Supplementary Information

Computational Study of Radicals Derived from Hydroxyurea and Its Methylated Analogues

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Table SI_1

• Gibbs Free Energies on different levels (a.u.) and energies of solvation (kJ/mol)

Name	UB3LYP/6-31G(d)	UB3LYP/ 6-311++G(d,p)	UBP86/ 6-311++G(d,p)	G3(MP2)RAD	G3B3	ΔG_{solv} UAHF	ΔG_{solv} UAKS
e1_0w	-299.7783	-299.886098	-299.9021	-299.4818	-299.6712	-58.1	-53.8
e1_1w	-376.1848	-376.338255	-376.3541	-375.8428	-376.0682	-59.9	-54.2
e2_0w	-299.7516	-299.861737	-299.8780	-299.4602	-299.6491	-70.1	-65.1
e2_1w	-376.1620	-376.316974	-376.3335	-375.8229	-376.0490	-66.2	-61.6
e3_0w	-299.7440	-299.853523	-299.8713	-299.4507	-299.6391	-72.1	-66.6
e3_1w	-376.1600	-376.311755	-376.3316	-375.8179	-376.0425	-60.7	-56.0
z1_0w	-299.7625	-299.871924	-299.8874	-299.4671	-299.6556	-84.5	-78.1
z1_1w	-376.1706	-376.326673	-376.3413	-375.8297	-376.0567	-88.1	-85.4
z2_0w	-299.7634	-299.870516	-299.8885	-299.2016	-299.6592	-51.2	-47.7
z2_1w	-376.1685	-376.322980	-376.3411	-375.8292	-376.0543	-55.0	-50.3
z3_0w	-299.7502	-299.857694	-299.8782	-299.4558	-299.6440	-64.2	-59.7
z3_1w	-376.1565	-376.309020	-376.3287	-375.8140	-376.0389	-68.1	-63.0
eTS_1_2_0w	-299.6845	-299.794695	-299.8198	-299.3923	-299.5821	-60.9	-56.3
eTS_1_2_1w	-376.1370	-376.288523	-376.3157	-375.7921	-376.0178	-57.2	-53.8
eTS_1_3_0w	-299.7117	-299.820056	-299.8460	-299.4155	-299.6036	-60.5	-54.6
eTS_1_3_1w	-376.1532	-376.303960	-376.3297	-375.8085	-376.0328	-53.1	-49.0
zTS_1_2_0w	-299.6803	-299.792006	-299.8174	-299.3908	-299.5779	-70.7	-65.6
zTS_1_2_1w	-376.1301	-376.281387	-376.3086	-375.7855	-376.0104	-70.3	-65.2
zTS_2_3_0w	-299.7505	-299.857218	-299.8793	-299.4527	-299.6445	-58.1	-52.8
zTS_2_3_1w	-376.1536	-376.304214	-376.3294	-375.8086	-376.0338	-77.6	-73.0
TS_1_0w	-299.7517	-299.861997	-299.8775	-299.4574	-299.6454	-74.6	-68.1
TS_1_1w	-376.1594	-376.314563	-376.3302	-375.8187	-376.0435	-75.4	-68.2
TS_2_0w	-299.7422	-299.852678	-299.8677	-299.4528	-299.6410	-71.8	-66.7
TS_2_1w	-376.1495	-376.304832	-376.3203	-375.8140	-376.0384	-71.9	-65.9
TS_3_0w	-299.7095	-299.821061	-299.8407	-299.4159	-299.6023	-68.5	-62.7
TS_3_1w	-376.1249	-376.278557	-376.2983	-375.7846	-376.0085	-78.5	-71.9
e4_0w	-339.0704	-339.185486	-339.1993	-338.7246	-338.9461	-42.3	-39.0
e4_1w	-415.4724	-415.629877	-415.6486	-415.0816	-415.3403	-55.6	-50.1
e5_0w	-339.0374	-339.152577	-339.1661	-338.6921	-338.9136	-51.8	-47.8
e5_1w	-415.4419	-415.603575	-415.6170	-415.0512	-415.3120	-66.1	-61.4
e6_0w	-339.0343	-339.152050	-339.1662	-338.6958	-338.9145	-50.2	-45.1
e6_1w	-415.4512	-415.610905	-415.6274	-415.0626	-415.3196	-43.6	-39.0
e7_0w	-339.0100	-339.126222	-339.1399	-338.6701	-338.8900	-55.0	-49.5
e7_1w	-415.4177	-415.576837	-415.5919	-415.0299	-415.2869	-60.5	-54.2
e8_0w	-339.0217	-339.136116	-339.1501	-338.7067	-338.8961	-52.8	-49.4
e8_1w	-415.4301	-415.587992	-415.6029	-415.0711	-415.2934	-53.8	-49.3
z4_0w	-339.0510	-339.167307	-339.1812	-338.7069	-338.9273	-68.5	-62.8
z4_1w	-415.4538	-415.612414	-415.6326	-415.0668	-415.3250	-74.2	-67.7
z5_0w	-339.0371	-339.152895	-339.1655	-338.6920	-338.9133	-52.8	-48.8
z5_1w	-415.4460	-415.6052	-415.6190	-415.0539	-415.3120	-52.9	-47.9
z6_0w	-339.0278	-339.1460	-339.1607	-338.6895	-338.9092	-63.6	-57.0

Name	UB3LYP/6-31G(d)	UB3LYP/ 6-311++G(d,p)	UBP86/ 6-311++G(d,p)	G3(MP2)RAD	G3B3	ΔG_{solv} UAHF	ΔG_{solv} UAKS
z6_1w	-415.4402	-415.6009	-415.6177	-415.0536	-415.3098	-60.4	-54.4
z7_0w	-339.0135	-339.1291	-339.1428	-338.6732	-338.8927	-50.8	-46.0
z7_1w	-415.4110	-415.5734	-415.5873	-415.0256	-415.2830	-65.2	-59.5
z8_0w	-339.0122	-339.1265	-339.1393	-338.6963	-338.8853	-56.7	-52.8
z8_1w	-415.4156	-415.5751	-415.5887	-415.0584	-415.2804	-66.7	-62.0
eTS_4_5_0w	-338.9470	-339.0621	-339.0822	-338.6056	-338.8254	-50.4	-46.1
eTS_4_5_1w	-415.3546	-415.5144	-415.5348	-414.9672	-415.2234	-51.4	-46.4
eTS_4_6_0w	-338.9882	-339.1046	-339.1268	-338.6445	-338.8650	-36.5	-31.9
eTS_4_6_1w	-415.4420	-415.6007	-415.6240	-415.0491	-415.3057	-35.4	-31.7
eTS_5_7_0w	-338.9632	-339.0776	-339.1004	-338.6191	-338.8396	-41.0	-36.1
eTS_5_7_1w	-415.4141	-415.5712	-415.5944	-415.0209	-415.2777	-57.6	-52.1
eTS_4_8_0w	-338.9671	-339.0830	-339.1119	-338.6488	-338.8391	-42.0	-39.3
eTS_4_8_1w	-415.3726	-415.5340	-415.5605	-415.0110	-415.2341	-44.6	-41.2
zTS_4_5_0w	-338.9424	-339.0581	-339.0778	-338.6023	-338.8210	-57.6	-52.8
zTS_4_5_1w	-415.3510	-415.5110	-415.5312	-414.9643	-415.2198	-58.3	-52.6
zTS_4_6_0w	-338.9799	-339.0966	-339.1188	-338.6363	-338.8574	-55.9	-49.2
zTS_4_6_1w	-415.4295	-415.5883	-415.6122	-415.0377	-415.2941	-56.5	-50.7
zTS_5_7_0w	-338.9639	-339.0785	-339.1017	-338.6191	-338.8395	-41.7	-36.5
zTS_5_7_1w	-415.4150	-415.5723	-415.5959	-415.0214	-415.2780	-57.7	-52.2
zTS_5_8_0w	-338.9666	-339.0837	-339.1078	-338.6481	-338.8380	-46.6	-43.5
zTS_5_8_1w	-415.3719	-415.5333	-415.5586	-415.0115	-415.2343	-51.2	-46.9
TS_4_0w	-339.0436	-339.1610	-339.1745	-338.7012	-338.9207	-61.7	-56.2
TS_4_1w	-415.4513	-415.6136	-415.6274	-415.0625	-415.3187	-62.4	-56.1
TS_5_0w	-339.0282	-339.1432	-339.1555	-338.6846	-338.9053	-53.8	-49.6
TS_5_1w	-415.4357	-415.5955	-415.6082	-415.0460	-415.3029	-53.8	-48.7
TS_6_0w	-339.0166	-339.1358	-339.1493	-338.6802	-338.8986	-60.9	-54.6
TS_6_1w	-415.4292	-415.5910	-415.6068	-415.0442	-415.2993	-57.4	-51.5
TS_7_0w	-338.9973	-339.1144	-339.1273	-338.6603	-338.8793	-59.0	-53.6
TS_7_1w	-415.3980	-415.5615	-415.5743	-415.0155	-415.2722	-69.4	-63.9
TS_8_0w	-338.9912	-339.1062	-339.1232	-338.6760	-338.8636	-47.3	-43.6
TS_8_1w	-415.3948	-415.5556	-415.5724	-415.0380	-415.2587	-57.7	-52.8
e10_0w	-414.2759	-414.4233	-414.4423	-413.8783	-414.1351	-70.0	-62.6
e10_1w	-490.6836	-490.8751	-490.8944	-490.2398	-490.5325	-75.5	-67.8
e11_0w	-414.2272	-414.3757	-414.4423	-413.8295	-414.0848	-82.5	-73.1
e11_1w	-490.6836	-490.8300	-490.8602	-490.1919	-490.4847	-75.5	-70.8
z10_0w	-414.2622	-414.4099	-414.4280	-413.8657	-414.1210	-89.6	-81.0
z10_1w	-490.6729	-490.8646	-490.8832	-490.2306	-490.5222	-83.3	-74.3
z11_0w	-414.2154	-414.3640	-414.4264	-413.8187	-414.0747	-96.5	-84.6
z11_1w	-490.6225	-490.8141	-490.8835	-490.0952	-490.4699	-100.8	-89.5
eTS_10_11_0w	-414.2345	-414.3818	-414.4069	-413.8315	-414.0892	-49.2	-43.8
eTS_10_11_1w	-490.6410	-490.8316	-490.8602	-490.1871	-490.4809	-77.1	-70.8
zTS_10_11_0w	-414.2275	-414.3758	-414.4018	-413.8251	-414.0820	-80.7	-69.7

