Microsolvation of Histamine Monocation in Aqueous Solution: The Effect on Structure, Hydrogen Bonding Ability and Vibrational Spectrum

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Supplementary Information

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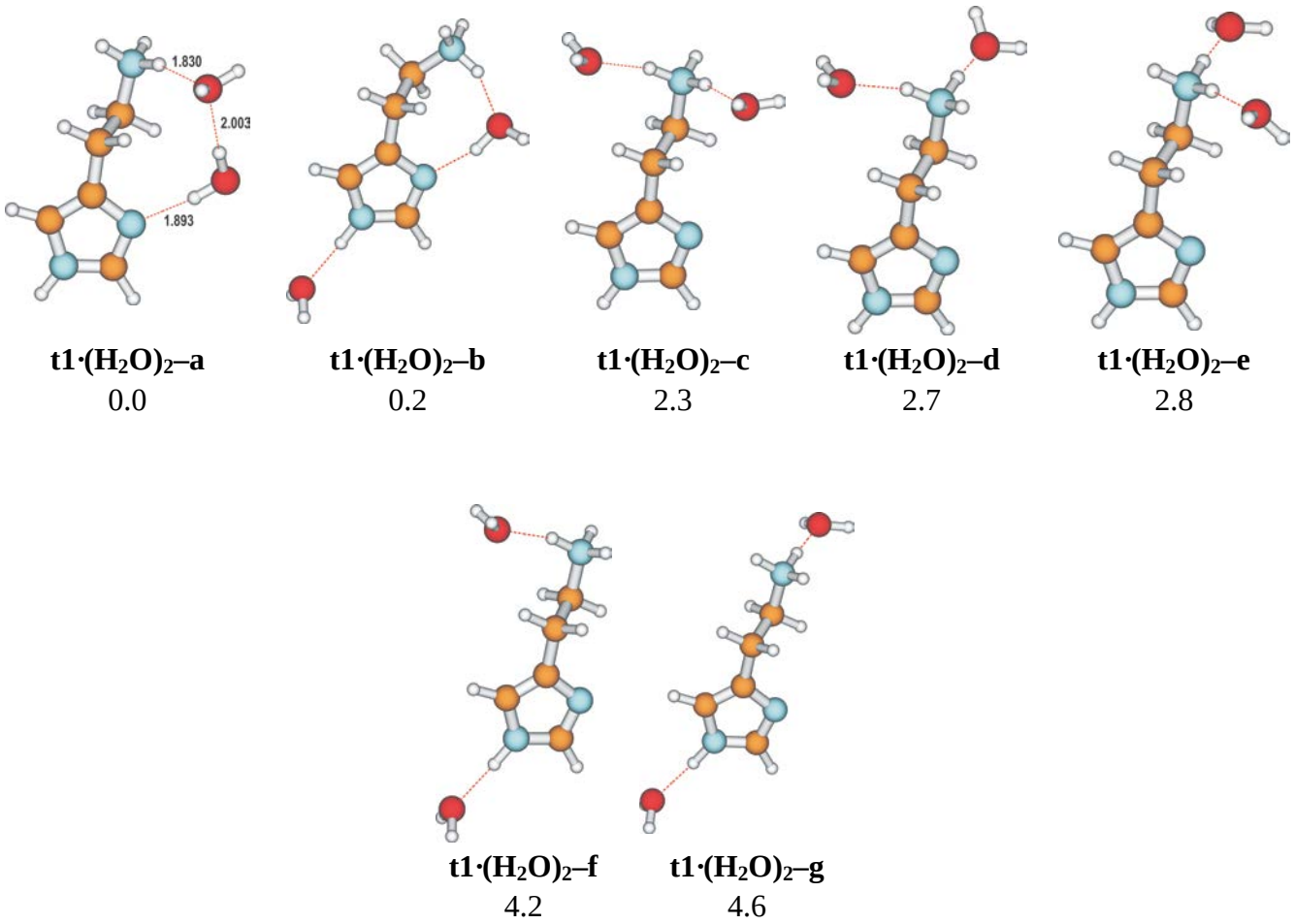
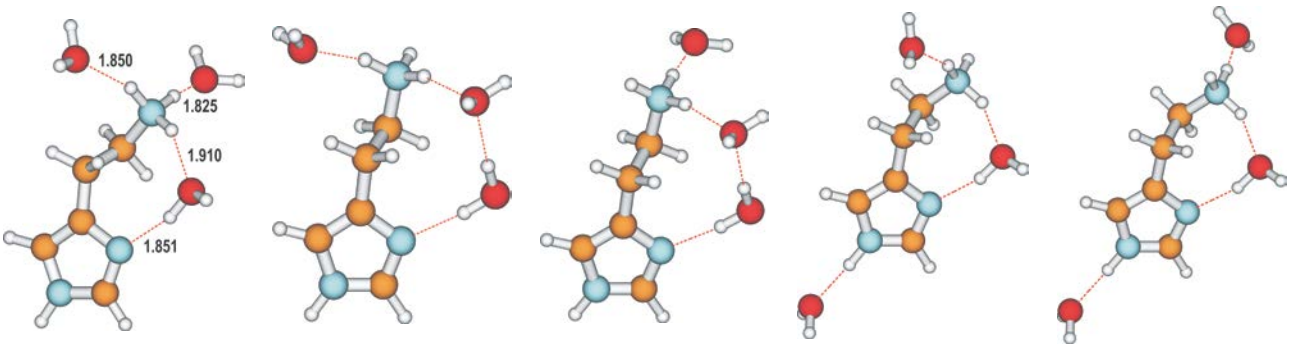


Figure S1. Investigated conformers of *trans* histamine explicitly solvated with 2 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



t1·(H$_2$O)$_3$–a	**t1·(H$_2$O)$_3$–b**	**t1·(H$_2$O)$_3$–c**	**t1·(H$_2$O)$_3$–d**	**t1·(H$_2$O)$_3$–e**
0.0	0.4	0.8	0.8	1.2

Figure S2. Investigated conformers of *trans* histamine explicitly solvated with 3 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.

