Supplementary Information for

Reaction pathways and free energy profiles for spontaneous hydrolysis of urea and tetramethylurea: Unexpected substituent effects

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Urea(H_2O) of SR-a in Figure 1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.704535	-0.076393	-0.012119
2	8	0	-0.021846	-1.107335	-0.059090
3	7	0	-2.080275	-0.130962	0.123965
4	1	0	-2.635737	0.630697	-0.244544
5	8	0	2.510840	0.016829	-0.037491
6	1	0	1.790846	-0.655126	-0.053184
7	1	0	3.152964	-0.281113	0.622635
8	1	0	-2.468733	-1.051956	-0.033628
9	7	0	-0.162277	1.180553	-0.083627
10	1	0	-0.679520	1.970214	0.277684
11	1	0	0.853302	1.222554	-0.005964

B3lYP/6-31+G* energy: -301.658788 Hartree
Zero-point vibrational energy: 0.088625 Hartree
Thermal correction to Gibbs free energy: 0.058132 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -301.7418316 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -301.8231799 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -301.770713 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.8498415 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -300.855515 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -300.9163744 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -301.0460054 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -301.1217937 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -300.9919506 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.2552013 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -301.3422227 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -301.3919361 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -300.9699271 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -301.0513669 Hartree
Solvent shift (FPCM/0.001 au contour): -0.026208826 Hartree

$OH^-(H_2O)_3$ of SR-a in Figure 1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-0.001590	-0.001083	0.735230
2	1	0	-0.002094	-0.003006	1.703932
3	8	0	1.616780	-1.855569	-0.244956
4	1	0	1.046296	-1.123472	0.177749
5	1	0	0.965452	-2.367795	-0.746417
6	8	0	-2.419773	-0.467475	-0.245370
7	1	0	-2.529925	0.352598	-0.748788
8	1	0	-1.499592	-0.346678	0.176335
9	8	0	0.804171	2.325149	-0.244374
10	1	0	1.571457	2.012932	-0.746324
11	1	0	0.451709	1.467239	0.179276

B3lYP/6-31+G* energy: -305.136485 Hartree
Zero-point vibrational energy: 0.082737 Hartree
Thermal correction to Gibbs free energy: 0.046521 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -305.2232863 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -305.3178539 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -305.2585016 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -305.3408226 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -304.335055 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -304.4179181 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -304.5780106 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -304.6640567 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -304.5277586 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -304.7972153 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -304.8876915 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -304.9395266 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -304.4565969 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -304.5745667 Hartree
Solvent shift (FPCM/0.001 au contour): -0.102735477 Hartree

TS1-a in Figure 1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.395045	-0.723671	0.537279
2	8	0	0.872627	-0.769629	0.532861
3	7	0	-1.039455	0.103391	1.498391
4	1	0	-2.028358	0.208951	1.272067
5	8	0	-0.949203	0.257856	-1.009981
6	1	0	-0.558088	-0.261205	-1.730663

7	1	0	-0.618598	1.032529	1.470207
8	8	0	2.609712	1.242883	0.388865
9	1	0	2.967856	1.393965	1.275550
10	1	0	1.912077	0.531107	0.510195
11	8	0	3.162557	-1.508386	-0.962784
12	1	0	3.416221	-0.583332	-0.800274
13	1	0	2.271102	-1.538498	-0.551602
14	8	0	-3.530780	0.037190	-0.596230
15	1	0	-2.561891	0.122804	-0.892686
16	1	0	-3.904129	0.921734	-0.719107
17	8	0	0.112521	2.700864	-0.282022
18	1	0	-0.282985	1.876584	-0.672225
19	1	0	1.047087	2.457612	-0.140205
20	7	0	-1.070544	-1.947940	0.222386
21	1	0	-2.075224	-1.895004	0.370340
22	1	0	-0.664287	-2.699605	0.773627

B3lYP/6-31+G* energy: - 606.760621 Hartree
Zero-point vibrational energy: 0.176210 Hartree
Thermal correction to Gibbs free energy: 0.131381 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -606.9546999 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -607.1303032 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -607.0173909 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -607.1761303 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -605.194225 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -605.335673 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -605.6246481 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -605.7850426 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -605.5217118 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -606.0519675 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -606.2277706 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -606.3282596 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -605.4308826 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -605.6307329 Hartree
Solvent shift (FPCM/0.001 au contour): -0.098589853 Hartree

INT-a in Figure 1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040094	-0.633192	0.546978
2	8	0	-1.273216	-0.140543	0.607633

3	7	0	0.552800	-0.682613	-0.831568
4	1	0	-0.106018	-1.190865	-1.426041
5	8	0	0.862492	0.215614	1.318679
6	1	0	1.685853	-0.296249	1.402966
7	8	0	-2.861583	-1.455167	-1.112485
8	1	0	-2.307295	-0.991608	-0.411855
9	1	0	-3.230131	-0.724597	-1.630482
10	8	0	-1.729377	2.364389	-0.062311
11	1	0	-1.556859	1.392308	0.187762
12	1	0	-1.974336	2.783946	0.775346
13	8	0	3.402590	-0.800775	-0.886197
14	1	0	3.493017	0.158721	-0.992615
15	1	0	2.416219	-0.936208	-0.890166
16	8	0	1.110421	2.592315	-0.286209
17	1	0	0.139096	2.730143	-0.339882
18	1	0	1.174457	1.868945	0.372979
19	1	0	0.531496	0.282537	-1.170422
20	7	0	0.110862	-1.996926	1.108758
21	1	0	-0.574911	-2.053985	1.861678
22	1	0	-0.186288	-2.673830	0.405663

B3lYP/6-31+G* energy: - 606.764021 Hartree
Zero-point vibrational energy: 0.177619 Hartree
Thermal correction to Gibbs free energy: 0.132904 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -606.9590285 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -607.1327711 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -607.0222513 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -607.1797663 Hartree
MP2/6-31+G*//B3LYP/6-31+G* energy: -605.2026 Hartree
MP2/6-31++G**//B3LYP/6-31+G* energy: -605.3437183 Hartree
MP2/6-311++G**//B3LYP/6-31+G* energy: -605.6334224 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -605.7926443 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -605.5291594 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -606.0602964 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -606.2361584 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -606.3366558 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -605.4398944 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -605.6390958 Hartree
Solvent shift (FPCM/0.001 au contour): -0.09985206 Hartree