Name	UB3LYP/6-31G(d)	UB3LYP/ 6-311++G(d,p)	UBP86/ 6-311++G(d,p)	G3(MP2)RAD	G3B3	ΔG_{solv} UAHF	ΔG_{solv} UAKS
zTS_10_11_1w	-490.6304	-490.8207	-490.8505	-490.1771	-490.4707	-90.2	-79.2
TS_10_0w	-414.2523	-414.4020	-414.4201	-413.8582	-414.1128	-85.2	-76.4
TS_10_1w	-490.6633	-490.8564	-490.8753	-490.2228	-490.5134	-82.4	-73.5
TS_11_0w	-414.2084	-414.3568	-414.3809	-413.8145	-414.0687	-92.1	-80.6
TS_11_1w	-490.6169	-490.8087	-490.8486	-490.1743	-490.4650	-95.0	-84.0
e13_0w	-299.7953	-299.9365	-299.9551	-299.5369	-299.7242	-304.2	-314.7
e13_1w	-376.2232	-376.4087	-376.4282	-375.9142	-376.1395	-282.4	-286.8
e14_0w	-339.0874	-339.2332	-339.2501	-338.7784	-338.9974	-279.4	-290.4
e14_1w	-415.5141	-415.7033	-415.7209	-415.1549	-415.4118	-263.8	-269.2
e15_0w	-339.0800	-339.2200	-339.2359	-338.7641	-338.9846	-288.2	-302.0
e15_1w	-415.5049	-415.6879	-415.7034	-415.1429	-415.3991	-259.4	-267.6
z13_0w	-299.7748	-299.9165	-299.9384	-299.5176	-299.7047	-329.8	-336.1
z13_1w	-376.2062	-376.3896	-376.4102	-375.9005	-376.1249	-309.2	-313.6
z14_0w	-339.0624	-339.2098	-339.2283	-338.7558	-338.9747	-320.0	-325.9
z14_1w	-415.4909	-415.6812	-415.6996	-415.1338	-415.3903	-299.6	-300.9
z15_0w	-339.0787	-339.2184	-339.2333	-338.7637	-338.9840	-291.5	-305.9
z15_1w	-415.4995	-415.6834	-415.6987	-415.1371	-415.3936	-273.5	-280.8

Table SI_2

- Reduction free energies (ΔG^{EA}_{aq} in kJ, at 298.15 K) and calculated standard reduction potentials (E^0 in V, at 298.15 K) for anion/radical pairs of hydroxyurea and its methylated analogues in water.[a]

Redox couple anion / radical	ΔG^{EA}_{aq}	E^0	E^0_{exp}
***z*1 / 13**	-396.6	+0.25	+0.47[b] ; +0.73[c]
	(-387.1)	(+0.35)	
***e*1 / 13**	-412.8	+0.08	
	(-388.8)	(+0.33)	
***z*4 /14**	-401.1	+0.20	
	(-345.9)	(+0.77)	-
***e*4 /14**	-398.3	+0.23	
	(-372.0)	(+0.59)	
z5 / 15	-430.8	-0.11	
	(-438.9)	(-0.19)	-
e5 / 15	-436.6	-0.17	
	(-387.1)	(-0.42)	

[a] All calculations were performed at G3B3 level and solvation effects were included by CPCM-B3LYP/6-311+g(d,p) model.

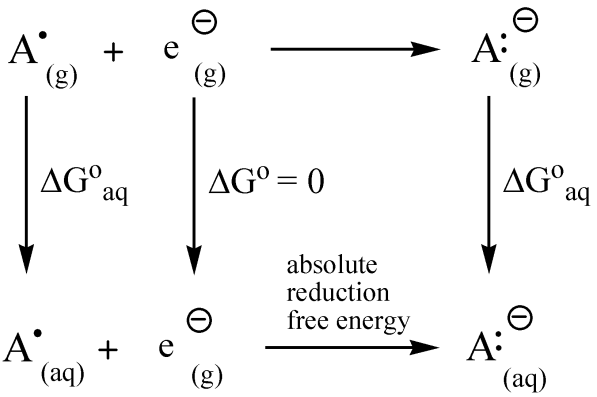

Figure SI_1.

- Thermodynamic cycle used in the computation of equilibrium reduction potentials.

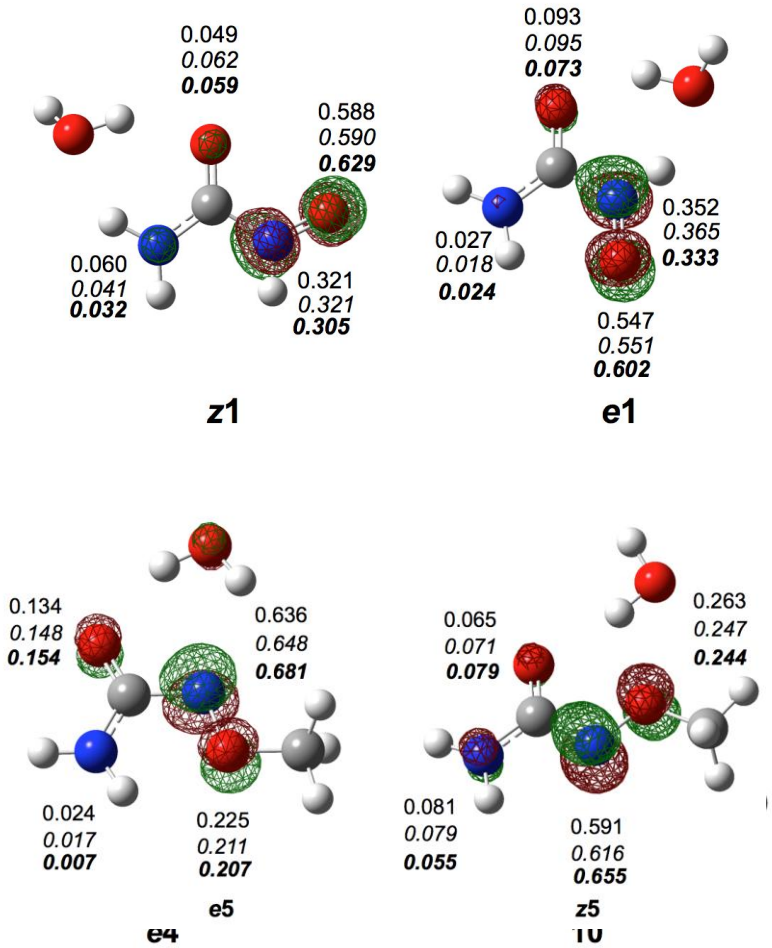

Figure SI_2.

- Mulliken (without explicit water, *with one explicit water molecule in italics*) and NPA spin distribution (*with one explicit water in bold*) calculated at B3LYP/6-311++G(d,p).

Table SI_3.

• RSE/BDE calculations on different systems

System	H^{298} (G3B3) (a.u.)	ΔH^{298}	RSE O-scale	RSE N-scale	BDE (exp)	BDE error
OH*	-75.693062					
H2O	-76.379942		0.0		497.1	0.3
NH2*	-55.835798					
NH3	-56.504485			0.0	450.1	0.2
C6H5O*						
C6H5OH			-121.6		362.8	2.9
CH3-C6H4-O*						
CH3-C6H4-OH			-129.4		360.2	2.1
Gly-Tyr*						
Gly-Tyr			-131.5			
HNHO*	-131.005728	0.0				
HNHOH	-131.622113		-185.1		318.0	4.2
*NHOH	-130.995078	28.0				
HNHOH	-131.622113			-109.4	341.0	2.1
e1*	-299.634943	0.0				
eHU	-300.253326	0.0	-179.8			
z1*	-299.620440	38.1				
zHU	-300.250398	7.7	-149.4			
e2*	-299.613327	56.8				
eHU	-300.253326	0.0		-75.3		
z2*	-299.624176	28.3				
zHU	-300.250398	7.7		-111.5		
e4*	-338.905473	0.0				
eNMHU	-339.520225	0.0	-189.4			
z4*	-338.888439	44.7				
zNMHU	-339.516986	8.5	-153.2			
e5*	-338.873536	83.9				
eOMHU	-339.510975	24.3		-82.0		
z5*	-338.873331	84.4		-97.2		
zOMHU	-339.505003	40.0				

B3LYP/6-31G(d) optimized structures

e1_0w
N 0.562377 1.273548 -0.000011
H 1.441445 1.764684 0.000034
H -0.317804 1.769175 0.000020
C 0.565989 -0.077767 -0.000002
O 1.523335 -0.831480 0.000005
N -0.754939 -0.622507 -0.000009
H -0.811292 -1.644640 0.000003
O -1.818379 0.083992 0.000007

e1_1w
N -0.163013 -1.027013 0.016523
C 0.220064 0.257697 0.005418
O -0.498821 1.257868 0.002664
N 1.631279 0.440706 0.005157
H 1.955382 1.411584 -0.001153
O 2.469749 -0.521264 -0.001683
H -1.167132 -1.207653 -0.029451
H 0.539084 -1.751695 -0.029125
O -2.886234 -0.263439 -0.096798
H -2.301075 0.523527 -0.134703
H -3.302056 -0.203117 0.776711

e2_0w
N 0.526250 1.255246 -0.031637
H 1.401231 1.744916 0.075974
H -0.341059 1.757127 0.078228
C 0.566592 -0.107397 -0.002996
O 1.590050 -0.775681 0.010774
N -0.673686 -0.815006 -0.012032
O -1.705817 0.091836 0.009650
H -2.501530 -0.468576 0.006056

e2_1w
N -1.835826 -0.936958 0.045751
H -2.837012 -0.939845 -0.074835
H -1.315916 -1.790114 -0.091626
C -1.208118 0.273341 0.005180
O -1.776468 1.356458 -0.004337
N 0.216356 0.273373 -0.001064
O 0.691271 -1.001679 -0.011053
H 1.676829 -0.845327 -0.031508
O 3.007055 0.290535 -0.081151
H 3.367748 0.441090 0.806694
H 2.318489 0.976731 -0.180289

e3_0w
N -0.348405 1.317815 -0.000203
H -1.174344 1.893767 0.000936
H 0.593101 1.699010 0.000223
C -0.387670 -0.011004 -0.000073
O -1.580898 -0.601258 0.000020
N 0.706919 -0.799608 -0.000042
O 1.804359 -0.097876 0.000075
H -1.390025 -1.561124 0.000232

e3_1w
N -1.762764 -0.823480 0.025044
H -2.036843 -1.791736 -0.015397
H -2.428202 -0.057920 0.006185
C -0.485900 -0.447972 0.000203
O 0.437426 -1.384284 -0.009249
N -0.125059 0.867617 -0.006424
O -1.155281 1.661304 0.000112
H 1.345923 -0.936638 -0.034202
O 2.533554 0.216238 -0.085482
H 1.789693 0.872557 -0.120065
H 2.933999 0.346548 0.788868

z1_0w
N 1.551380 -0.668854 -0.043132
H 2.429582 -0.191905 0.113040
H 1.491430 -1.588134 0.376095
C 0.452916 0.169015 -0.006843
O 0.487929 1.376893 -0.005044
N -0.770650 -0.569010 -0.035494
H -0.749673 -1.577820 -0.214497
O -1.907172 -0.000790 0.044644

z1_1w
N -0.093688 -1.495288 -0.088303
H 0.247774 -2.426304 0.098560
H -1.076131 -1.304866 0.073656
C 0.843902 -0.494263 -0.003116
O 2.043225 -0.651897 0.069772
N 0.229849 0.795617 -0.050303
H -0.793345 0.860275 -0.102699
O 0.912481 1.873019 -0.005411
O -2.695150 0.052186 0.045152
H -3.223187 0.395111 0.782341
H -3.256101 0.152600 -0.739026

