB3 Free Energy= -986.834550 A.U.

C	-0.759462	1.552803	0.834507
C	-0.736470	0.427734	1.893272
C	0.754171	-0.003821	1.916843
C	1.477358	1.253022	1.395670
O	0.604368	2.073776	0.784104
O	2.646136	1.506137	1.519750
O	1.200399	-0.447137	3.146971
O	-1.656022	-0.478420	1.867222
H	-1.031581	1.186231	-0.153039
C	-1.691541	2.645919	1.355962
H	-1.456881	3.609700	0.897086
C	-1.438439	2.666181	2.861613
H	-0.739267	3.453258	3.140972
O	-3.049374	2.281343	1.128698
H	-3.203847	2.283478	0.175398
H	-2.370993	2.776084	3.414663
O	-0.823608	1.391266	3.191141
H	-1.207873	0.875180	4.180229
O	0.974637	-0.941492	0.860722
O	-1.612226	0.314850	5.196594
H	-0.927506	0.373523	5.878587
H	-1.667342	-0.653769	4.922449
O	-1.678819	-2.042973	4.074599
H	-0.774389	-2.377247	4.134864
H	-1.690542	-1.552885	3.212708
O	0.234461	-2.171934	1.123107
H	-0.680805	-1.810924	1.237991
H	2.164365	-0.546912	3.102482

TS(9a$(H_2O)_2$ -> **DHA1**$(H_2O)_2$ + H_2O_2**)**

Charge = 0 Multiplicity = 1

CBS-QB3 Free Energy= -986.819849 A.U.

C	-1.393746	-0.177053	0.267136
C	-0.533639	0.788494	-0.528680
C	0.861765	0.190170	-0.612714
C	0.691599	-1.221922	-0.045029
O	-0.550358	-1.360672	0.467817
O	1.491585	-2.122771	-0.039293
O	1.685109	0.475323	-1.512672
O	-0.881303	1.845229	-1.003369
H	-1.621432	0.230617	1.252700
C	-2.685547	-0.626863	-0.432538
H	-2.452447	-0.905758	-1.467136
C	-3.746557	0.467458	-0.444576
H	-3.373203	1.347563	-0.966059
O	-3.250735	-1.733333	0.269526
H	-2.586411	-2.432534	0.317336
H	-4.617802	0.083437	-0.986866
O	-4.111995	0.884796	0.871467
H	-4.423099	0.098816	1.338318
O	1.307639	0.896044	0.990832
O	3.649173	-0.109964	1.421210
H	3.573859	-0.962077	1.878894

H	3.926895	-0.306855	0.373551
H	2.708298	0.282769	1.356028
O	4.104720	-0.460397	-0.958863
H	4.145783	-1.409246	-1.141886
H	3.208919	-0.164223	-1.292738
O	1.689678	2.254241	0.733250
H	0.882869	2.744905	0.955507

TS(10a$(H_2O)_2$ **->** **DHA5**$(H_2O)_2$ + H_2O_2**)**
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -986.828654 A.U.

C	-0.387106	0.952669	-1.362559
C	-0.290315	-0.043706	-0.205468
C	1.218972	-0.350540	-0.089901
C	1.859537	0.905615	-0.715879
O	0.927808	1.585990	-1.423617
O	2.996110	1.290842	-0.616605
O	1.719271	-0.946016	0.892535
O	-1.131085	-1.154365	-0.393094
H	-0.604937	0.502814	-2.327622
C	-1.425385	1.975900	-0.900590
H	-1.241650	2.959782	-1.339167
C	-1.239661	1.971948	0.611421
H	-0.552175	2.755727	0.932919
O	-2.737208	1.504417	-1.197171
H	-2.840420	1.495485	-2.157040
H	-2.190980	2.079449	1.132580
O	-0.655631	0.684006	0.956195
H	4.783096	-0.413501	0.677442
O	1.430272	-1.300325	-1.610023
O	4.367590	-1.284383	0.621478
H	4.183481	-1.568409	-0.810074
O	3.873593	-1.725366	-1.800719
H	2.820414	-1.542993	-1.777415
H	-1.119092	-1.661174	0.432700
O	1.005099	-2.653561	-1.335663
H	0.044489	-2.519742	-1.241629
H	3.410014	-1.118792	0.840106
H	4.013973	-2.661225	-2.012769

H_2O_2
Charge = 0 Multiplicity = 1
CBS-QB3 Free Energy= -151.415318

O	-0.800276	-2.610171	0.027887
H	-0.956819	-1.877504	0.642124
O	0.646406	-2.688373	0.027917
H	0.802927	-3.420966	0.642246

$O_2^{-\bullet}$
Charge = -1 Multiplicity = 2
CBS-QB3 Free Energy= -150.329270

-2.202490	-2.664906	0.000000

-0.855621 -2.664906 0.000000

H_2O_2 $(H_2O)_5$
charge: 0 multiplicity: 1
CBS-QB3 Free Energy= -533.201774 A.U.