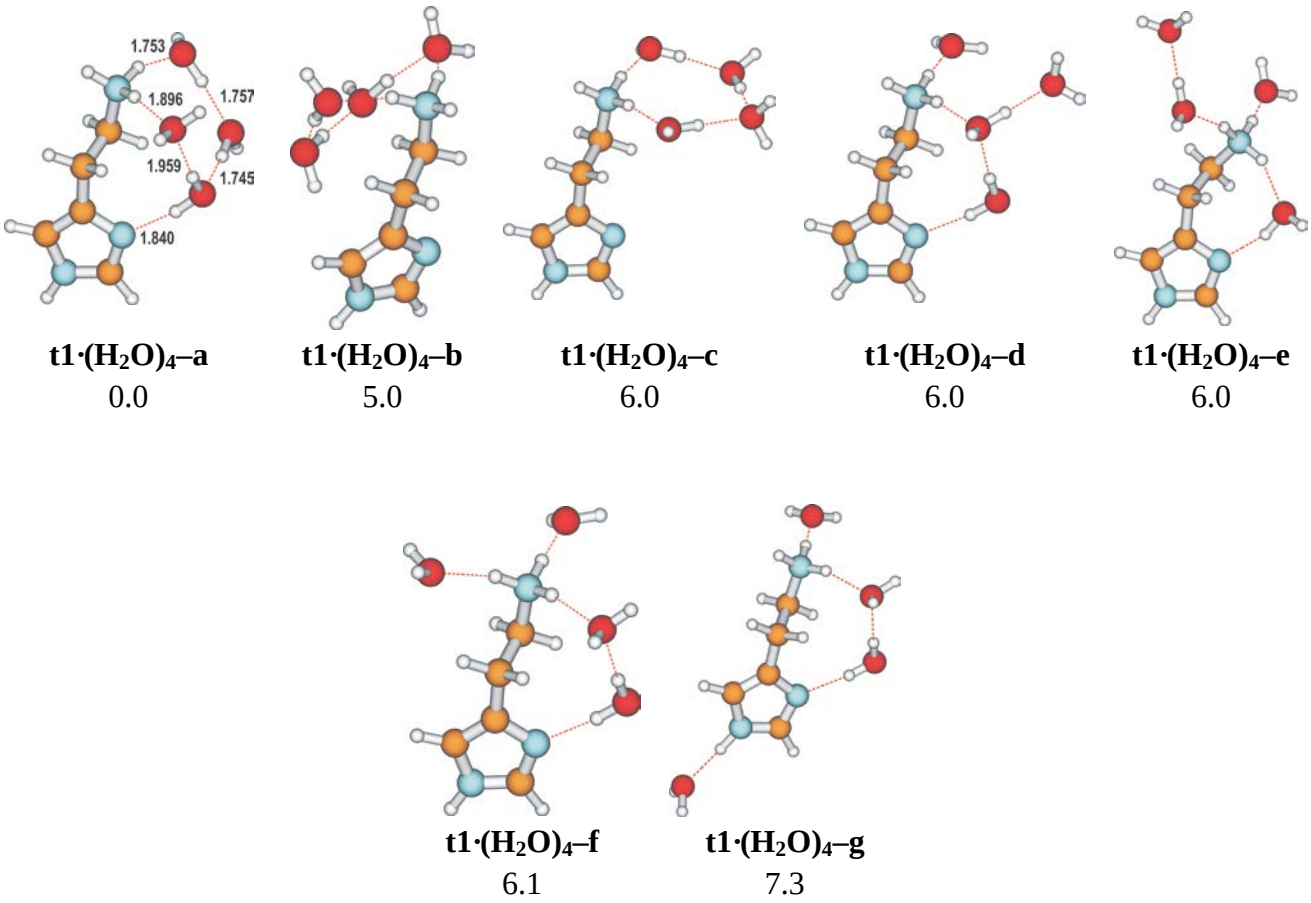
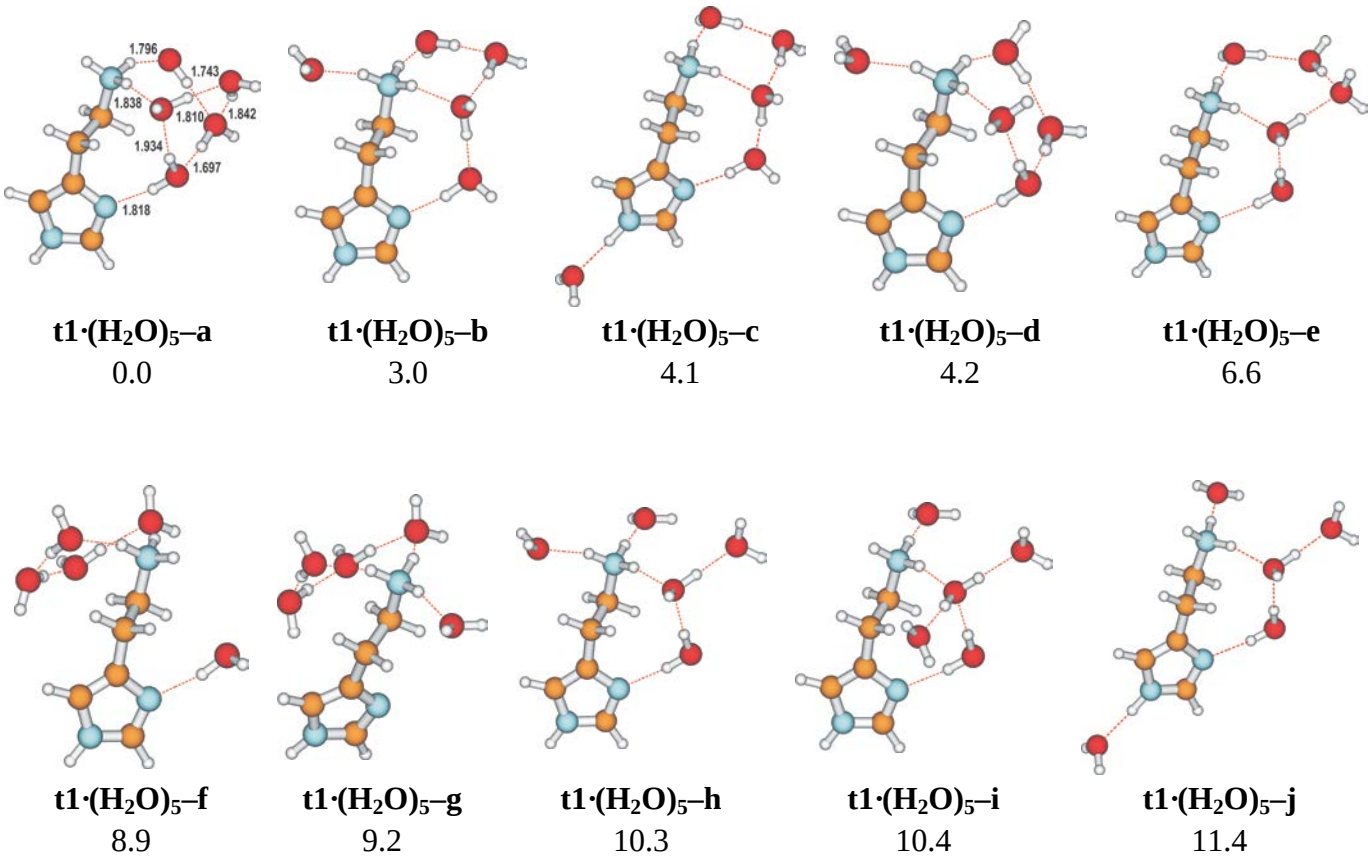