z2_0w
N -0.875093 1.478875 0.000000
H -0.531586 2.426737 0.000000
H -1.868242 1.299692 0.000000
C 0.000000 0.450492 0.000000
O 1.228445 0.544175 0.000000
N -0.664724 -0.817312 0.000000
O 0.275234 -1.767767 0.000000
H 1.149117 -1.271591 0.000000

z2_1w
N -0.547689 1.256502 -0.000098
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H -0.178573 2.196034 -0.000518
C 0.291415 0.208716 -0.000168
O -0.046432 -0.986466 -0.000467
N 1.667474 0.593743 0.000241
O 2.405894 -0.521240 0.000246
H 1.741088 -1.274515 -0.000028
O -2.928450 -0.319536 0.000171
H -2.522900 -0.786002 -0.749663
H -2.523445 -0.783774 0.751684

z3_0w
N -1.650293 -0.436877 -0.000105
H -2.432071 0.199381 0.000333
H -1.803117 -1.434966 0.000317
C -0.391886 0.011150 -0.000007
O -0.170468 1.303158 0.000006
N 0.650639 -0.867155 -0.000003
O 1.762365 -0.176190 0.000012
H 0.848907 1.281164 0.000005

z3_1w
N 2.207430 -0.383524 0.027255
H 2.842873 0.397346 -0.039715
H 2.542978 -1.327983 -0.080168
C 0.886499 -0.124525 0.002333
O 0.117908 -1.188611 -0.004401
N 0.556282 1.194730 0.009541
O -0.720763 1.449502 -0.002503
H -0.876538 -0.981213 -0.025339
O -2.432274 -0.595781 -0.091761
H -2.066876 0.326686 -0.129222
H -2.826378 -0.667010 0.792188

eTS_1_2_0w
N 0.691737 -0.750579 -0.128026
O 1.794651 0.094629 0.021102
C -0.592962 -0.093881 -0.012289
O -1.597735 -0.775939 0.039990
N -0.509686 1.256146 -0.007708
H 0.392314 1.709367 0.026204
H -1.360716 1.793855 0.035100
H 1.676492 -1.028427 0.473824

eTS_1_2_1w
H 3.039536 0.560776 0.766785
N 0.302714 0.148687 0.012108
O 0.799390 -1.080075 -0.001820
H 2.038319 -0.603147 -0.046748
O 2.630331 0.400663 -0.100541
H 1.545749 0.795385 -0.051818
C -1.113110 0.270660 0.005330
O -1.616309 1.383180 -0.009570
N -1.786758 -0.912481 0.043176
H -1.279866 -1.775351 -0.090148
H -2.784068 -0.885215 -0.101592

eTS_1_3_0w
N -0.777843 -0.559866 0.000147
H 0.126180 -1.627840 0.000203
C 0.487189 -0.008259 0.000003
O 1.278370 -1.010090 -0.000060
N 0.751251 1.290711 -0.000058
H 1.691583 1.653335 0.000010
H -0.048600 1.913742 0.000549
O -1.841639 0.134391 -0.000115

eTS_1_3_1w
N 0.081565 0.844075 -0.004832
H -1.570457 -0.731727 -0.045265
O -2.286161 0.244347 -0.090366
H -1.323169 0.869887 -0.053441
H -2.738027 0.343262 0.765133
C 0.421508 -0.502041 0.001673
O -0.512255 -1.378611 -0.008889
N 1.713543 -0.835730 0.025444
H 2.002088 -1.799718 -0.016900
H 2.372498 -0.066482 0.001265
O 1.068698 1.676590 -0.001384

zTS_1_2_0w
N 0.700667 -0.682055 -0.092867
O 1.875953 0.030722 0.002871
C -0.480204 0.153095 -0.007103
O -0.435794 1.361618 0.003254
N -1.597008 -0.627582 0.058729
H -1.536553 -1.611795 -0.158979
H -2.491322 -0.169581 -0.039645
H 1.662214 -1.108454 0.431205

zTS_1_2_1w
H 2.950322 0.654215 0.853747
N 0.291611 0.037873 -0.027915
O 0.910642 -1.119901 -0.092649
H 2.081820 -0.527128 -0.082148
O 2.580740 0.541336 -0.038146
H 1.421551 0.794371 0.010248
C -1.131439 -0.026080 0.014762
O -1.776077 -1.052250 0.080033
N -1.664620 1.243791 0.025951
H -1.114300 2.015276 -0.324733
H -2.662129 1.294608 -0.125851

zTS_2_3_0w
N -0.541263 1.634071 0.000000
H 0.038129 2.459360 0.000000
H -1.547929 1.718770 0.000000
C 0.000000 0.415550 0.000000
O 1.263012 0.200678 0.000000
N -0.830230 -0.702016 0.000000
O -0.011793 -1.731989 0.000000
H 1.100499 -0.945326 0.000000

zTS_2_3_1w
N 2.175244 -0.251374 0.025312
H 2.732512 0.588818 -0.009572
H 2.606339 -1.160025 -0.041083
C 0.829587 -0.143486 0.001652
O 0.147128 -1.225188 -0.015602
N 0.425108 1.184534 0.014193
O -0.867118 1.412980 -0.011149
H -1.067450 -1.079804 -0.043208
O -2.173584 -0.640255 -0.086387
H -1.699469 0.383706 -0.060818
H -2.603326 -0.784192 0.773338

TS_1_0w
N -1.331646 -0.892883 -0.088331
H -2.264333 -0.705561 -0.431284
H -0.958741 -1.825265 -0.191355
C -0.489117 0.159389 0.068833
O -0.775509 1.330064 -0.024016
N 0.868028 -0.301427 0.422823
H 1.115654 -0.228661 1.417031
O 1.811440 -0.059649 -0.419589

TS_1_1w
N 0.403293 1.183126 0.044713
H 1.412227 1.129278 -0.128941
H -0.116462 2.026383 -0.147909
C -0.244473 0.015707 0.199434
O 0.269151 -1.091406 0.257747
N -1.698573 0.191854 0.332295
H -2.070271 0.117843 1.286727
O -2.438683 -0.282819 -0.608523
O 2.885092 -0.124390 -0.295330
H 2.170570 -0.787448 -0.188930
H 3.413251 -0.216235 0.512237

TS_2_0w
N 1.139775 1.035547 -0.077192
H 2.100476 1.041102 -0.388963
H 0.684361 1.908251 0.141562
C 0.507632 -0.154906 0.092117
O 0.990817 -1.250065 -0.115076
N -0.825169 -0.012435 0.653746
O -1.675087 0.091812 -0.425593
H -2.558718 0.084323 -0.015828

TS_2_1w
N -0.332222 1.140386 -0.138224
H -1.336440 1.169016 0.058709
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C 0.242109 -0.073227 -0.240641
O -0.346640 -1.147769 -0.158100
N 1.652059 -0.041221 -0.574547
O 2.319646 -0.032287 0.629318
H 3.255730 -0.095484 0.367144
O -2.881332 -0.006968 0.329468
H -3.391112 -0.124095 -0.486683
H -2.176939 -0.688894 0.265329

TS_3_0w
N -1.204167 -1.073848 -0.106165
H -2.144631 -0.962331 0.255212
H -0.775358 -1.969701 0.075625
C -0.372832 0.010349 -0.014526
O -1.078607 1.177052 -0.042152
N 0.878723 -0.035015 0.296998
O 2.062262 -0.086115 -0.152785
H -0.434150 1.904485 -0.020017

TS_3_1w
N 2.050593 -0.090310 -0.281701
H 2.591334 -0.907757 -0.530322
H 2.477321 0.823804 -0.308323
C 0.778201 -0.193978 0.111489
O 0.297008 -1.420226 0.178035
N 0.081198 0.855405 0.599898
O -0.524142 1.715145 -0.189708
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O -2.196327 -0.620348 -0.271587
H -2.718687 -0.468636 0.532237
H -1.845005 0.276978 -0.481546

e4_0w
H 1.358418 -1.652316 -0.001514
H 2.630280 -0.431925 -0.002511
N 1.656588 -0.687892 0.001315
O 0.933526 1.498801 -0.000503
C 0.729147 0.296013 0.000014
N -0.612041 -0.229309 -0.000156
C -1.761392 0.673783 0.000391
H -2.364510 0.478031 0.891812
H -2.364694 0.478845 -0.891087
H -1.396344 1.699303 0.000783

O -0.806215 -1.495089 -0.000499

e4_1w
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H -1.596378 -2.451931 -0.075077
N -1.653055 -1.446584 -0.096798
O 0.585490 -1.193097 0.331534
C -0.525154 -0.731758 0.090381
N -0.747844 0.679561 -0.010841
C 0.331622 1.641535 0.233672
H 0.295727 1.973473 1.277792
H 0.148357 2.494693 -0.421071
H 1.301719 1.190246 0.018599
O -1.935294 1.110818 -0.226521
O 3.149124 -0.111989 -0.355219
H 2.348937 -0.650163 -0.204176
H 3.592778 -0.128440 0.506125

e5_0w
N -1.247113 1.208444 0.040849
H -0.460931 1.823095 -0.102260
H -2.181392 1.560859 -0.101874
C -1.088036 -0.147707 0.003768
O -2.007638 -0.953123 -0.014673
N 0.240660 -0.669027 0.017227
O 1.128026 0.363953 -0.011327
C 2.474331 -0.137393 -0.002542
H 2.641915 -0.765338 -0.881543
H 2.648179 -0.714935 0.909095
H 3.116526 0.744357 -0.029315

e5_1w
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H 3.247634 -1.374989 -0.001558
H 1.855186 -2.076574 -0.896090
H 1.857541 -2.075225 0.897636
O 1.584952 -0.219077 -0.000254
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O -1.545418 1.114623 -0.000850
H 1.529246 1.948390 -0.001263
H 0.132999 3.001197 -0.001346
O -2.633462 -1.665822 0.000589
H -2.586558 -0.693753 -0.000592
H -1.692182 -1.894446 -0.000824

e6_0w
H -1.184895 1.826937 -0.000418
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C -0.774890 -0.001577 -0.000541
N 0.630341 0.191033 -0.001211
C 1.612924 -0.897581 0.000158
H 2.231569 -0.805509 0.897618
H 2.248206 -0.790295 -0.883682
H 1.106554 -1.860128 -0.012457
O 1.067790 1.392613 0.000632
H -2.069858 -1.338633 0.001175

e6_1w
H -0.152892 2.034115 -0.018277
N -0.782340 1.230806 -0.011391
O -0.622345 -1.076392 -0.003954
C -0.098517 0.149182 -0.005911
N 1.318400 0.106956 0.000401
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H 3.108090 -0.901518 -0.061740
H 1.754984 -1.775794 -0.854397
O 1.962092 1.212576 0.019519
H -1.621744 -0.967859 -0.031509
O -3.127864 -0.187413 -0.081704
H -2.588163 0.643236 -0.120819
H -3.526491 -0.174120 0.802603