TS2-a in Figure 1:

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.406812	0.364364	-0.561053
2	8	0	-0.849150	0.671246	-0.748557
3	7	0	0.732352	0.261601	1.029406
4	1	0	0.513812	1.155504	1.472892
5	8	0	0.772911	-0.944783	-0.987751
6	1	0	1.721030	-1.058752	-0.693097
7	8	0	-1.472006	2.647078	0.957651
8	1	0	-1.296977	1.961518	0.244116
9	1	0	-2.304097	2.359724	1.360864
10	8	0	-2.857432	-1.015989	-0.434027
11	1	0	-2.092402	-0.368597	-0.573256
12	1	0	-3.002725	-1.405710	-1.308428
13	8	0	3.031669	-0.525174	0.472980
14	1	0	3.499025	-1.194448	0.992897
15	1	0	1.850374	-0.081099	1.037189
16	8	0	-0.803105	-2.492408	0.868189
17	1	0	-1.668144	-2.143504	0.560463
18	1	0	-0.198867	-2.193338	0.154639
19	1	0	0.118322	-0.464405	1.414832
20	7	0	1.339344	1.324995	-1.122468
21	1	0	1.044780	2.268028	-0.881135
22	1	0	2.290027	1.152951	-0.792103

B3lYP/6-31+G* energy: -606.748952 Hartree
Zero-point vibrational energy: 0.175918 Hartree
Thermal correction to Gibbs free energy: 0.134266 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -606.9447723 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -607.1173815 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -607.0070949 Hartree
B3lYP/ aug-cc-pVTZ//B3LYP/6-31+G* energy: -607.1645655 Hartree
MP2/6-31+G*//B3LYP/6-31+G* energy: -605.187739 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -605.3281668 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -605.6155384 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -605.7770263 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -605.5154091 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -606.0467482 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -606.2223397 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -606.3226476 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -605.4214425 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -605.6225995 Hartree
Solvent shift(FPCM/0.001 au contour): -0.101209686 Hartree

PC-a in Figure 1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.826777	-0.576599	-0.372553
2	8	0	1.692799	0.350045	-0.231754
3	7	0	-4.017223	0.198501	1.062011
4	1	0	-4.695743	0.236637	0.301714
5	8	0	-0.402943	-0.404590	-0.631728
6	1	0	-1.493688	-1.690407	-0.365121
7	8	0	4.004041	-0.605940	0.831546
8	1	0	3.231346	-0.165083	0.380535
9	1	0	3.998378	-0.235804	1.726208
10	8	0	1.006062	2.993695	-0.126718
11	1	0	1.249204	2.026474	-0.133978
12	1	0	1.085955	3.260253	-1.054183
13	8	0	-2.083573	-2.479208	-0.201222
14	1	0	-2.521817	-2.632640	-1.050628
15	1	0	-3.516155	-0.685190	0.949758
16	8	0	-1.753448	2.034030	-0.212223
17	1	0	-0.977533	2.595174	-0.013427
18	1	0	-1.326572	1.170480	-0.421056
19	1	0	-3.334937	0.937291	0.865076
20	7	0	1.286536	-1.891164	-0.272984
21	1	0	2.173752	-2.019864	0.200885
22	1	0	0.578444	-2.593339	-0.096856

B3lYP/6-31+G* energy: -606.830784 Hartree
Zero-point vibrational energy: 0.175495 Hartree
Thermal correction to Gibbs free energy: 0.124539 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -607.0159644 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -607.1924929 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -607.0787501 Hartree
B3lYP/ aug-cc-pVTZ//B3LYP/6-31+G* energy: -607.2396333 Hartree
MP2/6-31+G*//B3LYP/6-31+G* energy: -605.251338 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -605.3907138 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -605.6799955 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -605.8417192 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -605.5745467 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -606.1083553 Hartree

MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -606.2849787 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -606.3858982 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -605.4862267 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -605.6841056 Hartree
Solvent shift(FPCM/0.001 au contour): -0.091242038 Hartree

RC-b in Figure 2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.265546	-0.051991	-0.000330
2	1	0	-3.041874	-1.009134	-0.004623
3	7	0	-2.646152	-0.083720	-0.106944
4	1	0	-3.188619	0.658494	0.316022
5	8	0	-0.610774	-1.104896	-0.051643
6	7	0	-0.706756	1.179875	0.145102
7	1	0	-1.254802	2.008753	-0.037762
8	1	0	0.313208	1.278339	0.083847
9	1	0	1.132189	-1.372852	-0.060476
10	8	0	2.122279	-1.376007	-0.037380
11	1	0	2.372725	-1.912772	0.728612
12	1	0	2.366038	0.370085	0.023764
13	8	0	2.200259	1.346655	0.018935
14	1	0	2.670650	1.691938	-0.753808

B3lYP/6-31+G* energy: -378.080070 Hartree
Zero-point vibrational energy: 0.114040 Hartree
Thermal correction to Gibbs free energy: 0.079467 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1947923 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.300002 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.2319578 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.3320606 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.0861281 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.1688592 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.3388241 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.4349826 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.2703507 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.6013515 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.7108145 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.7733541 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.2332926 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.3426515 Hartree

Solvent shift(FPCM/0.001 au contour): -0.029329757 Hartree

TS1-b in Figure 2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.652799	-0.231075	-0.193343
2	1	0	-2.027195	-1.317920	0.752821
3	7	0	-1.896102	-0.384318	0.379127
4	1	0	-2.180350	0.356405	1.019653
5	8	0	0.035851	-1.093299	-0.688931
6	7	0	-0.532352	1.198538	-0.792964
7	1	0	-0.884622	1.212140	-1.753982
8	1	0	0.470826	1.401162	-0.750631
9	1	0	1.165553	-0.582177	-0.384417
10	8	0	2.294517	-0.176283	0.060563
11	1	0	3.165534	0.084984	0.390690
12	1	0	1.358192	0.343131	0.762801
13	8	0	0.151718	0.396611	0.943427
14	1	0	-0.008653	1.172949	1.499513