Figure S3. Investigated conformers of *trans* histamine explicitly solvated with 4 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



t1·(H$_2$O)$_5$–a
0.0

t1·(H$_2$O)$_5$–b
3.0

t1·(H$_2$O)$_5$–c
4.1

t1·(H$_2$O)$_5$–d
4.2

t1·(H$_2$O)$_5$–e
6.6

t1·(H$_2$O)$_5$–f
8.9

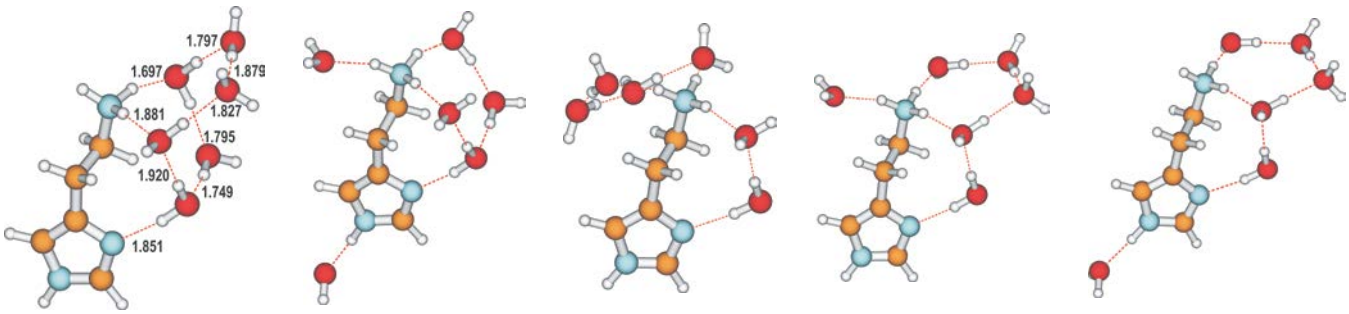
t1·(H$_2$O)$_5$–g
9.2

t1·(H$_2$O)$_5$–h
10.3

t1·(H$_2$O)$_5$–i
10.4

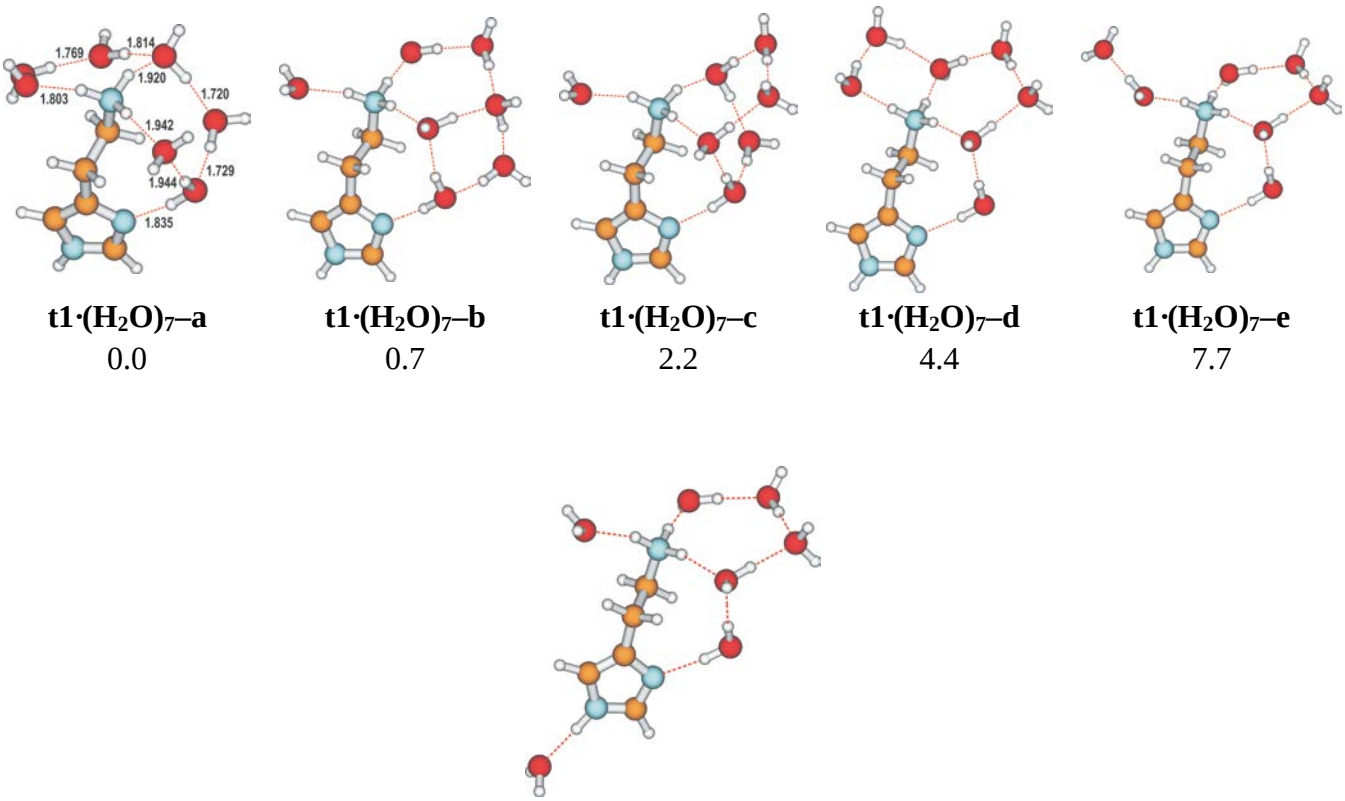
t1·(H$_2$O)$_5$–j
11.4

Figure S4. Investigated conformers of *trans* histamine explicitly solvated with 5 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



t1·(H$_2$O)$_6$–a	**t1·(H$_2$O)$_6$–b**	**t1·(H$_2$O)$_6$–c**	**t1·(H$_2$O)$_6$–d**	**t1·(H$_2$O)$_6$–e**
0.0	3.8	4.8	5.2	6.1

Figure S5. Investigated conformers of *trans* histamine explicitly solvated with 6 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