e7_0w
N -1.261106 1.323851 0.000221
C -1.022328 0.066598 0.000058
O -1.989589 -0.895831 -0.000027
N 0.241571 -0.519297 0.000110
O 1.197412 0.430227 -0.000685
C 2.495912 -0.180049 0.000290
H 2.623105 -0.798475 -0.893101
H 2.625788 -0.789715 0.899341
H 3.202136 0.651185 -0.004715
H -1.544408 -1.761888 -0.000408
H -2.273956 1.472557 0.000179

e7_1w
N 0.101453 -2.193190 0.041251
C 0.534469 -0.985754 -0.001315
O 1.838971 -0.642902 -0.038531
N -0.312568 0.132293 -0.002761
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H 1.948143 0.341689 -0.097724
H 0.906643 -2.825724 0.032474
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H 1.894205 2.405080 0.833349
H 0.767077 1.872810 -0.074651

e8_0w
H 1.927578 1.143156 0.002294
H 0.607608 2.337080 0.005328
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C 0.124260 0.333004 -0.000294
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C -2.079886 -0.524337 0.000301
H -1.925959 -1.137127 -0.889935
H -3.075427 -0.079781 0.000383
H -1.925762 -1.136729 0.890807
O 1.871333 -0.987860 0.000600

e8_1w
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H -0.172969 -2.198517 -0.002883
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C 0.454892 -0.280158 0.019310
N 0.262110 1.060411 0.035857
C 2.778471 0.228986 -0.037475
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H 3.688745 -0.371458 -0.054647
H 2.749076 0.867331 0.847466
O -0.987605 1.428107 0.021452
O -3.134578 -0.302136 -0.135272
H -3.543515 -0.207085 0.739040
H -2.552255 0.490550 -0.206573

z4_0w
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H 2.269267 1.235868 0.150124
N 1.265444 1.195648 0.027918
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C 0.787055 -0.102425 -0.010415
N -0.647949 -0.183266 0.004183
C -1.525057 0.990097 -0.103024
H -2.498896 0.616671 -0.418487
H -1.135435 1.692836 -0.844416
H -1.635032 1.496324 0.865534
O -1.189969 -1.333330 0.126442

z4_1w
H 1.127276 1.413677 1.376976
H 0.270100 2.608744 0.524340
N 0.743017 1.714204 0.490435
O -0.831613 1.058584 -1.047755
C 0.086649 0.797294 -0.300837
N 0.647886 -0.526073 -0.231993
C 1.927571 -0.834827 0.415901
H 2.294810 -1.753516 -0.041831
H 1.788935 -1.004154 1.491694
H 2.639588 -0.022606 0.253679
O -0.034852 -1.499002 -0.700507
O -2.323618 -0.594919 0.908362
H -1.860557 -1.190306 0.293967
H -2.561128 0.139141 0.320894

z5_0w
N -2.016768 -0.828990 -0.037975
H -1.792641 -1.799961 0.121297
H -2.965506 -0.517947 0.106081
C -1.025998 0.117806 -0.002103
O -1.210307 1.321286 0.006941
N 0.241247 -0.554589 -0.000952
O 1.198739 0.389363 -0.004749
C 2.497314 -0.220964 0.003802
H 2.626671 -0.839730 -0.888791
H 2.618751 -0.831917 0.902922
H 3.206016 0.608370 0.003245

z5_1w
C 3.215267 -0.133998 -0.007527
H 3.761595 -1.078119 -0.007727
H 3.455301 0.451465 0.884496
H 3.442681 0.444308 -0.907473
O 1.826917 -0.499057 0.003506
N 1.056996 0.602860 0.006051
C -0.308197 0.180258 0.009227
N -1.122032 1.264864 0.023302
O -0.695892 -0.988340 0.009209
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H -2.126992 1.091968 -0.036506
O -3.433277 -0.385554 -0.104293
H -2.591461 -0.893629 -0.141763
H -3.776014 -0.576483 0.782106

z6_0w
H -0.419155 2.090721 -0.000379
N -1.160366 1.393963 -0.000057
O -1.564253 -0.857100 0.000098
C -0.727122 0.192123 -0.000004
N 0.621624 -0.224856 -0.000142
C 1.698549 0.771215 0.000144
H 2.628531 0.205515 -0.000530
H 1.648649 1.401468 0.895135
H 1.648145 1.402543 -0.894089
O 0.925700 -1.467931 -0.000072
H -2.455108 -0.463781 0.000208

z6_1w
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N 0.668034 1.187970 -0.008799

O 0.751839 -1.106401 -0.016861
C 0.087462 0.036254 -0.008906
N -1.314830 -0.157484 0.004243
C -2.225944 0.992551 0.009808
H -3.231585 0.576071 0.019119
H -2.088572 1.606247 -0.887633
H -2.073520 1.610041 0.902259
O -1.810254 -1.336698 0.012282
H 1.727809 -0.880237 -0.048758
O 3.172069 0.048544 -0.077800
H 3.549236 0.073965 0.815486
H 2.544288 0.812729 -0.102834

z7_0w
N 2.054134 -0.926719 0.000168
C 1.056949 -0.107685 -0.000347
O 1.196565 1.242386 0.000186
N -0.204879 -0.676297 -0.000163
O -1.125394 0.343318 -0.000308
C -2.456436 -0.191024 0.000250
H -2.614130 -0.796237 0.896988
H -2.613886 -0.798817 -0.894768
H -3.119289 0.675725 -0.001049
H 0.304170 1.636134 -0.000155
H 2.925896 -0.389071 0.000509

z7_1w
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C 0.256182 0.072027 -0.032828
O 1.118689 1.150418 -0.030546
N -1.054458 0.533438 0.008043
O -1.914092 -0.503948 0.005570
C -3.265190 -0.022840 0.040121
H -3.470754 0.589565 -0.842824
H -3.435281 0.561629 0.949185
H -3.887110 -0.918881 0.038317
H 0.580226 1.961775 -0.031626
H 1.662696 -1.188836 -0.102253
O 3.628727 -0.293113 -0.031589
H 3.814323 -0.330762 0.919135
H 3.050919 0.484851 -0.121815

z8_0w
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H -2.079553 -1.502036 -0.173317
H -2.610539 0.152878 -0.092311
C -0.611990 -0.085284 0.003267
O 0.271909 -1.080023 -0.019043
N -0.455885 1.251030 -0.007001
O 0.780584 1.656193 -0.004087
C 1.702124 -0.868949 0.009293
H 2.030291 -0.311719 -0.866896
H 1.997327 -0.333976 0.910791
H 2.112995 -1.881172 0.004912

z8_1w
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H 1.690210 -1.167066 0.051023
H 0.454549 -2.433947 0.060348
C -0.275917 -0.565058 0.042100
O 0.180541 0.700115 -0.030293
N -1.535164 -1.038927 0.003949
O -2.457201 -0.136088 -0.158237
C -0.688127 1.849508 0.118118
H -1.325775 1.966543 -0.755634
H -1.306817 1.755865 1.009727
H 0.002710 2.691179 0.215617
O 3.057994 0.165026 -0.190948
H 2.298332 0.765728 -0.293554
H 3.436745 0.404767 0.668949

eTS_4_5_0w
N -1.233712 1.090013 0.341124
H -0.569543 1.842855 0.232454
H -2.189369 1.274223 0.603422
C -0.901863 -0.157967 -0.077505
O -1.611826 -1.148766 -0.035307
N 0.432982 -0.288440 -0.633430
O 1.202947 0.844077 -0.412735
C 1.831818 -0.543367 0.520453
H 1.231627 -1.239788 1.112500
H 2.519900 -1.032735 -0.156661
H 2.303799 0.189951 1.181075

eTS_4_5_1w
N -0.619089 1.057458 0.076501
H 0.029688 1.831208 0.074071
H -1.625317 1.169786 0.208986
C -0.178634 -0.167343 -0.263790
O -0.859646 -1.193765 -0.319384
N 1.221131 -0.277740 -0.614755
O 1.924973 0.869488 -0.288795
C 2.450292 -0.507651 0.723826
H 1.789037 -1.218982 1.226115
H 3.236224 -0.978963 0.148048
H 2.808247 0.235248 1.442577
O -3.297543 0.110572 0.214427
H -2.660950 -0.589551 -0.052280
H -3.563443 -0.147175 1.110078

eTS_4_6_0w
H 1.562180 1.772792 0.000035
N 1.683435 0.765372 0.000442
O 1.160964 -1.287150 -0.000362

C 0.690373 -0.080582 -0.000024
N -0.673730 0.196161 -0.000232
C -1.678231 -0.871613 0.000297
H -2.305576 -0.761451 -0.888429
H -2.297901 -0.768767 0.895352
H -1.171577 -1.835539 -0.005609
O -1.052769 1.419591 -0.000232
H 2.206529 -0.484119 0.000302

eTS_4_6_1w
H -0.298080 2.009401 -0.024768
N -0.852435 1.159448 -0.006314
O -0.684297 -1.116983 -0.001412
C -0.150919 0.060080 -0.001227
N 1.268230 0.111732 0.004706
C 2.096348 -1.095652 0.000010
H 2.711683 -1.103387 0.904505
H 2.749051 -1.066254 -0.877026
H 1.451720 -1.971628 -0.031269
O 1.842882 1.254457 0.013284
H -1.881240 -0.871036 -0.042379
O -2.888707 -0.163533 -0.090461
H -2.143710 0.735489 -0.055114
H -3.331586 -0.208952 0.773325

eTS_4_8_0w_done
H -2.289619 -0.196941 -0.004419
H -1.841894 -1.906781 -0.009024
N -1.590035 -0.932198 0.002556
O 0.702907 -1.251348 -0.000736
C -0.314401 -0.526436 0.000339
N -0.051985 0.837492 0.000946
C 2.152054 0.271414 -0.000044
H 2.181096 0.844410 0.917341
H 2.180510 0.852857 -0.912125
H 2.742758 -0.634351 -0.004492
O -1.015986 1.655582 -0.000960

eTS_4_8_1w_done
H -1.605675 0.941925 0.003690
H -0.586378 2.378125 -0.026336
N -0.673412 1.375232 0.041819
O 1.608450 1.093148 -0.019752
C 0.439877 0.637930 0.008962
N 0.421642 -0.757761 0.024749
C 2.646953 -0.699519 -0.015670
H 2.520613 -1.386396 -0.842689
H 2.606135 -1.153874 0.966022
H 3.431121 0.034027 -0.150143
O -0.651090 -1.432871 0.023070
O -3.111647 -0.121797 -0.121233
H -3.475308 -0.264959 0.766418
H -2.414801 -0.809445 -0.199374

eTS_5_7_0w
N -1.401784 1.149785 0.000315
C -0.985994 -0.097907 -0.000234
O -2.020158 -0.870441 0.000002
N 0.295947 -0.650001 0.000021
O 1.174487 0.382215 -0.000194
C 2.525066 -0.113613 0.000126
H 2.697304 -0.715474 -0.895779
H 2.697286 -0.714333 0.896803
H 3.158727 0.774009 -0.000427
H -2.491914 0.372744 0.000222
H -0.789604 1.959492 -0.000982

eTS_5_7_1w
N -0.776844 -1.021025 -0.005898
C -0.380435 0.232085 -0.001960
O -1.222143 1.209376 -0.006148
N 0.968267 0.663098 0.009576
O 1.760873 -0.436991 0.002141
C 3.145085 -0.050241 0.006094
H 3.364808 0.531086 0.905332
H 3.367042 0.540237 -0.886557
H 3.707902 -0.984708 0.001862
H -2.296464 0.655560 -0.045566
H -0.046469 -1.722448 -0.024820
O -3.089967 -0.305419 -0.087731
H -3.523838 -0.368522 0.779167
H -2.090940 -0.972508 -0.046075

zTS_4_5_0w
N 1.726755 -0.912130 -0.020158
H 1.535165 -1.686547 -0.640820
H 2.696706 -0.701038 0.169011
C 0.856296 0.149835 -0.018133
O 1.096825 1.260486 0.407162
N -0.413200 -0.289107 -0.580066
O -1.342279 0.721917 -0.526181
C -1.787028 -0.612831 0.565969
H -2.388290 -1.275209 -0.043925
H -1.125071 -1.140346 1.260129
H -2.365372 0.130557 1.122307

zTS_4_5_1w
N -0.874483 1.230352 -0.191745
H -0.467143 2.065820 -0.585257
H -1.884923 1.146884 -0.060543
C -0.163171 0.076630 -0.194131
O -0.610652 -1.034347 0.073166
N 1.220930 0.348169 -0.537256
O 1.965067 -0.807014 -0.526948