B3lYP/6-31+G* energy: - 378.005611 Hartree
Zero-point vibrational energy: 0.109005 Hartree
Thermal correction to Gibbs free energy: 0.077424 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1209941 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2226383 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.1574688 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.2552684 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.0072618 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.0935134 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.2622344 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.3582982 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.1979265 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.5284171 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.636741 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.6985275 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.15704 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.269324 Hartree
Solvent shift(FPCM/0.001 au contour): -0.027435262 Hartree

INT-b in Figure 2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.677301	-0.215208	0.015563
2	1	0	1.676044	-0.249680	-1.712813
3	7	0	1.819861	-0.048453	-0.730009
4	1	0	2.301094	0.829222	-0.574608
5	8	0	-0.113769	-1.179507	-0.374845
6	7	0	0.861745	0.101422	1.386679
7	1	0	1.692503	-0.362219	1.748483
8	1	0	0.051180	-0.176630	1.933475
9	1	0	-1.187133	-0.927848	-0.131905
10	8	0	-2.257618	-0.183001	0.103267
11	1	0	-2.947420	-0.301018	-0.567238
12	1	0	-1.530697	0.726218	-0.176185
13	8	0	-0.455444	1.291081	-0.413755
14	1	0	-0.275969	1.953835	0.273383

B3lYP/6-31+G* energy: - 378.032094 Hartree
Zero-point vibrational energy: 0.116423 Hartree
Thermal correction to Gibbs free energy: 0.084145 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.151393 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2543431 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.1891316 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.2855477 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.0500814 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.133643 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.303883 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.3986501 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.2356821 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.566239 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.6752803 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.737549 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.20095 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.3105666 Hartree
Solvent shift(FPCM/0.001 au contour): -0.026951084 Hartree

TS2-b in Figure 2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.570314	-0.119743	-0.005851
2	1	0	1.722359	-1.769904	0.273624
3	7	0	1.667422	-0.975923	-0.358459
4	1	0	1.536980	-1.302629	-1.311353
5	8	0	-0.137160	-0.634486	1.077547
6	7	0	1.116332	1.311886	0.375273
7	1	0	2.127493	1.392191	0.270286
8	1	0	0.812484	1.634793	1.294078
9	1	0	-1.099774	-0.468296	0.926808
10	8	0	-2.604091	0.032659	0.009552
11	1	0	-3.202635	-0.644926	-0.337668
12	1	0	-1.918288	0.197010	-0.686004
13	8	0	-0.165970	0.336583	-1.072935
14	1	0	0.370982	1.450435	-0.625672

B3lYP/6-31+G* energy: - 377.990490 Hartree
Zero-point vibrational energy: 0.111123 Hartree
Thermal correction to Gibbs free energy: 0.079019 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1052605 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2063285 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.1419317 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.2371175 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -376.9992308 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.082729 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.2521504 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.3469139 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.1869467 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.5177153 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.6266403 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.688824 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.1472 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.2593469 Hartree
Solvent shift(FPCM/0.001 au contour): -0.024781003 Hartree

PC-b in Figure 2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.466185	-0.057305	-0.080965
2	1	0	-2.918884	-1.393254	0.498693
3	7	0	-2.665345	-0.686837	-0.176722
4	1	0	-3.132486	-0.675342	-1.070860

5	8	0	-0.859562	-0.305209	1.093955
6	7	0	3.521445	-1.002132	-0.304001
7	1	0	4.186156	-1.084908	0.462834
8	1	0	2.892098	-0.227366	-0.091614
9	1	0	0.006216	0.174137	1.097235
10	8	0	1.315659	1.220482	0.345036
11	1	0	1.467422	2.129526	0.644993
12	1	0	0.657203	1.269581	-0.389410
13	8	0	-1.006291	0.676047	-0.959126
14	1	0	4.048242	-0.756326	-1.139952

B3lYP/6-31+G* energy: -378.077965 Hartree
Zero-point vibrational energy: 0.112921 Hartree
Thermal correction to Gibbs free energy: 0.073921 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1851004 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2900295 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.2219705 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.3235514 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.0765602 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.1579954 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.3276847 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.4247474 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.2591867 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.5913766 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.7007441 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.7631784 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.2237375 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.3328632 Hartree
Solvent shift(FPCM/0.001 au contour): -0.020270045 Hartree

RC-c1 in Figure 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.898218	0.012927	0.026817
2	1	0	0.744232	2.020014	0.054883
3	7	0	0.281789	1.186712	0.394522
4	1	0	-0.735596	1.210767	0.388058
5	8	0	1.998623	-0.053475	-0.504175
6	7	0	0.130332	-1.137319	0.307887
7	1	0	-0.358287	-1.116422	1.199371

8	1	0	0.690604	-1.977109	0.203370
9	1	0	-1.824693	-0.639936	-0.476108
10	8	0	-2.457497	0.047065	-0.190226
11	1	0	-3.119414	0.130659	-0.892129

B3lYP/6-31+G* energy: -301.654297 Hartree
Zero-point vibrational energy: 0.088628 Hartree
Thermal correction to Gibbs free energy: 0.057575 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -301.7362315 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -301.8178901 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -301.7649692 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.8437875 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -300.852119 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -300.9125851 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -301.0427357 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -301.1173616 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -300.987895 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.2504068 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -301.337245 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -301.3868619 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -300.966275 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -301.0474908 Hartree
Solvent shift(FPCM/0.001 au contour): -0.027576942 Hartree

TS-c1 in Figure 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.405378	0.091578	0.107211
2	1	0	1.702781	-1.355189	-0.273586
3	7	0	0.955553	-0.863765	-0.757509
4	1	0	0.248593	-1.530559	-1.059149
5	8	0	0.935116	0.556610	1.095335
6	7	0	-0.527980	1.066465	-0.701134
7	1	0	-0.351277	1.070813	-1.707250
8	1	0	-0.441678	2.003035	-0.304578
9	1	0	-1.425990	0.526495	-0.372806
10	8	0	-1.382412	-0.785702	0.397134
11	1	0	-1.579340	-0.850231	1.344852