t1·(H$_2$O)$_7$–a
0.0

t1·(H$_2$O)$_7$–b
0.7

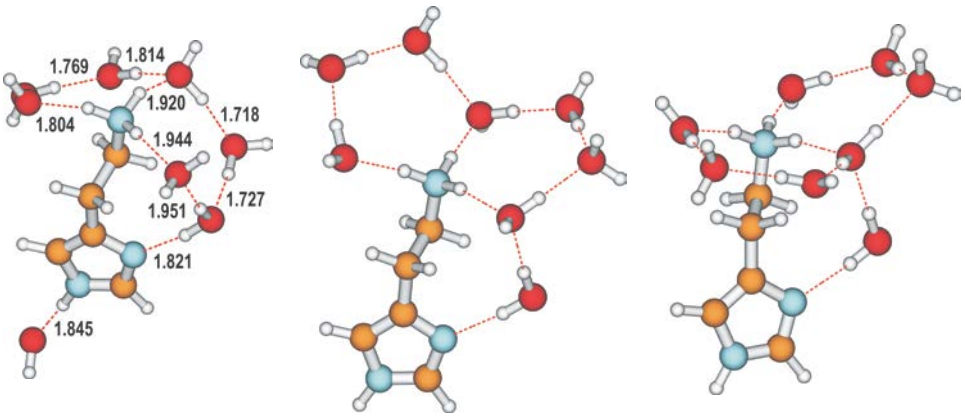
t1·(H$_2$O)$_7$–c
2.2

t1·(H$_2$O)$_7$–d
4.4

t1·(H$_2$O)$_7$–e
7.7

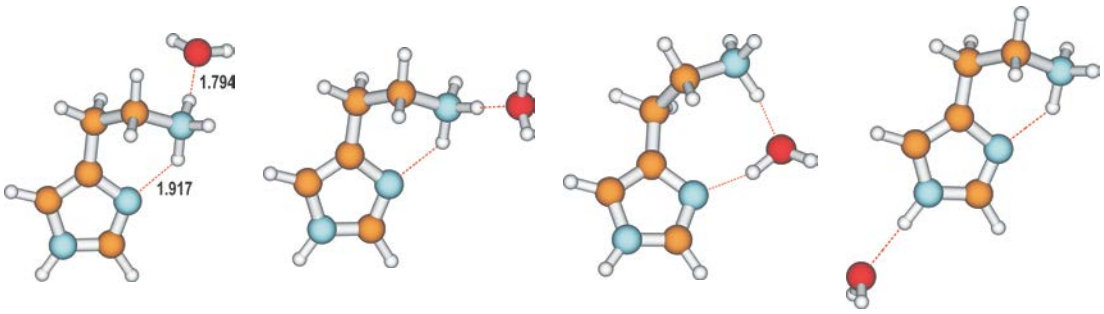
t1·(H$_2$O)$_7$–f
8.3

Figure S6. Investigated conformers of *trans* histamine explicitly solvated with 7 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



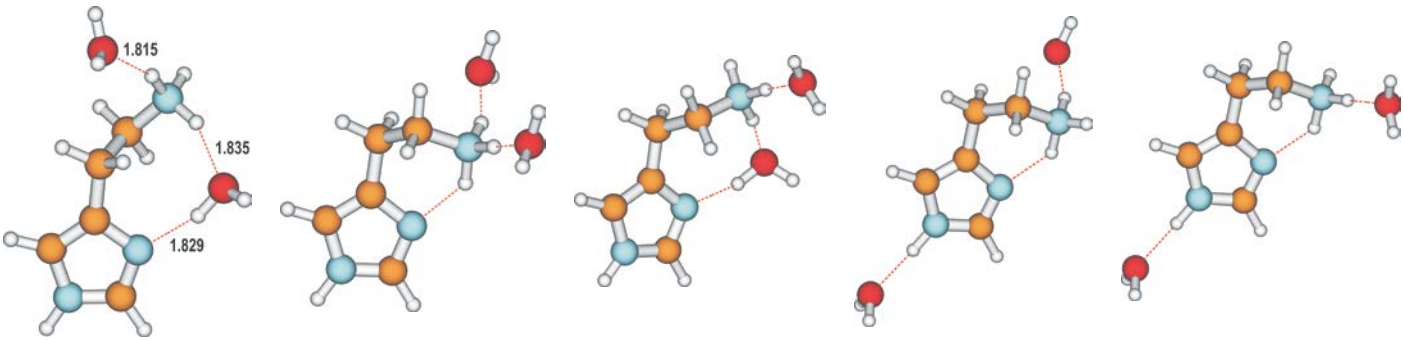
t1·(H$_2$O)$_8$–a 0.0 **t1·(H$_2$O)$_8$–b** 2.4 **t1·(H$_2$O)$_8$–c** 3.0

Figure S7. Investigated conformers of *trans* histamine explicitly solvated with 8 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



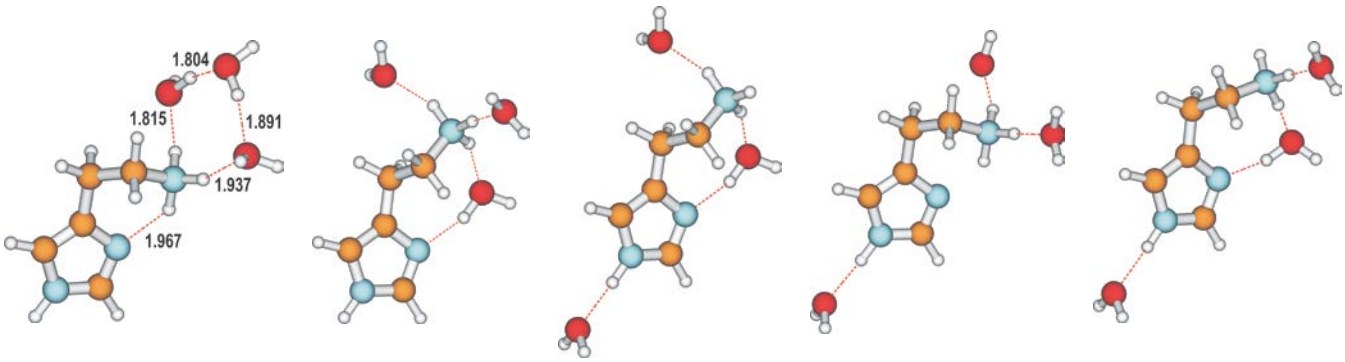
g1·(H$_2$O)$_1$–a	**g1·(H$_2$O)$_1$–b**	**g1·(H$_2$O)$_1$–c**	**g1·(H$_2$O)$_1$–d**
0.0	0.1	0.4	1.3

Figure S8. Investigated conformers of *gauche* histamine explicitly solvated with 1 water molecule. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



g1·(H$_2$O)$_2$–a	**g1·(H$_2$O)$_2$–b**	**g1·(H$_2$O)$_2$–c**	**g1·(H$_2$O)$_2$–d**	**g1·(H$_2$O)$_2$–e**
0.0	0.4	0.7	1.1	1.5

Figure S9. Investigated conformers of *gauche* histamine explicitly solvated with 2 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



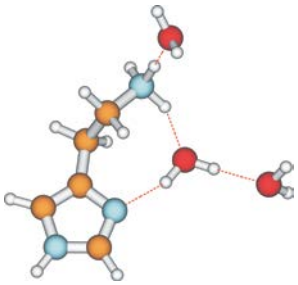
g1·$(H_2O)_3$–a
0.0

g1·$(H_2O)_3$–b
2.4

g1·$(H_2O)_3$–c
3.2

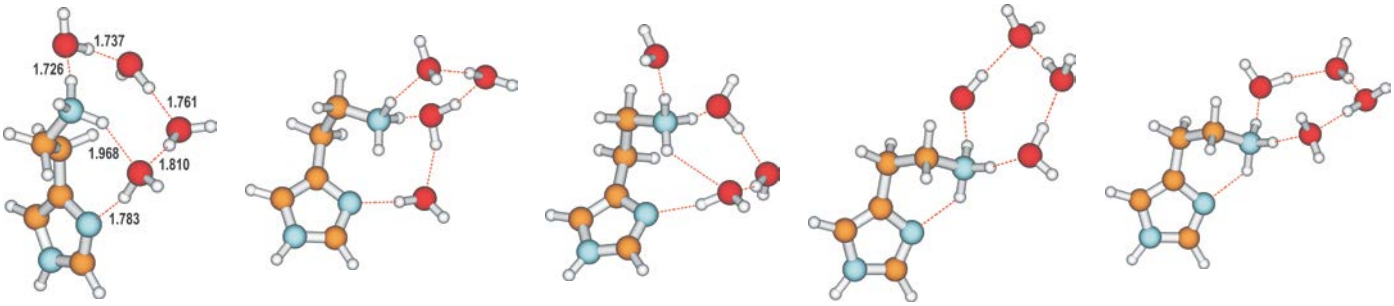
g1·$(H_2O)_3$–d
3.6

g1·$(H_2O)_3$–e
3.8



g1·$(H_2O)_3$–f
3.9

Figure S10. Investigated conformers of *gauche* histamine explicitly solvated with 3 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