C 2.450385 0.278778 0.803595
H 3.224001 0.903935 0.376041
H 1.783732 0.813838 1.486999
H 2.824838 -0.620166 1.301423
O -3.280560 -0.187850 0.330452
H -3.735607 -0.496793 -0.467697
H -2.484151 -0.761920 0.381894

zTS_4_6_0w
H 0.934760 2.084763 0.056828
N 1.342889 1.157718 0.006244
O 1.551747 -0.944221 -0.011140
C 0.694681 0.011119 -0.001438
N -0.683954 -0.186932 -0.008150
C -1.602766 0.958465 -0.008857
H -1.536647 1.507947 0.936872
H -2.604090 0.547624 -0.128667
H -1.371778 1.630963 -0.841106
O -1.157202 -1.376267 0.016754
H 2.257366 0.179603 0.006267

zTS_4_6_1w
H -0.152913 1.977448 -0.040737
N -0.727797 1.147198 0.000194
O -0.819595 -1.120987 -0.000294
C -0.143870 -0.034711 -0.000789
N 1.268225 -0.159857 0.004317
C 2.139274 1.021278 0.009075
H 3.159252 0.641685 0.035916
H 1.952726 1.641594 0.892913
H 1.993461 1.620353 -0.897185
O 1.804720 -1.320414 -0.000182
H -1.983457 -0.736624 -0.047196
O -2.902431 0.075785 -0.093094
H -2.038251 0.882812 -0.046944
H -3.347793 0.066872 0.770506

zTS_5_7_0w
N 2.079410 -0.762861 0.000356
C 0.972305 -0.045693 0.000039
O 1.306248 1.201339 -0.000131
N -0.293987 -0.610088 -0.000120
O -1.197785 0.392943 0.000061
C -2.532000 -0.140282 0.000021
H -2.690596 -0.745424 0.896830
H -2.689951 -0.746954 -0.895859
H -3.188604 0.730308 -0.000930
H 2.453573 0.513035 -0.000058
H 2.108083 -1.778723 -0.001431

zTS_5_7_1w
N -1.258391 1.212997 0.000833
C -0.371033 0.233810 -0.001622
O -0.732155 -1.001618 -0.012372
N 0.974807 0.629051 0.009317
O 1.753627 -0.472226 0.001572
C 3.138800 -0.095616 0.006094
H 3.366760 0.482555 0.906090
H 3.368982 0.493986 -0.885820
H 3.692819 -1.035149 0.000634
H -1.943404 -0.941074 -0.050657
H -0.875011 2.151641 -0.012496
O -3.061195 -0.398119 -0.088246
H -3.481518 -0.527602 0.777991
H -2.432362 0.627845 -0.041256

zTS_5_8_0w
N -2.099603 -0.231121 0.035704
H -2.542269 -1.125778 -0.103618
H -2.637199 0.618470 -0.068894
C -0.753374 -0.128980 0.000750
O -0.004920 -1.128877 -0.011608
N -0.290937 1.193552 -0.001073
O 0.986150 1.227493 -0.006690
C 1.981865 -0.670220 0.007084
H 2.379342 -0.235961 -0.902028
H 2.359934 -0.234633 0.923822
H 1.953191 -1.752843 0.007682

zTS_5_8_1w
N 1.078642 -1.410930 0.013999
H 2.012562 -1.005286 -0.051145
H 0.910898 -2.404148 -0.066771
C 0.014715 -0.595089 0.011059
O 0.135677 0.661494 0.029408
N -1.224596 -1.240650 -0.001751
O -2.181997 -0.393313 0.003504
C -1.612514 1.677148 -0.012789
H -2.178009 1.606507 -0.933625
H -2.205068 1.629832 0.892365
H -0.864096 2.460820 -0.012428
O 2.990288 0.703612 -0.101583
H 3.294498 0.933519 0.789798
H 2.085949 1.073124 -0.144187

TS_4_0w
N 1.524683 0.831003 -0.526941
H 2.529344 0.755328 -0.437019
H 1.156377 1.308253 -1.337064
C 0.767746 -0.110092 0.099893
O 1.165882 -0.941928 0.881853
N -0.657236 0.028500 -0.255026
O -1.183151 -0.984518 -0.847450
C -1.509435 0.823399 0.637076

H -2.444019 1.021507 0.108718
H -1.719155 0.267331 1.559028
H -1.006388 1.762786 0.883069

TS_4_1w
N 0.730072 0.952222 -0.698229
H 1.754424 0.919248 -0.679613
H 0.243171 1.482015 -1.405983
C 0.087863 -0.029239 -0.036461
O 0.610753 -0.877038 0.672045
N -1.370416 0.024069 -0.211906
O -1.894722 -0.989675 -0.804846
O 3.259919 -0.077100 0.045126
H 2.543406 -0.652554 0.388287
H 3.639796 0.324440 0.841374
C -2.159527 0.702498 0.822516
H -3.164410 0.851096 0.422779
H -2.211410 0.086483 1.728786
H -1.700182 1.666189 1.060381

TS_5_0w
N 1.660378 1.054628 -0.078255
H 2.630854 1.080870 -0.357040
H 1.193320 1.913186 0.169653
C 1.055038 -0.151124 0.088992
O 1.569843 -1.232950 -0.114348
N -0.285788 -0.041506 0.636931
O -1.118975 0.066519 -0.441237
C -2.486350 0.020252 -0.009283
H -2.680894 0.817691 0.714340
H -3.082233 0.165864 -0.912062
H -2.702248 -0.952786 0.440799

TS_5_1w
N -0.898342 1.147872 -0.131512
H -1.908379 1.163107 0.032997
H -0.375066 1.996590 -0.282191
C -0.316083 -0.056663 -0.291503
O -0.893268 -1.138162 -0.209787
N 1.080979 -0.001932 -0.668887
O 1.782405 0.015855 0.503032
O -3.445565 -0.040750 0.259047
H -2.750239 -0.702396 0.047104
H -3.632662 -0.196647 1.197344
C 3.189804 -0.064506 0.232238
H 3.496338 0.761845 -0.415925
H 3.677735 0.007753 1.205753
H 3.422909 -1.020357 -0.245036

TS_6_0w
H 1.118107 1.535842 -1.191776
N 1.591325 0.890863 -0.559025
O 1.140250 -0.880685 0.823377
C 0.766535 0.086141 -0.035978
N -0.660210 0.062027 -0.255111
C -1.546242 0.661261 0.747016
H -1.659196 -0.005999 1.610362
H -2.517585 0.812530 0.272591
H -1.132539 1.618724 1.075281
O -1.110330 -0.905076 -0.975926
H 2.112284 -0.829645 0.886664

TS_6_1w
H 0.194689 1.690787 -1.199886
N 0.787785 1.039244 -0.688642
O 0.607336 -0.880426 0.562332
C 0.092485 0.119656 -0.137804
N -1.351959 0.058409 -0.202051
C -2.131349 0.552189 0.937214
H -2.108196 -0.171215 1.761551
H -3.159427 0.683954 0.595022
H -1.720251 1.507342 1.275744
O -1.848386 -0.886848 -0.920678
H 1.608505 -0.803767 0.514301
O 3.143243 -0.164737 0.111129
H 3.519207 0.320902 0.861904
H 2.630327 0.513441 -0.392503

TS_7_0w
N -1.652723 -1.198245 -0.068630
C -1.053273 -0.099623 0.095574
O -1.598890 1.133145 -0.111845
N 0.277191 -0.053724 0.629245
O 1.117616 -0.029743 -0.448100
C 2.483398 -0.026752 -0.004374
H 2.697359 -0.948867 0.542650
H 2.670505 0.840372 0.636036
H 3.083456 0.028625 -0.913967
H -0.940767 1.807555 0.128905
H -2.612390 -1.032869 -0.385566

TS_7_1w
N -0.849645 1.315359 -0.161508
C -0.271809 0.210466 -0.319970
O -0.893118 -1.022360 -0.282264
N 1.117198 0.114531 -0.658977
O 1.788982 -0.034667 0.521918
C 3.203504 -0.084893 0.277851
H 3.537159 0.858778 -0.161807
H 3.441570 -0.915428 -0.393401
H 3.661342 -0.236225 1.256607
H -0.244604 -1.705652 -0.524219
H -1.857553 1.180573 -0.007903
O -3.583897 -0.077196 0.321839

H -2.918924 -0.731407 0.045619
H -3.577774 -0.139524 1.289282

TS_8_0w_done
N -0.594019 1.809717 0.122115
H 0.016283 2.513180 -0.279855
H -1.575145 1.944671 -0.078744
C -0.156545 0.507010 0.014363
O 1.201518 0.451903 0.011954
N -0.905843 -0.497274 -0.275969
O -1.628750 -1.448283 0.135936
C 1.771788 -0.861980 0.018382
H 1.495249 -1.404420 0.927509
H 1.437830 -1.428853 -0.856711
H 2.851218 -0.710816 -0.014812