B3lYP/6-31+G* energy: -301.574547 Hartree

Zero-point vibrational energy: 0.086627 Hartree
Thermal correction to Gibbs free energy: 0.058104 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -301.6554513 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -301.7359617 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -301.6841692 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.7595877 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -300.771378 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -300.8299214 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -300.9579854 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -301.0338826 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -300.9081129 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.1689693 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -301.2551139 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -301.3043184 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -300.8813739 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -300.9656492 Hartree
Solvent shift(FPCM/0.001 au contour): -0.035037769 Hartree

PC-c1 in Figure 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.748958	0.092821	0.000225
2	1	0	-2.708245	0.642460	-0.117263
3	7	0	-2.095629	-0.141790	0.048535
4	1	0	-2.444818	-1.072458	-0.128586
5	8	0	-0.255519	1.218019	-0.007613
6	7	0	2.500496	-0.041398	0.001900
7	1	0	3.086146	-0.137202	0.829559
8	1	0	2.092244	0.895625	0.004392
9	1	0	3.099828	-0.127310	-0.816975
10	8	0	-0.044816	-1.050724	-0.007120
11	1	0	0.937205	-0.814085	-0.007658

B3lYP/6-31+G* energy: -301.668719 Hartree
Zero-point vibrational energy: 0.089051 Hartree
Thermal correction to Gibbs free energy: 0.058080 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -301.748995 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -301.829324 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -301.7755627 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.8556622 Hartree

MP2/6-31+G* //B3LYP/6-31+G* energy: -300.86356 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -300.9218392 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -301.0504848 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -301.125603 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -300.995489 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -301.2596046 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -301.3463023 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -301.3957669 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -300.9757973 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -301.0555723 Hartree
Solvent shift(FPCM/0.001 au contour): -0.020368766 Hartree

RC-c2 in Figure 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.362125	0.028607	0.035281
2	1	0	-1.433355	1.634743	-1.193316
3	7	0	-0.901609	1.222927	-0.439813
4	1	0	0.081133	1.473881	-0.341108
5	8	0	-2.444384	-0.466504	-0.253136
6	7	0	-0.453743	-0.633020	0.898763
7	1	0	-0.945610	-1.301791	1.483280
8	1	0	0.148378	-0.014698	1.439718
9	1	0	1.030939	-1.397617	-0.169138
10	8	0	1.911326	-1.351906	-0.610919
11	1	0	2.376262	-2.175389	-0.403155
12	1	0	2.245381	0.366226	-0.072117
13	8	0	1.963993	1.227771	0.314509
14	1	0	2.709604	1.838758	0.227869

B3lYP/6-31+G* energy: -378.074553 Hartree
Zero-point vibrational energy: 0.114039 Hartree
Thermal correction to Gibbs free energy: 0.079295 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1888441 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2940962 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.2253382 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.3250894 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.082916 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.1656207 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.3361021 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.4310027 Hartree

MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.2667973 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.5970224 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.7063768 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.76887 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.2299549 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.3390106 Hartree
Solvent shift(FPCM/0.001 au contour): -0.031683881 Hartree

TS-c2 in Figure 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.935689	0.154869	-0.003727
2	1	0	0.976729	1.657898	-1.309346
3	7	0	0.476993	1.364170	-0.477220
4	1	0	-0.535927	1.450546	-0.556420
5	8	0	2.043693	-0.311245	-0.139163
6	7	0	0.169916	-0.214708	1.298137
7	1	0	0.639411	0.188202	2.113657
8	1	0	0.187934	-1.238740	1.313853
9	1	0	-0.831963	0.080139	1.226883
10	8	0	-2.197202	0.370517	0.073206
11	1	0	-3.143036	0.173728	0.124058
12	1	0	-1.697137	-0.396053	-0.463495
13	8	0	-0.527800	-1.235589	-0.748888
14	1	0	-0.288029	-1.480634	-1.654490

B3lYP/6-31+G* energy: -378.0019387 Hartree
Zero-point vibrational energy: 0.113815 Hartree
Thermal correction to Gibbs free energy: 0.082689 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1173079 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2216737 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.1530715 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.2499303 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.014833 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.0947651 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.2626508 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.3592754 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.1980749 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.5267928 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.63534 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.6973395 Hartree

CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -377.1566416 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.2680172 Hartree
Solvent shift(FPCM/0.001 au contour): -0.038507256 Hartree

PC-c2 in Figure 3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.050970	0.798842	0.014776
2	1	0	1.284842	2.324515	-0.082976
3	7	0	1.198199	1.327901	0.043837
4	1	0	2.017623	0.729551	-0.025424
5	8	0	-1.088926	1.454164	-0.030312
6	7	0	-2.699289	-1.091018	-0.011040
7	1	0	-2.862865	-0.082214	-0.041000
8	1	0	-3.181715	-1.469285	0.802247
9	1	0	-3.115126	-1.506725	-0.842726
10	8	0	2.716007	-1.208095	-0.122433
11	1	0	3.133134	-1.678095	0.614257
12	1	0	1.755778	-1.374251	-0.044099
13	8	0	-0.030767	-0.559190	0.060375
14	1	0	-0.988740	-0.889761	0.040440

B3lYP/6-31+G* energy: -378.083800 Hartree
Zero-point vibrational energy: 0.113741 Hartree
Thermal correction to Gibbs free energy: 0.078187 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -378.1949582 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -378.2993241 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -378.2303657 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -378.3313517 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -377.087948 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -377.1687031 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -377.3378245 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -377.4340595 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -377.2692091 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -377.6010137 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -377.7102787 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -377.7726563 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: - -377.2337376 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -377.3422703 Hartree
Solvent shift(FPCM/0.001 au contour): -0.024507031 Hartree

$Me_4U(H_2O)$ of SR-d in Figure 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.090595	-0.113889	-0.243522
2	8	0	-0.893542	-0.764487	-0.627441
3	7	0	1.326953	-0.718340	-0.068321
4	8	0	-3.455640	-1.041611	0.551349
5	1	0	-2.594926	-1.025181	0.084482
6	1	0	-4.014820	-1.648680	0.045857
7	7	0	0.015473	1.241651	0.017004
8	6	0	2.197133	-0.384216	1.058432
9	1	0	3.236863	-0.261726	0.728536
10	1	0	1.867506	0.535061	1.541956
11	1	0	2.166713	-1.189817	1.807100
12	6	0	1.446210	-2.099467	-0.525798
13	1	0	1.049992	-2.810895	0.214003
14	1	0	0.894150	-2.229840	-1.456794
15	1	0	2.505522	-2.319867	-0.697234
16	6	0	-1.314266	1.848743	0.016681
17	1	0	-2.039851	1.182224	0.482640
18	1	0	-1.267686	2.780834	0.589807
19	1	0	-1.655800	2.076833	-1.003783
20	6	0	1.099471	2.161127	-0.323180
21	1	0	1.347916	2.812764	0.524790
22	1	0	1.991748	1.611459	-0.623218
23	1	0	0.794286	2.798644	-1.165874