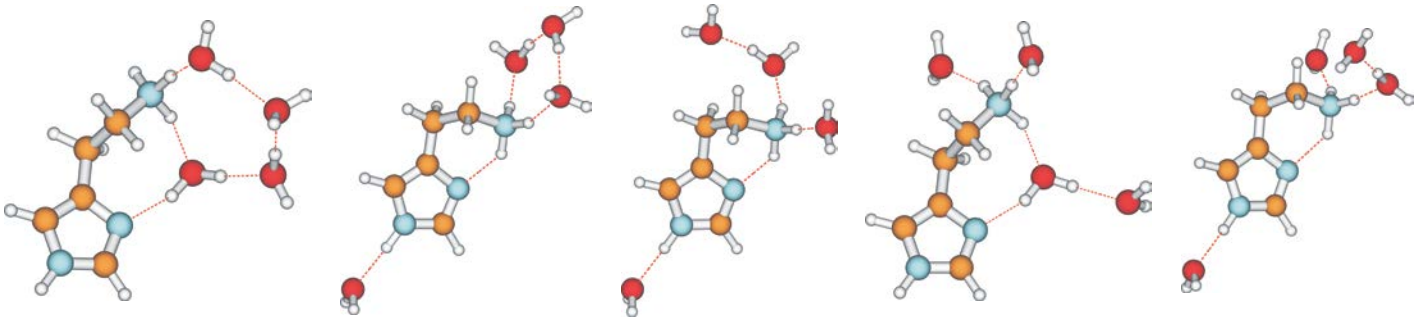
g1·(H$_2$O)$_4$–a
0.0

g1·(H$_2$O)$_4$–b
0.6

g1·(H$_2$O)$_4$–c
1.0

g1·(H$_2$O)$_4$–d
2.3

g1·(H$_2$O)$_4$–e
2.9



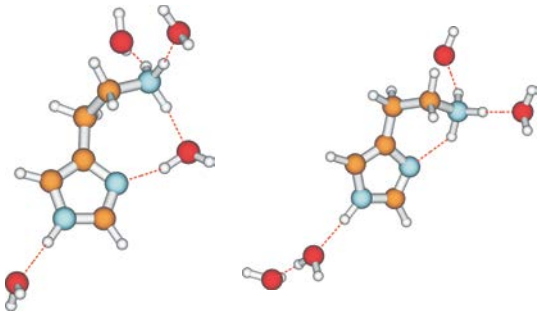
g1·(H$_2$O)$_4$–f
3.3

g1·(H$_2$O)$_4$–g
4.1

g1·(H$_2$O)$_4$–h
6.3

g1·(H$_2$O)$_4$–i
6.9

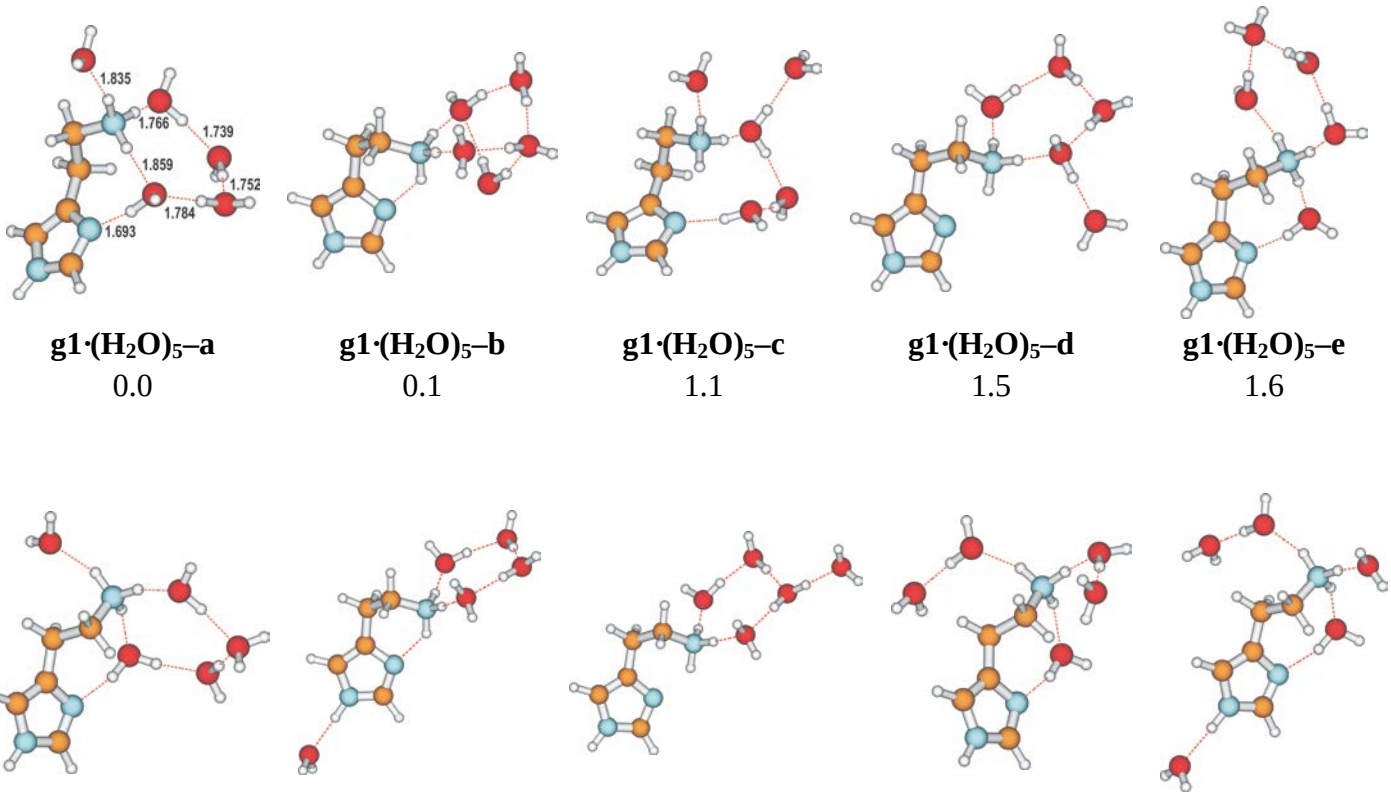
g1·(H$_2$O)$_4$–j
6.9



g1·(H$_2$O)$_4$–k
6.9

g1·(H$_2$O)$_4$–l
7.3

Figure S11. Investigated conformers of *gauche* histamine explicitly solvated with 4 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