TS_8_1w_done
N 0.524209 -1.468356 -0.296867
H 1.509618 -1.335827 -0.052749
H 0.123005 -2.373014 -0.096634
C -0.308135 -0.404733 -0.096316
O 0.377977 0.783874 -0.176543
N -1.518433 -0.462469 0.347019
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C -0.423420 1.969306 -0.057653
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H -0.921729 1.996144 0.915988
H 0.272559 2.803457 -0.154394
O 3.069462 -0.177697 0.287076
H 2.379388 0.509437 0.242907
H 3.531067 -0.100618 -0.562266

e10_0w
C 1.136252 -0.310862 -0.020246
O 1.291679 -1.520042 -0.021982
N -0.172096 0.255249 0.172155
O -0.347672 1.524500 0.187565
N 2.084518 0.639728 -0.173386
H 3.034570 0.349925 -0.340646
H 1.820253 1.614058 -0.183054
C -1.369363 -0.597200 0.352182
H -1.089221 -1.618593 0.102659
H -1.648998 -0.528038 1.413878
O -2.391603 -0.179766 -0.497032
H -2.524137 0.768641 -0.324241

e10_1w
C -1.679011 0.015902 -0.030742
O -2.240003 1.096717 -0.038603
N -0.268822 -0.076850 0.272105
O 0.294793 -1.232269 0.280915
N -2.234167 -1.192723 -0.270523
H -3.217824 -1.234063 -0.483647
H -1.665698 -2.025617 -0.238671
C 0.557609 1.151342 0.473685
H -0.150785 1.974995 0.539098
H 1.068846 0.998969 1.433048
O 1.428582 1.371929 -0.578977
H 2.184935 0.748317 -0.467948
O 3.073978 -0.762896 -0.013850
H 3.361377 -1.188259 -0.836350
H 2.209688 -1.178639 0.189859

e11_0w
C 1.068536 -0.344545 -0.067101
O 1.213366 -1.560855 -0.037658
N -0.215658 0.211618 -0.218861
O -0.310425 1.577595 0.170721
N 2.086687 0.563869 -0.046164
H 2.995216 0.194599 0.190771
H 1.877075 1.524912 0.180508
C -1.343990 -0.562604 0.292663
H -1.109606 -1.625975 0.103338
H -1.420854 -0.457907 1.397450
O -2.532241 -0.218239 -0.230500
H -0.751910 1.990851 -0.590767

e11_1w
C -1.538257 -0.013776 -0.181762
O -2.139576 0.995769 -0.542244
N -0.158620 0.035384 0.062110
O 0.364027 -1.026958 0.834637
N -2.093118 -1.248522 -0.047449
H -3.099173 -1.296091 -0.092805
H -1.580065 -1.958114 0.455073
C 0.404160 1.325495 0.397233
H -0.244411 2.084364 -0.088028
H 0.324086 1.520918 1.489594
O 1.692295 1.505606 0.042572
H 1.147339 -1.316728 0.294071
O 2.603437 -1.105935 -0.666417
H 2.461863 -0.135513 -0.681672
H 3.395634 -1.225044 -0.120073

z10_0w
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O 2.188637 0.145597 -0.106008
N -0.074585 0.637446 0.100625
O 0.096106 1.875395 -0.177285
N 0.681473 -1.581375 0.126703
H 1.432057 -2.238819 -0.037586
H -0.242505 -1.851086 -0.194907
C -1.413381 0.194305 0.521750
H -1.341783 -0.355498 1.462862

H -1.982671 1.117757 0.655066
O -2.010511 -0.699012 -0.397868
H -2.173631 -0.215809 -1.225105

z10_1w
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O -2.279992 -1.076294 -0.293288
N -0.223612 -0.340484 0.513411
O 0.286932 -1.516297 0.524597
N -1.723440 1.155521 -0.473735
H -2.560848 1.315219 -1.017872
H -0.913002 1.727591 -0.694876
C 0.598945 0.799309 0.987691
H -0.037187 1.462865 1.577115
H 1.361716 0.337866 1.622819
O 1.128985 1.544160 -0.070226
H 1.784931 0.950502 -0.513595
O 2.619110 -0.618608 -0.851513
H 1.977608 -1.231747 -0.436779
H 3.459226 -0.791403 -0.400637

z11_0w
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O 2.058855 0.651885 0.132894
N -0.214406 0.304880 -0.188111
O -0.382606 1.694755 -0.008795
N 1.259096 -1.496782 -0.076770
H 2.233499 -1.769607 -0.128027
H 0.674879 -1.984385 -0.746243
C -1.315674 -0.404507 0.462530
H -0.955905 -1.391531 0.804268
H -1.596579 0.150696 1.382006
O -2.437716 -0.550367 -0.273420
H -0.438961 2.041582 -0.914868

z11_1w
C 1.544380 -0.266527 0.098548
O 2.137555 -1.258671 -0.262499
N 0.161759 -0.046797 -0.081703
O -0.483788 -1.097363 -0.751386
N 2.156947 0.814286 0.745438
H 3.119566 0.597180 0.977223
H 1.647430 1.210518 1.527465
C -0.323309 1.236848 -0.557470
H 0.371743 2.041387 -0.259863
H -0.312920 1.235570 -1.673823
O -1.596283 1.546581 -0.225047
H -1.227594 -1.317738 -0.136330
O -2.699114 -0.920523 0.830178
H -2.538838 0.025055 0.635527
H -3.483719 -1.146512 0.307219

eTS_10_11_0w
C 1.292513 0.273401 -0.000011
O 1.630600 1.444539 -0.000175
N -0.100674 -0.025867 -0.000249
O -0.442636 -1.290085 -0.000254
N 2.118129 -0.804269 0.000738
H 3.113015 -0.639140 -0.000958
H 1.758701 -1.746523 -0.001152
C -1.831317 0.853339 0.000121
H -1.680143 1.435946 0.922991
H -1.680651 1.436165 -0.922701
O -2.546804 -0.190705 0.000185
H -1.529567 -1.145927 -0.000309

eTS_10_11_1w
C -1.684907 0.140269 0.020250
O -2.113497 1.282170 0.109645
N -0.276111 -0.068709 0.110401
O 0.116226 -1.317684 -0.006689
N -2.432403 -0.983682 -0.135245
H -3.416090 -0.869041 -0.324917
H -1.978600 -1.864318 -0.328284
C 1.010968 1.407850 0.238019
H 0.279762 2.163858 -0.063633
H 1.087918 1.268200 1.328767
O 2.001262 1.164850 -0.512269
H 2.507455 -0.049306 -0.176906
O 2.533289 -1.129867 0.057570
H 1.326997 -1.317337 0.053606
H 2.897546 -1.249781 0.949609

zTS_10_11_0w
C -1.324873 -0.030234 0.008487
O -2.066123 -0.975168 0.165472
N 0.101235 -0.132818 -0.096196
O 0.575251 -1.338293 -0.144376
N -1.699963 1.286527 -0.043575
H -2.692460 1.461828 -0.111345
H -1.080510 1.979537 -0.439248
C 1.670731 0.909825 0.122589
H 1.527234 1.612385 -0.717984
H 1.411513 1.344969 1.103271
O 2.528637 -0.021582 0.034345
H 1.648053 -1.071895 -0.086279

zTS_10_11_1w
C -1.709038 -0.161886 -0.011984
O -2.360190 -1.134560 0.300825
N -0.266844 -0.141635 -0.071839
O 0.253609 -1.336685 -0.141286
N -2.220110 1.084604 -0.287415
H -3.225500 1.115463 -0.392432

H -1.691940 1.707882 -0.883675
C 0.850799 1.232878 0.553015
H 0.098861 2.032505 0.548898
H 0.940120 0.744033 1.540308
O 1.878699 1.365247 -0.184923
H 2.514706 0.157665 -0.182193
O 2.649802 -0.937000 -0.201697
H 1.446060 -1.225623 -0.157888
H 3.100439 -1.214678 0.612219

TS_10_0w
C 1.140571 0.035657 -0.098755
O 2.069622 -0.421282 -0.722830
N -0.160364 -0.663900 -0.013560
O -0.463445 -1.196629 1.121834
N 1.123702 1.197138 0.600247
H 1.940346 1.791337 0.564722
H 0.251096 1.571827 0.945056
C -1.290271 -0.178787 -0.810499
H -0.915678 0.205700 -1.761100
H -1.947706 -1.039127 -0.976924
O -1.957038 0.880762 -0.156424
H -2.366339 0.493569 0.636328

TS_10_1w
C 1.630806 -0.136131 0.043101
O 2.638035 -0.162491 -0.624538
N 0.291678 -0.272631 -0.569089
O -0.357633 -1.352318 -0.285930
N 1.542209 0.006521 1.389814
H 2.393288 0.220497 1.892233
H 0.658138 0.285527 1.794651
C -0.479080 0.962224 -0.845910
H 0.233335 1.709819 -1.203262
H -1.189933 0.705401 -1.639264
O -1.103438 1.442595 0.308331
H -1.920629 0.896590 0.422566
O -2.981401 -0.539562 0.206534
H -3.277163 -0.936046 1.039960
H -2.209107 -1.081372 -0.070282

TS_11_0w
C 1.116454 -0.029655 0.124232
O 1.396805 0.316771 1.252931
N -0.226135 0.084458 -0.461746
O -0.581288 1.476683 -0.312927
N 1.960611 -0.631726 -0.752199
H 2.934698 -0.724047 -0.499849
H 1.684035 -0.741088 -1.715841
C -1.189610 -0.676391 0.356661
H -0.864058 -1.734194 0.389049
H -1.159761 -0.304628 1.407724
O -2.462950 -0.550066 -0.047479
H -1.117849 1.623993 -1.109019

TS_11_1w
C 1.605822 -0.169266 -0.038812
O 2.156018 0.131648 -1.076910
N 0.156851 -0.088037 0.178919
O -0.449021 -0.802710 -0.900589
N 2.228262 -0.560270 1.104981
H 3.223534 -0.733520 1.069972
H 1.683104 -0.981611 1.842262
C -0.281693 1.308388 0.105753
H 0.297392 1.910290 0.832922
H -0.020932 1.713324 -0.904165
O -1.603057 1.509767 0.236736
H -1.260299 -1.171876 -0.471330
O -2.895413 -1.066065 0.279805
H -2.695554 -0.112035 0.376523
H -3.536028 -1.102268 -0.447467

e13_0w
N -0.434373 1.323192 -0.114155
C -0.550546 -0.090268 -0.028029
O -1.648761 -0.694453 0.029400
N 0.660632 -0.672304 -0.034079
H 0.648529 -1.690716 0.024610
O 1.853936 -0.006392 0.038658
H -1.114053 1.760935 0.500550
H 0.543590 1.521930 0.136186

e13_1w
N -1.624900 1.016335 0.382508
C -1.149964 -0.234427 -0.048330
O -1.804054 -1.290066 0.044738
N 0.070150 -0.126057 -0.637093
H 0.579647 -1.003577 -0.712017
O 0.861394 1.003401 -0.422606
H -2.230168 0.914756 1.187994
H -0.804466 1.617456 0.512793
O 2.886516 -0.448632 0.359002
H 2.191623 0.227118 0.024654
H 2.495552 -0.698763 1.209577

e14_0w
H 1.033097 1.650395 0.136128
H 2.399841 0.660000 0.478503
N 1.591417 0.824016 -0.112646
O 1.087608 -1.463734 0.025455
C 0.698297 -0.271977 -0.026394
N -0.584996 0.152659 -0.016759
C -1.678920 -0.774911 -0.002158
H -2.341487 -0.595616 -0.866059