B3lYP/6-31+G* energy: -458.777147 Hartree
Zero-point vibrational energy: 0.200505 Hartree
Thermal correction to Gibbs free energy: 0.161277 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -458.965217 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -459.072682 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -458.9896271 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -459.1135268 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -457.486515 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -457.6057153 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -457.780636 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -457.8960512 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -457.6938239 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -458.1071502 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -458.2381285 Hartree

MP2/CBS //B3LYP/6-31+G(d) energy: -458.3123583 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -457.7293943 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -457.8284386 Hartree
Solvent shift (FPCM/0.001 au contour): -0.018773258 Hartree

$OH^-(H_2O)_3$ of SR-d in Figure 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.001590	-0.001083	0.735230
2	1	0	-0.002094	-0.003006	1.703932
3	8	0	1.616780	-1.855569	-0.244956
4	1	0	1.046296	-1.123472	0.177749
5	1	0	0.965452	-2.367795	-0.746417
6	8	0	-2.419773	-0.467475	-0.245370
7	1	0	-2.529925	0.352598	-0.748788
8	1	0	-1.499592	-0.346678	0.176335
9	8	0	0.804171	2.325149	-0.244374
10	1	0	1.571457	2.012932	-0.746324
11	1	0	0.451709	1.467239	0.179276

B3lYP/6-31+G* energy: -305.136485 Hartree
Zero-point vibrational energy: 0.082737 Hartree
Thermal correction to Gibbs free energy: 0.046521 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -305.2232863 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -305.3178539 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -305.2585016 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -305.3408226 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -304.335055 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -304.4179181 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -304.5780106 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -304.6640567 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -304.5277586 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -304.7972153 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -304.8876915 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -304.9395266 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -304.4565969 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -304.5745667 Hartree
Solvent shift (FPCM/0.001 au contour): -0.102735477 Hartree

TS1-d in Figure 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.142586	-0.620993	0.396868
2	8	0	1.118437	-0.737031	0.526276
3	7	0	-0.844530	-0.092273	1.509912
4	8	0	-0.388845	0.835994	-0.864886
5	1	0	0.118957	0.469828	-1.607475
6	8	0	3.115901	0.994737	0.256525
7	1	0	3.559305	1.002463	1.117026
8	1	0	2.299662	0.429327	0.395122
9	8	0	3.169378	-1.663039	-1.221335
10	1	0	3.582701	-0.800235	-1.042482
11	1	0	2.325468	-1.572505	-0.725925
12	8	0	-2.414966	2.244218	-1.786090
13	1	0	-1.649405	1.672523	-1.451376
14	1	0	-2.040210	3.137348	-1.802322
15	8	0	1.157434	3.096267	-0.430513
16	1	0	0.543167	2.329002	-0.581185
17	1	0	1.995656	2.641549	-0.223411
18	7	0	-0.768545	-1.672193	-0.364841
19	6	0	-0.410414	-3.025537	0.013964
20	1	0	-0.356284	-3.665290	-0.879989
21	1	0	0.566945	-3.027948	0.498306
22	1	0	-1.151215	-3.479073	0.704343
23	6	0	-2.016288	-1.575691	-1.091174
24	1	0	-2.244077	-0.535462	-1.315231
25	1	0	-1.918721	-2.119226	-2.045415
26	1	0	-2.871250	-2.030272	-0.551779
27	6	0	-0.122157	0.924780	2.271280
28	1	0	-0.647270	1.083490	3.221618
29	1	0	0.886292	0.567901	2.484561
30	1	0	-0.052698	1.882646	1.734740
31	6	0	-2.269845	0.196631	1.409006
32	1	0	-2.488381	1.041620	0.739394
33	1	0	-2.818142	-0.679887	1.063666
34	1	0	-2.639948	0.439164	2.412850

B3lYP/6-31+G* energy: -763.870157 Hartree
Zero-point vibrational energy: 0.287434 Hartree
Thermal correction to Gibbs free energy: 0.234299 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -764.1693078 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -764.370761 Hartree

B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -764.2290198 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -764.430983 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -761.8203705 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -762.0205068 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -762.353967 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -762.5535801 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -762.2198783 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -762.8985195 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -763.1178537 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -763.242628 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -762.185871 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -762.403999 Hartree
Solvent shift(FPCM/0.001 au contour): -0.0929143 Hartree

INT-d in Figure 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.259589	-0.300312	-0.227654
2	8	0	0.992016	-0.664100	-0.145735
3	7	0	-0.881182	0.153984	1.099810
4	8	0	-0.363109	0.903978	-1.095467
5	1	0	-1.260222	1.272637	-1.002759
6	8	0	2.870359	-2.053339	1.321636
7	1	0	2.043807	-1.749096	0.873648
8	1	0	3.468345	-1.309630	1.138616
9	8	0	3.249346	0.665222	-0.387588
10	1	0	2.338290	0.232296	-0.306178
11	1	0	3.595349	0.320933	-1.224233
12	8	0	-2.947224	1.976074	0.606162
13	1	0	-2.518682	2.812784	0.840479
14	1	0	-2.276833	1.269658	0.856088
15	8	0	1.691992	2.955956	-1.228825
16	1	0	2.410691	2.379594	-0.895419
17	1	0	0.943914	2.324678	-1.279259
18	7	0	-1.126414	-1.377717	-0.767464
19	6	0	-1.129914	-0.968681	2.014818
20	1	0	-1.841073	-1.668491	1.573830
21	1	0	-0.203889	-1.516675	2.251536
22	1	0	-1.549429	-0.571287	2.948444
23	6	0	-0.499593	-2.128535	-1.845621
24	1	0	-0.450124	-1.556310	-2.793384