g1·$(H_2O)_5$–a
0.0

g1·$(H_2O)_5$–b
0.1

g1·$(H_2O)_5$–c
1.1

g1·$(H_2O)_5$–d
1.5

g1·$(H_2O)_5$–e
1.6

g1·$(H_2O)_5$–f
2.4

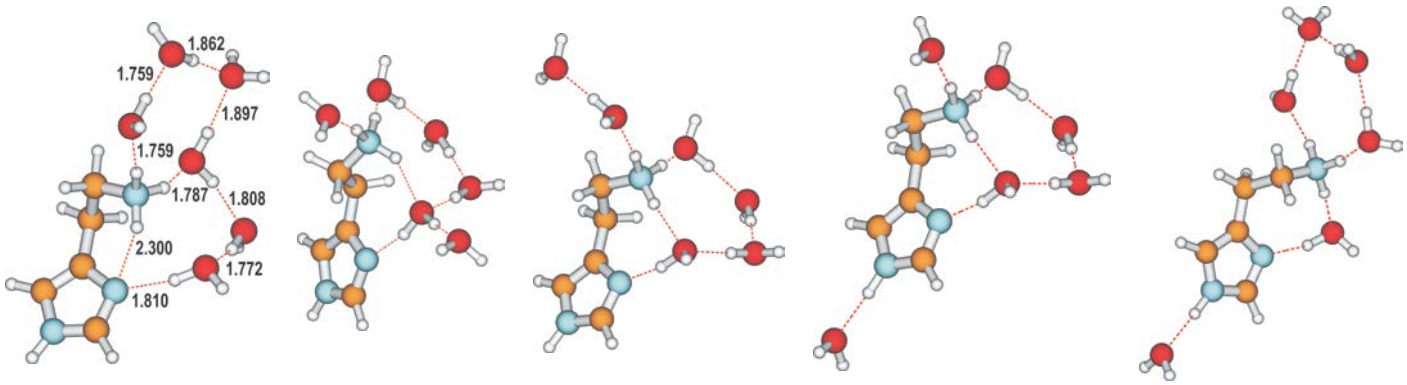
g1·$(H_2O)_5$–g
2.9

g1·$(H_2O)_5$–h
2.9

g1·$(H_2O)_5$–i
4.6

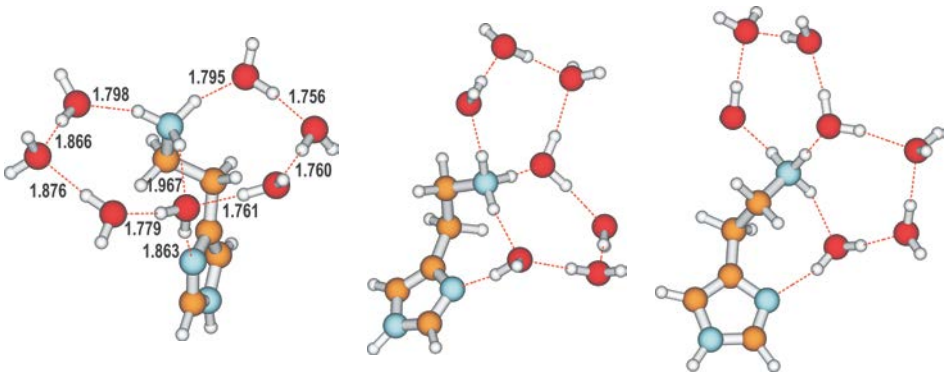
g1·$(H_2O)_5$–j
5.4

Figure S12. Investigated conformers of *gauche* histamine explicitly solvated with 5 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



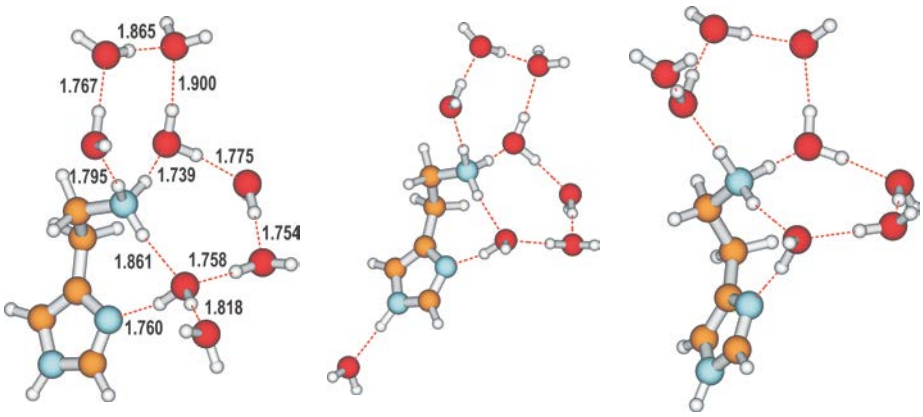
g1·(H$_2$O)$_6$–a	**g1·(H$_2$O)$_6$–b**	**g1·(H$_2$O)$_6$–c**	**g1·(H$_2$O)$_6$–d**	**g1·(H$_2$O)$_6$–e**
0.0	2.9	3.3	3.9	5.5

Figure S13. Investigated conformers of *gauche* histamine explicitly solvated with 6 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



g1·(H$_2$O)$_7$–a	**g1·(H$_2$O)$_7$–b**	**g1·(H$_2$O)$_7$–c**
0.0	0.7	3.5

Figure S14. Investigated conformers of *gauche* histamine explicitly solvated with 7 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.



g1·$(H_2O)_8$–a
0.0

g1·$(H_2O)_8$–b
0.0

g1·$(H_2O)_8$–c
0.3

Figure S15. Investigated conformers of *gauche* histamine explicitly solvated with 8 water molecules. Relative total electronic energies (in kcal mol^{-1}) are obtained with (PCM)/M06–2X/6–311+G(d,p) method.

molecule: **t1**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -360.60992 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.977074	-1.057397	0.295244
2	6	0	-0.450443	0.215488	0.267689
3	6	0	-1.416628	1.116326	-0.090367
4	7	0	-2.554250	0.372251	-0.278349
5	6	0	-2.240936	-0.922666	-0.036126
6	6	0	0.991920	0.462340	0.579360
7	6	0	1.862014	-0.225066	-0.463915
8	7	0	3.318781	-0.089886	-0.122710
9	1	0	-2.966588	-1.717131	-0.116484
10	1	0	-1.395619	2.185049	-0.220574
11	1	0	1.225047	0.065711	1.572443
12	1	0	1.188212	1.536620	0.590319
13	1	0	1.648425	-1.291095	-0.512127
14	1	0	1.727790	0.215552	-1.450227
15	1	0	3.908120	-0.552440	-0.818669
16	1	0	3.606935	0.890760	-0.082887
17	1	0	3.531446	-0.510446	0.785420
18	1	0	-3.461522	0.724107	-0.546361

molecule: **t2**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -360.60687 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.431425	-0.705752	-0.173331
2	7	0	-1.162957	-1.012013	0.196766
3	6	0	-0.463920	0.168028	0.306843
4	6	0	-1.369400	1.143059	-0.017393
5	7	0	-2.593510	0.589116	-0.313567
6	6	0	0.981159	0.236513	0.674568
7	6	0	1.862582	-0.108691	-0.522735
8	7	0	3.313479	-0.058078	-0.137998
9	1	0	-3.186327	-1.462769	-0.319577
10	1	0	-1.200527	2.208674	-0.045831
11	1	0	1.191506	-0.443651	1.505127
12	1	0	1.201343	1.251177	1.013048
13	1	0	1.674506	-1.114470	-0.894284
14	1	0	1.725981	0.605561	-1.332263
15	1	0	3.916589	-0.254492	-0.940146
16	1	0	3.576779	0.863424	0.221464
17	1	0	3.536870	-0.745244	0.586786
18	1	0	-0.809773	-1.940316	0.381564