H -2.288169 -0.623446 0.905562
H -1.296111 -1.798795 -0.029138
O -0.921155 1.482741 0.031064

e14_1w
H 0.675631 -1.906913 0.222351
H 2.136054 -1.797391 -0.678391
N 1.572566 -1.437231 0.082886
O 2.156129 0.716294 -0.599399
C 1.316260 -0.063134 -0.102918
N 0.086507 0.283672 0.341806
C -0.399606 1.634417 0.282926
H -0.654852 1.998775 1.292392
H -1.314559 1.662228 -0.326300
H 0.369981 2.274120 -0.155556
O -0.806064 -0.667415 0.805583
O -2.949533 -0.423428 -0.725776
H -2.078881 -0.605014 -0.226786
H -3.451063 0.017797 -0.023866

e15_0w
C -2.362005 -0.145638 0.272873
H -3.169346 0.584648 0.068199
H -2.206997 -0.222878 1.372029
H -2.674774 -1.146867 -0.094391
O -1.212471 0.310878 -0.394221
N -0.157508 -0.763396 -0.220464
C 1.029571 -0.171479 0.005349
N 1.096428 1.261301 0.180099
O 2.107481 -0.827092 0.104250
H 0.308788 1.741168 -0.263339
H 2.004408 1.591011 -0.149501

e15_1w
C -2.134855 -1.178885 0.469139
H -3.183095 -1.339643 0.170379
H -2.114666 -0.570754 1.389129
H -1.674372 -2.153969 0.697600
O -1.488089 -0.544760 -0.602166
N -0.050347 -0.452353 -0.270722
C 0.268225 0.818003 0.009742
N -0.754663 1.814924 0.052556
O 1.446760 1.186699 0.267511
H -1.530051 1.569679 -0.554937
H -0.341271 2.712454 -0.175907
O 2.708658 -1.347287 -0.016531
H 2.564461 -0.388972 0.151661
H 1.775213 -1.558710 -0.214562

z13_0w
N -1.518656 -0.826287 -0.000050
C -0.392296 0.157542 -0.000052
O -0.606807 1.387916 0.000023
N 0.767918 -0.503815 -0.000118
H 0.643993 -1.521815 -0.000282
O 2.002885 -0.016542 0.000091
H -2.101457 -0.542402 0.795277
H -2.102217 -0.541310 -0.794422

z13_1w
N 2.167759 -0.217212 -0.465157
C 0.818939 -0.170549 0.095666
O 0.344076 -1.197288 0.620453
N 0.245044 1.026991 -0.060209
H 0.742300 1.671944 -0.677812
O -0.983792 1.412781 0.352007
H 2.743803 0.534397 -0.087604
H 2.557141 -1.098263 -0.141210
H -1.635116 -1.291750 -0.064169
H -2.037060 0.121398 -0.210074
O -2.382075 -0.788354 -0.436906

z14_0w
H 1.106842 1.693812 0.788949
H 2.362227 0.898621 0.097180
N 1.381540 1.141930 -0.024397
O 1.437712 -1.186569 -0.067685
C 0.714979 -0.172807 -0.023653
N -0.629027 -0.136313 -0.000408
C -1.391865 1.090955 -0.082606
H -2.147292 0.952755 -0.870306
H -0.780161 1.969017 -0.319737
H -1.944011 1.262844 0.858568
O -1.413196 -1.229088 0.099751

z14_1w
H 1.632863 1.336138 1.257827
H 2.883243 0.310710 0.948452
N 2.092793 0.792979 0.528825
O 1.697372 -1.437014 0.024849
C 1.239365 -0.286255 0.040457
N 0.023535 0.103035 -0.386580
C -0.417879 1.476168 -0.498665
H -0.785259 1.630554 -1.524528
H 0.386043 2.192723 -0.303088
H -1.262209 1.647710 0.184745
O -0.926096 -0.794057 -0.790471
O -2.902302 -0.272164 0.858065
H -3.454433 0.082339 0.144762
H -2.095248 -0.585874 0.305823

z15_0w
C -2.484838 -0.261652 -0.008012
H -3.304306 0.481210 -0.016199

H -2.594730 -0.916745 0.886800
H -2.570331 -0.911526 -0.908740
O -1.287618 0.468725 0.010620
N -0.203845 -0.533231 0.030671
C 0.973579 0.107885 -0.012383
N 2.067568 -0.866135 -0.117097
O 1.276269 1.328878 -0.001279
H 1.750432 -1.784039 0.212908
H 2.831219 -0.531559 0.477844

z15_1w
C 3.112038 -0.249038 0.213311
H 3.722185 -1.160594 0.126775
H 3.254883 0.178095 1.224728
H 3.488117 0.500101 -0.509126
O 1.794077 -0.619599 -0.032725
N 0.999240 0.602595 0.102963
C -0.257964 0.324329 -0.203788
N -1.091453 1.498733 -0.158452
O -0.806221 -0.771681 -0.538471
H -0.686864 2.193577 0.463693
H -2.019767 1.224464 0.159210
O -3.329106 -0.660853 0.302179
H -2.445479 -0.753160 -0.177318
H -3.062027 -0.926460 1.195464

H2O
O 0.000000 0.000000 0.119746
H 0.000000 0.761572 -0.478982
H 0.000000 -0.761572 -0.478982

OH*
O 0.000000 0.000000 0.109213
H 0.000000 0.000000 -0.873700

NH3
N -0.000336 0.000000 -0.119105
H 0.470383 -0.812097 0.277581
H 0.470343 0.812120 0.277581
H -0.938377 -0.000023 0.278575

NH2*
N 0.000000 0.000000 0.144460
H 0.000000 0.804525 -0.505611
H 0.000000 -0.804525 -0.505611

NH2OH
N -0.697714 -0.000969 -0.117642
H -1.004741 -0.818312 0.415000
O 0.733812 -0.001062 -0.102653
H 1.023476 0.008510 0.828696
H -1.005234 0.825082 0.401023

NH2O*
N -0.028172 0.546984 0.000000
H 0.211287 1.029752 0.868651
O -0.028172 -0.736049 0.000000
H 0.211287 1.029752 -0.868651

*NHOH
N -0.709428 -0.177925 -0.000030
O 0.627324 0.149270 -0.000031
H 1.074018 -0.715652 0.000241
H -1.126613 0.766965 0.000224

eHU
N 0.556089 1.285652 0.081335
C 0.607276 -0.079995 0.024834
O 1.621723 -0.751427 -0.066421
N -0.642795 -0.719106 0.200789
H -0.660292 -1.595492 -0.315211
O -1.767828 0.065234 -0.195394
H -2.298166 0.111213 0.617705
H 1.410423 1.757169 -0.176755
H -0.319841 1.730803 -0.155092

zHU
N -1.697387 -0.483730 0.085497
C -0.466946 0.128345 -0.010467
O -0.289765 1.341532 -0.006644
N 0.607168 -0.761404 -0.120287
H 0.585530 -1.518484 0.559238
O 1.857877 -0.107711 0.012362
H 1.580518 0.831948 0.116785
H -2.474405 0.148572 -0.055786
H -1.803328 -1.386729 -0.359648

eNMHU
H -1.172935 1.708385 0.356956
H -2.512684 0.617130 0.358151
N -1.578555 0.837630 0.044782
O -1.131646 -1.412947 -0.042451
C -0.749597 -0.251869 -0.055867
N 0.604218 0.064251 -0.300379
C 1.607658 -0.892431 0.148845
H 1.786164 -0.816737 1.229724
H 2.542963 -0.706090 -0.385775
H 1.237972 -1.888865 -0.091893
O 0.954034 1.390696 0.104341
H 1.211409 1.816819 -0.730974

zNMHU
H -1.265492 1.757842 -0.674775
H -2.515893 0.801166 -0.042411

N -1.527356 1.018147 -0.036197
O -1.188411 -1.241246 0.222559
C -0.744453 -0.120186 -0.023384
N 0.601830 0.063368 -0.323326
C 1.367663 1.170477 0.237417
H 2.318713 1.236074 -0.295883
H 1.564424 1.018539 1.306720
H 0.821219 2.104910 0.097461
O 1.337238 -1.137695 -0.135783
H 0.625837 -1.759354 0.147147

eOMHU
C 2.339337 0.020742 0.351314
H 3.106521 0.655537 -0.115629
H 2.730418 -1.002738 0.477512
H 2.046627 0.430846 1.331689
O 1.228719 0.039096 -0.568921
N 0.151844 -0.737763 -0.018539
H 0.068851 -1.618423 -0.537010
C -1.100621 -0.074836 0.033247
N -1.020191 1.295925 0.063893
O -2.130782 -0.734781 0.139227
H -0.185226 1.730112 -0.324458
H -1.904547 1.787581 -0.019399

zOMHU
C -2.206233 0.182583 0.433279
H -3.125953 0.459460 -0.101451
H -1.769554 1.075156 0.908619
H -2.424091 -0.592093 1.188446
O -1.332742 -0.328585 -0.590710
N -0.125446 -0.786103 0.000096
H 0.098201 -1.679567 -0.447233
C 0.929296 0.164094 -0.030516
N 2.176579 -0.434480 0.145172
O 0.757437 1.365610 -0.162585
H 2.222446 -1.322943 0.641532
H 2.905090 0.227806 0.402986

Comparison of geometrical parameters (bond distance and angles) between optimization in gas phase and in implicit CPCM solvent for selected structures

e1_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.3407 1.3379 0.0028
1.0213 1.0207 0.0006
1.01 1.0137 -0.0037
1.2317 1.2362 -0.0045
1.423 1.4212 0.0018
1.951 1.9495 0.0015
1.0236 1.0313 -0.0077
1.2761 1.2771 -0.001
1.9625 2.002 -0.0395
0.9814 0.9811 0.0003
0.9693 0.9736 -0.0043
Angle
116.7477 117.1268 -0.3791
119.2447 120.2809 -1.0362
123.6763 122.5812 1.0951
127.6889 127.191 0.4979
113.9918 114.5589 -0.5671
118.3181 118.25 0.0681
103.5134 103.9121 -0.3987
115.8488 116.6081 -0.7593
123.6865 123.2017 0.4848
120.4604 120.1902 0.2702
141.0512 140.8839 0.1673
82.2318 80.1645 2.0673
112.0119 106.2035 5.8084
103.9269 103.628 0.2989
148.2011 150.7044 -2.5033

e2_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0084 1.0128 -0.0044
1.0085 1.0119 -0.0034
1.364 1.3538 0.0102
1.2232 1.2333 -0.0101
1.4245 1.4243 0.0002
1.3607 1.353 0.0077
2.2239 3.3271 -1.1032
0.9981 1.0084 -0.0103
1.7499 1.6385 0.1114
0.9701 0.976 -0.0059
0.9771 0.9759 0.0012
Angle
119.5459 119.3509 0.195
117.1214 118.6136 -1.4922
120.6204 121.2636 -0.6432
124.8967 124.6886 0.2081
117.4093 118.1903 -0.781
117.6829 117.1176 0.5653
110.4286 109.8251 0.6035
161.0128 178.4342 -17.4214
88.0436 68.6235 19.4201
101.4203 104.611 -3.1907
148.5274 179.9818 -31.4544
110.9421 108.9456 1.9965
85.5859 108.7338 -23.1479
104.2338 104.0786 0.1552
115.8366 77.7573 38.0793

e3_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0071 1.0141 -0.007
1.0145 1.0163 -0.0018
1.3312 1.3247 0.0065
1.315 1.3147 0.0003
1.3642 1.3717 -0.0075
1.0131 1.0151 -0.002
1.3005 1.3035 -0.003
1.9181 1.9944 -0.0763
1.656 1.6397 0.0163
0.9926 0.988 0.0046
0.9705 0.9759 -0.0054
Angle
123.1095 121.5699 1.5396
122.1068 122.0151 0.0917
114.5789 116.4148 -1.8359
118.2146 118.2846 -0.07
121.7253 122.5434 -0.8181
120.0586 119.172 0.8866
108.3734 108.8227 -0.4493
112.2708 112.4186 -0.1478
105.4748 105.4086 0.0662
142.1385 142.1653 -0.0268
162.085 164.5587 -2.4737
85.6385 86.5946 -0.9561
111.193 108.9576 2.2354
104.5857 104.5095 0.0762
138.1 135.4039 2.6961

z1_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0091 1.013 -0.0039
1.0137 1.0184 -0.0047