25	1	0	0.513970	-2.403685	-1.554153
26	1	0	-1.085699	-3.040254	-2.028703
27	6	0	-2.491804	-1.014807	-1.114018
28	1	0	-2.970776	-0.458833	-0.305361
29	1	0	-2.561491	-0.405143	-2.036999
30	1	0	-3.073333	-1.932349	-1.282303
31	6	0	0.021513	1.112860	1.761260
32	1	0	0.963315	0.640649	2.075325
33	1	0	0.261216	1.933875	1.082152
34	1	0	-0.484895	1.517309	2.648030

B3lYP/6-31+G* energy: -763.881257 Hartree
Zero-point vibrational energy: 0.289453 Hartree
Thermal correction to Gibbs free energy: 0.237493 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -764.183611 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -764.383749 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -764.2436195 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -764.4447349 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -761.8441533 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -762.0439901 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -762.378719 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -762.5763917 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -762.2437534 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -762.9222924 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -763.1412111 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -763.2657068 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -762.2097447 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -762.4281285 Hartree
Solvent shift(FPCM/0.001 au contour): -0.090332011 Hartree

TS2-d in Figure 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.322945	-0.202620	-0.283919
2	8	0	0.869751	-0.705459	-0.249040
3	7	0	-0.812780	0.214550	1.245353
4	8	0	-0.389674	1.055264	-0.960038
5	1	0	-1.192835	1.565050	-0.629942
6	8	0	2.746040	-2.221568	1.129958
7	1	0	1.914024	-1.880647	0.727485
8	1	0	3.389509	-1.563138	0.815941

9	8	0	3.265807	0.317397	-0.651506
10	1	0	2.312650	0.009455	-0.530222
11	1	0	3.491550	0.044996	-1.553114
12	8	0	-2.432748	2.008280	0.515351
13	1	0	-2.272459	2.880620	0.905773
14	1	0	-1.626221	1.021265	1.079716
15	8	0	1.905377	2.860208	-1.026313
16	1	0	2.576344	2.168338	-0.858138
17	1	0	1.078898	2.335152	-1.080021
18	7	0	-1.345325	-1.152969	-0.761690
19	6	0	-1.298983	-0.926325	2.036539
20	1	0	-2.209406	-1.324050	1.589037
21	1	0	-0.539655	-1.715848	2.062969
22	1	0	-1.508248	-0.589258	3.059623
23	6	0	-0.839783	-2.112925	-1.733481
24	1	0	-0.648201	-1.657534	-2.725558
25	1	0	0.088697	-2.555183	-1.372724
26	1	0	-1.590829	-2.904134	-1.865950
27	6	0	-2.622809	-0.592800	-1.193999
28	1	0	-2.990667	0.161670	-0.495292
29	1	0	-2.559572	-0.117117	-2.190391
30	1	0	-3.359670	-1.406890	-1.252755
31	6	0	0.303543	0.896540	1.933298
32	1	0	1.122082	0.195823	2.117202
33	1	0	0.664076	1.714916	1.308408
34	1	0	-0.063884	1.301247	2.884389

B3lYP/6-31+G* energy: -763.869555 Hartree
Zero-point vibrational energy: 0.287690 Hartree
Thermal correction to Gibbs free energy: 0.238130 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -764.172319 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -764.371606 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -764.2315009 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -764.4303473 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -761.8317082 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -762.0313066 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -762.363784 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -762.5630893 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -762.231568 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -762.9101033 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -763.128679 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -763.2529437 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -762.1946108 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -762.4136298 Hartree

Solvent shift(FPCM/0.001 au contour): -0.091913764 Hartree

PC-d in Figure 5:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.780822	-0.579193	-0.471691
2	8	0	2.339680	0.436852	0.060624
3	7	0	-4.258630	-0.602294	0.751576
4	8	0	0.869637	-0.550201	-1.351613
5	1	0	-1.111061	-0.615373	-1.120336
6	8	0	2.932705	2.148470	2.284345
7	1	0	2.839815	1.344589	1.732928
8	1	0	2.459955	2.804477	1.741520
9	8	0	1.625748	2.976386	-0.345495
10	1	0	1.849876	1.998335	-0.269678
11	1	0	2.318002	3.340198	-0.917061
12	8	0	-1.993934	-0.201528	-1.212845
13	1	0	-1.745443	0.686055	-1.548226
14	1	0	-3.464780	-0.528019	0.107639
15	8	0	-0.270552	1.849163	-2.236178
16	1	0	0.128116	2.477009	-1.600940
17	1	0	0.250723	1.026530	-2.064534
18	7	0	2.249072	-1.841449	-0.067354
19	6	0	-5.478822	-0.236076	0.051583
20	1	0	-5.572534	-0.838024	-0.859230
21	1	0	-6.353432	-0.441963	0.686510
22	1	0	-5.524785	0.834328	-0.240220
23	6	0	3.131081	-1.968175	1.075039
24	1	0	3.798873	-2.829735	0.931122
25	1	0	3.730961	-1.063676	1.172745
26	1	0	2.576300	-2.123909	2.017950
27	6	0	1.523677	-3.037985	-0.444048
28	1	0	0.962134	-2.840517	-1.356968
29	1	0	2.229420	-3.863035	-0.620056
30	1	0	0.816078	-3.359799	0.341363
31	6	0	-4.010220	0.233727	1.916107
32	1	0	-4.783264	0.055615	2.678235
33	1	0	-3.039122	-0.024484	2.351719

34	1	0	-4.004434	1.320665	1.693310

B3lYP/6-31+G* energy: -763.953545 Hartree
Zero-point vibrational energy: 0.289353 Hartree
Thermal correction to Gibbs free energy: 0.229808 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -764.244806 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -764.447696 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -764.3010912 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -764.50986 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -761.8823246 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -762.0789142 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -762.412637 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -762.6118317 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -762.2716537 Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -762.9560947 Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -763.1777898 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -763.3039604 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -762.2454714 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -762.4577975Hartree
Solvent shift(FPCM/0.001 au contour): -0.082351784 Hartree