molecule: **g1**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -360.61813 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.716194	-1.140251	0.005639
2	7	0	-0.440098	-0.882975	-0.183346
3	6	0	-0.317191	0.493367	-0.153856
4	6	0	-1.544724	1.055846	0.058229
5	7	0	-2.420066	0.001107	0.151726
6	6	0	1.018713	1.148058	-0.339213
7	6	0	2.113364	0.446773	0.456858
8	7	0	2.289601	-0.954818	-0.052983
9	1	0	-2.169624	-2.117739	0.047321
10	1	0	-1.862932	2.080232	0.149101
11	1	0	0.970587	2.186330	-0.009030
12	1	0	1.296237	1.163614	-1.398734
13	1	0	3.071438	0.954041	0.366265
14	1	0	1.844485	0.363852	1.509074
15	1	0	2.895168	-1.508859	0.553182
16	1	0	1.341988	-1.392118	-0.109430
17	1	0	2.698280	-0.960072	-0.989323
18	1	0	-3.415493	0.064755	0.307850

molecule: **g2**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -360.60794 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.129609	-0.971686	-0.091718
2	6	0	2.311165	0.190901	0.489369
3	7	0	1.224072	0.989528	0.352642
4	6	0	0.281660	0.298344	-0.370127
5	6	0	0.865237	-0.916294	-0.631450
6	6	0	-1.057962	0.868509	-0.724815
7	6	0	-2.190115	-0.107798	-0.436105
8	7	0	-2.195776	-0.474561	1.019337
9	1	0	3.194768	0.506654	1.021939
10	1	0	0.448514	-1.745830	-1.182664
11	1	0	-1.104364	1.116806	-1.787424
12	1	0	-1.223516	1.800199	-0.178011
13	1	0	-3.161463	0.326074	-0.661836
14	1	0	-2.073837	-1.038514	-0.988393
15	1	0	-2.922556	-1.160391	1.234904
16	1	0	-1.292468	-0.879818	1.288056
17	1	0	-2.357336	0.342942	1.613406
18	1	0	1.127017	1.926936	0.716967

molecule: **t1·$(H_2O)_2$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49490 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.302894	0.848845	-0.111974
2	6	0	1.131907	-0.456143	0.297979
3	6	0	2.350850	-1.063539	0.422171
4	7	0	3.273269	-0.104309	0.084677
5	6	0	2.600347	1.024733	-0.228386
6	6	0	-0.234137	-1.021169	0.521942
7	6	0	-0.990799	-1.119180	-0.798052
8	7	0	-2.404323	-1.549265	-0.551164
9	8	0	-3.203651	0.785848	0.818431
10	8	0	-1.089954	2.374123	-0.502448
11	1	0	3.095667	1.934735	-0.528130
12	1	0	2.633204	-2.060064	0.716354
13	1	0	-0.787559	-0.375920	1.212182
14	1	0	-0.151923	-2.008429	0.981858
15	1	0	-1.042923	-0.150744	-1.295471
16	1	0	-0.534401	-1.845708	-1.468083
17	1	0	-2.887911	-0.827171	0.014782
18	1	0	-2.918056	-1.664852	-1.426370
19	1	0	-2.447216	-2.440147	-0.052183
20	1	0	4.276327	-0.217743	0.075635
21	1	0	-0.236108	1.925919	-0.349469
22	1	0	-1.734510	1.900694	0.038204
23	1	0	-4.024395	1.199765	0.526277
24	1	0	-3.243243	0.794785	1.781853

molecule: **t1·$(H_2O)_2$–b**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49464 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.274046	-0.993395	-0.326225
2	7	0	-2.126262	0.039714	-0.023091
3	6	0	-1.378346	1.148527	0.143302
4	7	0	-0.098126	0.893415	-0.035344
5	6	0	-0.018806	-0.450501	-0.333323
6	6	0	1.306932	-1.090254	-0.598553
7	6	0	2.220436	-1.050206	0.638512
8	7	0	3.583254	-0.551323	0.269419
9	8	0	2.468550	1.902330	-0.102916
10	1	0	-1.803676	2.108981	0.388847
11	1	0	-1.623037	-1.996064	-0.506967
12	1	0	1.790053	-0.552285	-1.420844
13	1	0	1.166987	-2.118805	-0.930561
14	1	0	1.842979	-0.349937	1.382343
15	1	0	2.336108	-2.028787	1.098444
16	1	0	4.223172	-0.579529	1.064466
17	1	0	4.002797	-1.099627	-0.482911
18	1	0	3.470923	0.440115	-0.033172
19	1	0	-3.143564	-0.018691	0.063780
20	1	0	1.495908	1.725612	-0.091380
21	1	0	2.618962	2.628840	-0.713480
22	8	0	-4.973230	-0.188102	0.211919
23	1	0	-5.580281	0.267332	-0.379113
24	1	0	-5.408976	-0.198648	1.069358

molecule: **t1·$(H_2O)_2$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49118 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.413149	0.547372	-0.157640
2	6	0	3.218437	-0.735248	0.229517
3	7	0	1.944266	-1.054195	0.213503
4	6	0	1.282884	0.079795	-0.207182
5	6	0	2.181887	1.085937	-0.439071
6	6	0	-0.206347	0.108435	-0.338437
7	6	0	-0.864176	-0.066102	1.025729
8	7	0	-2.349944	-0.111290	0.871669
9	8	0	-2.778803	2.403616	-0.319393
10	1	0	4.034286	-1.384234	0.507661
11	1	0	2.058017	2.102147	-0.773082
12	1	0	-0.535770	-0.700461	-0.997807
13	1	0	-0.523090	1.056678	-0.778599
14	1	0	-0.552212	-0.998871	1.493793
15	1	0	-0.625517	0.765347	1.688318
16	1	0	-2.816582	-0.210524	1.773393
17	1	0	-2.683049	0.764683	0.429478
18	1	0	-2.613944	-0.919817	0.279659
19	1	0	4.302613	1.019077	-0.227624
20	1	0	-3.089454	2.518912	-1.223038
21	1	0	-3.128518	3.153623	0.171922
22	8	0	-2.574043	-2.405251	-0.737091
23	1	0	-2.924670	-2.397845	-1.633326
24	1	0	-2.807753	-3.265746	-0.374925