1.3742 1.3534 0.0208
2.1127 1.9776 0.1351
1.2118 1.2228 -0.011
1.4294 1.4318 -0.0024
1.0266 1.031 -0.0044
1.2762 1.278 -0.0018
2.0716 1.9694 0.1022
0.9695 0.9746 -0.0051
0.9694 0.9746 -0.0052
Angle
118.1413 119.9237 -1.7824
115.4501 118.2183 -2.7682
120.9629 121.8575 -0.8946
149.4459 149.8574 -0.4115
125.7478 126.5439 -0.7961
111.2359 111.7973 -0.5614
122.9929 121.6588 1.3341
119.1244 119.5785 -0.4541
122.0645 121.1416 0.9229
118.7991 119.2799 -0.4808
152.4717 149.6552 2.8165
63.1294 67.254 -4.1246
129.3705 121.4007 7.9698
121.3925 121.5181 -0.1256
114.6015 119.5353 -4.9338
115.6639 119.4432 -3.7793
105.2664 104.883 0.3834

z2_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0222 1.0246 -0.0024
1.0094 1.0129 -0.0035
1.3424 1.34 0.0024
1.9509 1.865 0.0859
1.242 1.2464 -0.0044
1.4289 1.427 0.0019
1.8106 1.8305 -0.0199
1.3373 1.3364 0.0009
1.0047 1.0063 -0.0016
0.9718 0.9767 -0.0049
0.9718 0.9739 -0.0021
Angle
122.4068 124.3762 -1.9694
117.7306 116.2727 1.4579
119.8625 119.351 0.5115
145.8643 152.0874 -6.2231
125.5268 125.8685 -0.3417
113.0571 113.0101 0.047
121.4161 121.1212 0.2949
107.8835 108.2863 -0.4028
105.0545 106.1245 -1.07
92.5721 88.1519 4.4202
92.558 105.3372 -12.7792
101.1561 103.6104 -2.4543

z3_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.009 1.0145 -0.0055
1.008 1.0145 -0.0065
1.3463 1.3351 0.0112
1.3127 1.3119 0.0008
1.36 1.3682 -0.0082
1.0161 1.0152 0.0009
1.3023 1.3076 -0.0053
1.7575 1.8146 -0.0571
1.6041 1.6115 -0.0074
0.9929 0.9875 0.0054
0.9704 0.9757 -0.0053
Angle
120.5573 119.7976 0.7597
117.8918 119.297 -1.4052
120.3226 120.9053 -0.5827
114.7483 115.5431 -0.7948
115.135 115.8822 -0.7472
130.1074 128.5747 1.5327
114.061 114.2464 -0.1854
115.3305 114.7803 0.5502
128.8124 130.9376 -2.1252
82.4083 82.5038 -0.0955
109.7855 107.984 1.8015
104.5964 104.5772 0.0192
150.7734 147.4298 3.3436
177.8481 181.5172 -3.6691
178.1495 178.19 -0.0405

TS_1_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0252 1.0243 0.0009
1.0091 1.0144 -0.0053
1.344 1.3344 0.0096
1.9413 1.9781 -0.0368
1.2218 1.2287 -0.0069
1.4707 1.467 0.0037
1.9767 1.9876 -0.0109
1.0269 1.0329 -0.006
1.2877 1.2894 -0.0017
0.9806 0.9801 0.0005
0.9693 0.9738 -0.0045
Angle
121.2284 121.317 -0.0886
116.628 117.4709 -0.8429

119.9714 121.1871 -1.2157
142.6653 142.1293 0.536
126.152 126.3443 -0.1923
112.5119 113.271 -0.7591
121.3201 120.3834 0.9367
104.7287 104.6018 0.1269
115.6697 116.8346 -1.1649
117.2641 116.9638 0.3003
116.3873 117.3545 -0.9672
82.7921 81.2655 1.5266
113.7773 106.8799 6.8974
104.0384 103.6889 0.3495
146.0408 148.1794 -2.1386

TS_2_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0237 1.0231 0.0006
1.0085 1.0143 -0.0058
1.3466 1.3393 0.0073
1.9603 2.002 -0.0417
1.228 1.2352 -0.0072
1.4493 1.4471 0.0022
1.9339 1.9377 -0.0038
1.3766 1.3706 0.006
0.9742 0.9841 -0.0099
0.9694 0.9736 -0.0042
0.9825 0.9818 0.0007
Angle
121.6618 121.0352 0.6266
117.2723 117.7298 -0.4575
120.8653 121.217 -0.3517
141.5207 141.0756 0.4451
125.3821 125.4464 -0.0643
114.3657 114.7767 -0.411
120.0803 119.6477 0.4326
105.1198 105.0277 0.0921
105.6908 105.8878 -0.197
103.31 104.1194 -0.8094
111.7545 106.065 5.6895
80.9294 79.1381 1.7913
103.7804 103.6318 0.1486
149.0402 151.5705 -2.5303

TS_3_1w
OPT_no_solv OPT_CPCM Diff
Bond Distance
1.0112 1.019 -0.0078
1.0092 1.0164 -0.0072
1.3358 1.3173 0.0185
1.319 1.3103 0.0087
1.3511 1.3839 -0.0328
1.0119 1.018 -0.0061
1.3149 1.3355 -0.0206
1.9744 2.0562 -0.0818
1.6958 1.6482 0.0476
0.9706 0.9757 -0.0051
0.9863 0.9831 0.0032
Angle
119.9781 119.065 0.9131
121.2672 121.5989 -0.3317
118.7409 119.3344 -0.5935
115.7545 117.3019 -1.5474
122.5143 122.3361 0.1782
121.0399 120.1236 0.9163
105.2446 106.6173 -1.3727
121.8854 112.6915 9.1939
85.4392 83.7628 1.6764
156.9773 158.3349 -1.3576
109.0374 109.7807 -0.7433
96.4859 95.6701 0.8158
103.0504 103.9581 -0.9077
150.4094 149.8872 0.5222

eTS_1_2_1w
OPT_no_solv OPT_CPCM
Bond Distance
0.9723 0.9802 -0.0079
1.3254 1.3232 0.0022
1.4027 1.5022 -0.0995
1.4211 1.4164 0.0047
1.3283 1.4444 -0.1161
1.1666 1.1016 0.065
1.1552 1.1022 0.053
1.2211 1.2321 -0.011
1.362 1.356 0.006
1.0096 1.0128 -0.0032
1.0081 1.0126 -0.0045
Angle
95.4435 95.0091 0.4344
116.9277 116.0775 0.8502
147.4723 148.8835 -1.4112
90.9744 90.7577 0.2167
141.6106 139.2366 2.374
108.3087 108.2749 0.0338
107.5325 108.1249 -0.5924
79.3753 83.9852 -4.6099
132.5637 130.9142 1.6495
119.2624 118.9848 0.2776
114.7133 115.7156 -1.0023
126.0113 125.2854 0.7259
119.3696 119.3527 0.0169
117.5038 118.4318 -0.928
120.0558 119.4301 0.6257

zTS_1_2_1w
OPT_no_solv OPT_CPCM
Bond Distance
0.972 0.9794 -0.0074
1.3145 1.3166 -0.0021
1.3603 1.4717 -0.1114
1.4251 1.4196 0.0055
1.3127 1.4285 -0.1158
1.18 1.1098 0.0702
1.1875 1.1193 0.0682
1.2136 1.2269 -0.0133
1.3773 1.3635 0.0138
1.0105 1.0141 -0.0036
1.0103 1.0135 -0.0032
Angle
95.7406 95.337 0.4036
115.6072 115.0165 0.5907
148.5988 149.6165 -1.0177
91.2625 90.6564 0.6061
141.8504 139.7361 2.1143
107.4651 108.1007 -0.6356
108.0007 108.0198 -0.0191
77.3924 82.5349 -5.1425
133.7257 131.6359 2.0898
124.7472 124.6311 0.1161
110.2076 110.6517 -0.4441
124.9968 124.6964 0.3004
119.3597 120.3207 -0.961
115.3016 117.8161 -2.5145
116.5637 117.6632 -1.0995

eTS_1_3_1w
OPT_no_solv OPT_CPCM
Bond Distance
1.4058 1.4466 -0.0408
1.3884 1.3969 -0.0085
1.2913 1.2938 -0.0025
1.2112 1.1708 0.0404
1.2408 1.2873 -0.0465
1.1489 1.1253 0.0236
0.9725 0.9781 -0.0056
1.2808 1.2798 0.001
1.3346 1.3307 0.0039
1.0071 1.0132 -0.0061
1.0132 1.0153 -0.0021
Angle
105.2257 105.1214 0.1043
138.7728 138.8384 -0.0656
115.969 116.0396 -0.0706
157.6962 157.4945 0.2017
86.6915 87.5404 -0.8489
108.8903 108.4373 0.453
107.8055 107.8113 -0.0058
145.9596 145.5362 0.4234
119.0136 118.3416 0.672
118.6542 119.1291 -0.4749
122.3314 122.5293 -0.1979
105.3789 105.8867 -0.5078
121.0587 121.1383 -0.0796
116.0634 117.5967 -1.5333
122.6408 121.2636 1.3772

zTS_2_3_1w
OPT_no_solv OPT_CPCM
Bond Distance
1.0088 1.0137 -0.0049
1.0079 1.0136 -0.0057
1.3502 1.3447 0.0055
1.2791 1.2726 0.0065
1.3883 1.4003 -0.012
1.2236 1.2963 -0.0727
1.3125 1.3158 -0.0033
1.3246 1.3975 -0.0729
1.1911 1.1344 0.0567
1.1287 1.0893 0.0394
0.9719 0.9875 -0.0156
Angle
120.8163 119.6901 1.1262
118.9074 120.2885 -1.3811
119.8121 120.019 -0.2069
117.6724 118.8513 -1.1789
111.5091 111.649 -0.1399
130.8151 129.4995 1.3156
115.4324 117.3803 -1.9479
116.9469 116.9926 -0.0457
165.14 164.0115 1.1285
86.7823 88.376 -1.5937
108.9008 108.0447 0.8561
107.4615 107.3319 0.1296