RC-e in Figure 6:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.267488	0.310694	-0.122376
2	7	0	-1.241052	-1.049933	0.073220
3	8	0	-2.230929	0.879411	-0.634752
4	7	0	-0.120277	1.050404	0.298273
5	1	0	1.424516	0.781229	-0.842068
6	8	0	2.298327	0.719523	-1.298936
7	1	0	2.103723	0.561146	-2.234873
8	1	0	3.174031	-0.614234	-0.376328
9	8	0	3.381605	-1.363445	0.223584
10	1	0	4.312418	-1.263537	0.469184
11	6	0	-2.465918	-1.781536	-0.237078
12	1	0	-2.500336	-2.684244	0.382198
13	1	0	-3.333801	-1.157316	-0.025143
14	1	0	-2.502348	-2.078000	-1.295652
15	6	0	-0.037197	-1.878440	0.125531
16	1	0	-0.005672	-2.536876	-0.753804
17	1	0	0.873030	-1.284896	0.129330
18	1	0	-0.041244	-2.510570	1.022545

19	6	0	-0.238777	2.488050	-0.007615
20	1	0	-1.013278	2.971549	0.602666
21	1	0	0.728580	2.958298	0.191478
22	1	0	-0.498851	2.625462	-1.057595
23	6	0	0.323066	0.848915	1.693485
24	1	0	1.318723	1.285313	1.815500
25	1	0	-0.367519	1.341186	2.395220
26	1	0	0.383187	-0.207819	1.946035

B3lYP/6-31+G* energy: -535.188554 Hartree
Zero-point vibrational energy: 0.225887 Hartree
Thermal correction to Gibbs free energy: 0.181454 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -535.4076102 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -535.5385568 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -535.4404007 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -535.5843945 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -533.7108106 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -533.8525861 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -534.0682379 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -534.0222697 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -533.9676158Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -534.4471616Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -534.6001791 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -534.6870141 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -533.9872021 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -534.1151401 Hartree
Solvent shift(FPCM/0.001 au contour): -0.015876977 Hartree

TS-e in Figure 6:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.479395	-0.598034	-0.332527
2	7	0	1.427126	0.102613	0.381350
3	8	0	0.718974	-1.534935	-1.068543
4	7	0	-0.924701	-0.607046	0.354459
5	1	0	-1.281479	0.375422	0.438209
6	8	0	-1.839436	2.037676	0.208612
7	1	0	-2.740332	2.246553	-0.077772
8	1	0	-1.270913	1.850616	-0.657903
9	8	0	-0.430703	0.998429	-1.536729
10	1	0	0.154226	1.325955	-2.234959
11	6	0	2.796702	-0.072700	-0.105533

12	1	0	3.486604	0.231945	0.687238
13	1	0	2.967569	-1.118925	-0.358578
14	1	0	2.986864	0.542010	-0.998252
15	6	0	1.178634	1.427934	0.948624
16	1	0	1.299991	2.208525	0.187630
17	1	0	0.171329	1.526984	1.350751
18	1	0	1.895588	1.590439	1.760909
19	6	0	-1.900811	-1.305848	-0.537810
20	1	0	-1.614964	-2.353165	-0.629901
21	1	0	-2.891171	-1.207999	-0.085952
22	1	0	-1.853532	-0.806310	-1.504420
23	6	0	-0.864189	-1.237727	1.705102
24	1	0	-1.871127	-1.252874	2.129499
25	1	0	-0.486674	-2.257323	1.602035
26	1	0	-0.198014	-0.661921	2.346947

B3lYP/6-31+G* energy: -535.127862 Hartree
Zero-point vibrational energy: 0.226244 Hartree
Thermal correction to Gibbs free energy: 0.187873 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -535.3521202 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -535.482388 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -535.3848094 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -535.5269789 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -533.6623746 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -533.8024414 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -534.0154312 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -534.1514769 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -533.92005Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -534.3966379Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -534.548375 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -534.6344476 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -533.9348143 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -534.0655751 Hartree
Solvent shift(FPCM/0.001 au contour): -0.026446037 Hartree

PC-e in Figure 6:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.236317	0.288995	0.209325
2	7	0	-1.653861	-0.761008	-0.408801
3	8	0	-3.060066	0.248915	1.112757

4	7	0	2.531695	-0.294259	0.123389
5	1	0	2.146918	0.650466	0.160722
6	8	0	0.963096	2.389867	0.095227
7	1	0	1.123301	3.165711	-0.461643
8	1	0	0.045246	2.110872	-0.087706
9	8	0	-1.813394	1.513204	-0.293285
10	1	0	-2.355747	2.163248	0.188641
11	6	0	-1.900316	-2.103484	0.105763
12	1	0	-0.965658	-2.541442	0.478375
13	1	0	-2.625928	-2.049633	0.916669
14	1	0	-2.293872	-2.743256	-0.693721
15	6	0	-0.661626	-0.643699	-1.479024
16	1	0	-0.852833	-1.433508	-2.214590
17	1	0	-0.759175	0.320811	-1.976568
18	1	0	0.357174	-0.754082	-1.083451
19	6	0	2.881720	-0.734425	1.469774
20	1	0	3.160775	-1.796024	1.450877
21	1	0	3.726542	-0.173941	1.915072
22	1	0	2.014552	-0.624700	2.129774
23	6	0	3.668134	-0.323391	-0.789959
24	1	0	4.541413	0.257874	-0.434292
25	1	0	3.998543	-1.359855	-0.937333
26	1	0	3.367256	0.074489	-1.765813

B3lYP/6-31+G* energy: -535.195556 Hartree
Zero-point vibrational energy: 0.226233 Hartree
Thermal correction to Gibbs free energy: 0.178222 Hartree
B3lYP/6-31++G**//B3LYP/6-31+G* energy: -535.4086347 Hartree
B3lYP/6-311++G**//B3LYP/6-31+G* energy: -535.539609 Hartree
B3lYP/aug-cc-pVDZ//B3LYP/6-31+G* energy: -535.4405035 Hartree
B3lYP/ aug-cc-pVTZ //B3LYP/6-31+G* energy: -535.5869776 Hartree
MP2/6-31+G* //B3LYP/6-31+G* energy: -533.7033275 Hartree
MP2/6-31++G** //B3LYP/6-31+G* energy: -533.8433137 Hartree
MP2/6-311++G** //B3LYP/6-31+G* energy: -534.0585253 Hartree
MP2/6-311++G(2d,2p)//B3LYP/6-31+G* energy: -534.0149259 Hartree
MP2/aug-cc-pVDZ //B3LYP/6-31+G* energy: -533.9550502Hartree
MP2/aug-cc-pVTZ //B3LYP/6-31+G* energy: -534.4372105Hartree
MP2/aug-cc-pVQZ //B3LYP/6-31+G* energy: -534.5909248 Hartree
MP2/CBS //B3LYP/6-31+G(d) energy: -534.6781419 Hartree
CCSD(T)/6-31++G**// B3LYP /6-31+G* energy: -533.9800121 Hartree
CCSD(T)/aug-cc-pVDZ// B3LYP /6-31+G* energy: -534.1049951 Hartree
Solvent shift (FPCM/0.001 au contour): -0.018076818 Hartree