O	-0.673982	1.321027	1.732277
H	0.172686	1.652400	1.331201
O	-1.671252	1.864742	0.826018
H	-1.633487	1.240993	0.052430
O	-1.573652	0.245610	-1.339794
H	-0.616513	0.052745	-1.366518
H	-1.966364	-0.590221	-1.009221
O	-2.419358	-2.161057	-0.179322
H	-1.663208	-2.026212	0.429379
H	-2.099037	-2.815332	-0.812396
O	-0.205996	-1.385304	1.282704
H	0.177879	-1.795397	2.067064
H	-0.440292	-0.467191	1.544465
O	1.563954	2.044593	0.405442
H	1.231780	2.723763	-0.194982
H	1.557139	1.221821	-0.129721
O	1.143101	-0.350259	-0.881394
H	1.737612	-0.918647	-1.385126
H	0.832670	-0.880648	-0.115838

HOO$^-(H_2O)_5$
charge: -1 multiplicity: 1
CBS-QB3 Free Energy= -532.741063 A.U.

O	0.619397	-1.181444	-1.298704
H	1.179987	-0.911579	0.284462
O	-0.660975	-1.909346	-1.185137
H	-0.957791	-1.673907	-0.281798
O	-1.375024	-1.038108	1.414384
H	-0.412232	-0.878773	1.516925
H	-1.717598	-0.181781	1.080295
O	-2.172195	1.404905	0.305540
H	-1.465060	1.351598	-0.384869
H	-1.823890	2.041799	0.941299
O	-0.086513	1.170110	-1.377151
H	-0.062331	1.527660	-2.271029
H	0.223280	0.126629	-1.408037
O	1.383017	-0.651418	1.226043
H	1.407028	0.324599	1.180679
O	1.309663	2.152172	0.713225
H	2.221843	2.274798	0.424427
H	0.830272	1.878354	-0.107185

HOO$^{\bullet}(H_2O)_5$
charge: 0 multiplicity: 2
CBS-QB3 Free Energy= -532.560088 A.U.

O	-0.081060	-1.241876	-2.096552
H	1.824310	-0.948695	1.750145

O	-0.486691	-2.161001	-1.239044
H	-0.753681	-1.667881	-0.343890
O	-1.125988	-1.070327	0.923734
H	-0.293017	-0.758836	1.356805
H	-1.660430	-0.259102	0.758287
O	-2.461189	1.263949	0.326728
H	-1.746682	1.467561	-0.314096
H	-2.272737	1.833619	1.082699
O	-0.268881	1.443993	-1.323852
H	-0.276798	1.933712	-2.155523
H	-0.196206	0.496942	-1.573633
O	1.221116	-0.252617	2.038469
H	1.466764	0.525739	1.485470
O	1.826328	1.873025	0.407045
H	2.619656	1.579212	-0.056994
H	1.106063	1.768849	-0.252429

$\mathbf{O_2}^{-\bullet}(H_2O)_5$
charge: -1 multiplicity: 2
CBS-QB3 Free Energy= -532.117716 A.U.

O	-1.601836	-0.185026	1.603572
O	-0.903403	0.950620	1.521851
H	-0.946967	1.238993	-0.402817
O	-0.889428	1.244928	-1.373642
H	1.091869	1.278749	-1.394604
H	-0.719566	0.307723	-1.592769
O	0.233481	-1.335159	-1.880680
H	0.135652	-1.711850	-0.980887
H	1.003406	-0.743259	-1.791446
O	0.069847	-2.102878	0.773800
H	-0.158992	-2.960487	1.149839
H	-0.598208	-1.452334	1.131296
O	1.977643	0.885873	-1.292915
H	1.981204	0.613147	-0.348220
O	1.703755	0.090313	1.359205
H	0.813551	0.510886	1.453202
H	1.451300	-0.839912	1.220712