Table S1. Calculated Gibbs free energy barriers (in kcal/mol) for various reaction pathways of the hydrolysis of urea and Me_4U in both the gas phase and aqueous solution at 298.15 K.[a]

Theoretical level	Urea hydrolysis				Me_4U hydrolysis	
	Alkaline	APOE	One-water APNE	Two-water APNE	Alkaline	Two-water APNE
B3LYP/6-31+G*	46.4 (29.1)	59.1 (56.2)	45.4 (50.0)	41.3 (45.6)	46.2 (27.7)	31.5 (38.0)
B3LYP/6-31++G**	48.7 (31.3)	60.4 (55.9)	46.3 (51.0)	42.7 (47.0)	47.7 (29.2)	32.2 (38.8)
B3LYP/6-311++G**	50.8 (33.4)	63.0 (58.5)	47.1 (51.7)	43.3 (47.6)	49.4 (30.9)	32.6 (39.3)
B3LYP/aug-cc-pVDZ	49.9 (32.5)	60.7 (56.2)	46.4 (51.0)	43.2 (47.5)	48.0 (29.5)	32.3 (38.9)
B3LYP/aug-cc-pVTZ	52.4 (35.0)	63.8 (59.3)	48.5 (53.2)	45.0 (49.3)	52.6 (34.1)	33.4 (40.1)
MP2/6-31+G*	37.8 (20.4)	57.1 (54.2)	46.3 (50.9)	40.6 (44.8)	35.3 (17.4)	27.8 (34.4)
MP2/6-31++G**	39.8 (22.4)	58.3 (53.8)	47.5 (52.2)	42.3 (46.6)	36.5 (18.6)	28.9 (35.5)
MP2/6-311++G**	41.3 (23.9)	57.0 (54.1)	48.8 (53.5)	43.9 (48.2)	37.5 (19.6)	30.5 (37.2)
MP2/6-311++G(2d,2p)	41.5 (24.1)	57.8 (55.0)	48.0 (52.7)	42.9 (47.1)	38.6 (20.7)	30.2 (36.8)
MP2/aug-cc-pVDZ	38.7 (21.2)	56.6 (52.1)	45.7 (50.4)	41.0 (45.3)	35.6 (17.7)	27.2 (33.9)
MP2/aug-cc-pVTZ	39.5 (22.1)	56.7 (52.2)	46.8 (51.4)	41.9 (46.2)	38.2 (20.3)	29.1 (35.7)
MP2/aug-cc-pVQZ	40.7 (23.3)	57.0 (52.5)	47.2 (51.9)	42.4 (46.7)	39.6 (21.6)	29.9 (36.5)
MP2/CBS	41.5 (24.1)	57.3 (52.8)	47.4 (52.1)	42.7 (47.0)	40.4 (22.4)	30.4 (37.0)
CCSD(T)/6-31++G**	39.2 (21.8)	58.2 (53.7)	48.9 (53.6)	43.8 (48.1)	34.6 (16.7)	30.3 (36.9)
CCSD(T)/aug-cc-pVDZ	38.1 (20.7)	56.5 (52.0)	47.0 (51.7)	42.4 (46.7)	33.9 (16.0)	28.5 (35.1)
Best estimate[b]	40.9 (23.5)	57.2 (52.7)	48.7 (53.4)	44.1 (48.4)	38.7 (20.7)	31.7 (38.2)
Experimental value[c]	Uncertain				32.9	

[a]All energy calculations were performed by using the geometries optimized in the gas phase at the B3LYP/6-31+G* level. The obtained free energy barriers were based on the single-point energy calculations at various levels, plus the zero-point vibration and thermal corrections calculated at the B3LYP/6-31+G* level and the solvent shifts calculated at the

HF/6-31+G* level (using the default 0.001 a.u. contour). Values given in the parentheses are the Gibbs free energy barriers calculated in the gas phase.
[b]The best estimate was the extrapolated MP2/CBS value plus the shift from the MP2/aug-cc-pVDZ value to the corresponding CCSD(T)/aug-cc-pVDZ value.
[c]Experimental value from literature (B. P. Callahan, Y. Yuan and R. Wolfenden, *J. Am. Chem. Soc.*, 2005, 127, 10828).

Table S2. Imaginary vibrational frequencies for the rate-determining transition states, tunneling factor (transmission coefficient), and rate constants for urea and Me_4U hydrolysis at 298.15 K.

	Urea hydrolysis				Me_4U hydrolysis	
	Alkaline	APOE	One-water APNE	Two-water APNE	Alkaline	Two-water APNE
	TS2-a	TS2-b	TS-c1	TS-c2	TS1-d	TS-e
Imaginary frequency (i cm^{-1})	-460.93	-1679.52	-629.51	-239.08	-221.31	-189.54
g(tunneling factor) [a]	1.21	3.75	1.39	1.06	1.05	1.03
k(298.15K, s^{-1}) [b]	6.0×10^{-18}	1.9×10^{-29}	1.3×10^{-23}	2.3×10^{-20}	2.2×10^{-16}	3.0×10^{-11}

[a] $g = 1 - (ih\nu^{\neq}/RT)^2/24$, see references 1-2.
[b] $k=g(k_bT/h)\exp(\Delta S^{\neq}_m/R-\Delta H^{\neq}_m/RT)$, see references 1-2.

References

1. W. Si and S. Zhuo, Indian Journal of Chemistry, 2008, 47A, 560-564.
2. E. Wigner, Z. Phys. Chem. B., 1932, 19, 203.