molecule: **t1·$(H_2O)_2$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49068 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.484683	0.132090	-0.660876
2	6	0	-3.252590	-1.067440	-0.077232
3	7	0	-2.078033	-1.096990	0.510240
4	6	0	-1.524955	0.147428	0.296807
5	6	0	-2.385788	0.922816	-0.432469
6	6	0	-0.163879	0.492840	0.810963
7	6	0	0.888453	-0.399304	0.164702
8	7	0	2.249529	-0.082880	0.691385
9	8	0	2.366251	2.534020	-0.317911
10	1	0	-3.967843	-1.874562	-0.112295
11	1	0	-2.315798	1.934641	-0.794392
12	1	0	-0.135257	0.358545	1.897283
13	1	0	0.059872	1.539853	0.594549
14	1	0	0.689965	-1.451155	0.365739
15	1	0	0.925656	-0.245240	-0.913707
16	1	0	2.950007	-0.719037	0.267142
17	1	0	2.489856	0.895014	0.451633
18	1	0	2.290970	-0.190101	1.705459
19	1	0	-4.316035	0.395528	-1.168869
20	1	0	2.454844	3.339299	0.201543
21	1	0	2.805990	2.717280	-1.154187
22	8	0	3.804386	-1.951656	-0.702142
23	1	0	4.628468	-1.746767	-1.154757
24	1	0	3.899080	-2.855793	-0.386574

molecule: **t1·$(H_2O)_2$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49048 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.828866	0.302611	-1.013889
2	6	0	3.075086	-0.085299	-1.163147
3	1	0	3.641227	-0.070749	-2.081550
4	7	0	3.601009	-0.523368	0.005083
5	1	0	4.539289	-0.868799	0.142467
6	6	0	2.627173	-0.409087	0.965941
7	1	0	2.791156	-0.691641	1.992115
8	6	0	1.536717	0.106932	0.318943
9	6	0	0.185562	0.427900	0.873679
10	1	0	0.191957	0.291258	1.957904
11	1	0	-0.060886	1.474155	0.667903
12	6	0	-0.874423	-0.465349	0.241013
13	1	0	-0.869619	-0.364076	-0.843883
14	1	0	-0.718830	-1.512470	0.498366
15	7	0	-2.240360	-0.079674	0.705319
16	8	0	-3.956748	-1.918542	-0.550487
17	1	0	-4.259221	-1.781584	-1.453578
18	1	0	-3.780629	-2.861509	-0.474481
19	1	0	-2.951022	-0.709449	0.287804
20	1	0	-2.318535	-0.138079	1.721313
21	8	0	-2.418336	2.533661	-0.334179
22	1	0	-2.310905	3.347406	0.167707
23	1	0	-2.080509	2.722484	-1.215129
24	1	0	-2.440093	0.894542	0.416204

molecule: **t1·$(H_2O)_2$–f**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.48821 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.354421	-0.028429	-0.036640
2	6	0	2.103115	-1.356262	0.001287
3	7	0	0.828576	-1.619378	-0.196200
4	6	0	0.226377	-0.393528	-0.372797
5	6	0	1.160545	0.603793	-0.273204
6	6	0	-1.244137	-0.274971	-0.619400
7	6	0	-2.023845	-0.802674	0.577780
8	7	0	-3.496221	-0.728157	0.312886
9	8	0	-3.749919	2.013994	-0.021270
10	1	0	2.879258	-2.086411	0.172690
11	1	0	1.079051	1.675170	-0.351506
12	1	0	-1.514607	-0.850200	-1.510893
13	1	0	-1.507155	0.769705	-0.799754
14	1	0	-1.775639	-1.842231	0.784158
15	1	0	-1.833500	-0.204374	1.468168
16	1	0	-4.036266	-1.090372	1.100000
17	1	0	-3.771475	0.263076	0.153369
18	1	0	-3.755438	-1.274133	-0.510943
19	1	0	3.264240	0.419232	0.086391
20	1	0	-4.056489	2.428736	-0.834083
21	1	0	-4.057810	2.580393	0.693567
22	8	0	4.879552	1.306783	0.309202
23	1	0	5.575911	1.285844	-0.353912
24	1	0	5.333087	1.332947	1.156971

molecule: **t1·$(H_2O)_2$–g**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.48758 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.575143	-0.680304	-0.491632
2	7	0	2.524116	0.130607	0.076331
3	6	0	1.963389	0.698980	1.167483
4	7	0	0.718793	0.306778	1.339137
5	6	0	0.464813	-0.563192	0.302590
6	6	0	-0.868523	-1.223425	0.147414
7	6	0	-1.952059	-0.176285	-0.073664
8	7	0	-3.306221	-0.807478	-0.169030
9	8	0	-5.054888	1.318263	-0.524772
10	8	0	5.185743	0.473972	-0.961691
11	1	0	2.502257	1.387125	1.800611
12	1	0	1.765380	-1.256155	-1.381998
13	1	0	-1.101896	-1.802644	1.046585
14	1	0	-0.836992	-1.916041	-0.696802
15	1	0	-1.989545	0.529734	0.754397
16	1	0	-1.792868	0.372308	-1.001219
17	1	0	-3.533286	-1.329990	0.679269
18	1	0	-4.033738	-0.072815	-0.304120
19	1	0	-3.359638	-1.461126	-0.952436
20	1	0	3.476742	0.277228	-0.262101
21	1	0	-4.833136	1.996294	-1.170914
22	1	0	-5.405885	1.787978	0.238433
23	1	0	5.963261	0.112266	-0.526026
24	1	0	5.479108	1.293959	-1.370181

molecule: **t1·$(H_2O)_3$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93585 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.577507	1.051115	-0.822164
2	7	0	-3.623894	0.168173	-0.697192
3	6	0	-3.195922	-0.878978	0.040235
4	7	0	-1.940293	-0.722218	0.396322
5	6	0	-1.538939	0.486737	-0.136095
6	6	0	-0.142241	0.975501	0.079099
7	6	0	0.888966	0.051511	-0.588342
8	7	0	2.066893	-0.155062	0.300861
9	8	0	0.279159	-1.719619	1.786566
10	8	0	2.596179	2.600425	0.641060
11	1	0	-3.828358	-1.716853	0.287785
12	1	0	-2.662801	1.974487	-1.369211
13	1	0	0.049212	1.001778	1.156882
14	1	0	-0.033378	1.994941	-0.290624
15	1	0	0.466214	-0.935449	-0.773209
16	1	0	1.250375	0.459708	-1.530761
17	1	0	2.791531	-0.703105	-0.190849
18	1	0	2.454370	0.757111	0.586453
19	1	0	1.740603	-0.682955	1.124458
20	1	0	-4.548537	0.278805	-1.087022
21	1	0	2.180344	3.125826	1.331922
22	1	0	3.430742	3.040536	0.451620
23	1	0	-0.602569	-1.507797	1.406860
24	1	0	0.131337	-1.987164	2.697219
25	8	0	3.705695	-1.680832	-1.430702
26	1	0	4.386038	-1.284047	-1.983341
27	1	0	4.021536	-2.567182	-1.229903

molecule: **t1·$(H_2O)_3$–b**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93529 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.178442	0.285289	0.117893
2	7	0	-1.909381	0.620877	0.050214
3	6	0	-1.221941	-0.541976	-0.226029
4	6	0	-2.102031	-1.584786	-0.319596
5	7	0	-3.342626	-1.038114	-0.099288
6	6	0	0.266738	-0.541719	-0.360598
7	6	0	0.926829	-0.230007	0.979112
8	7	0	2.406493	-0.119372	0.800077
9	8	0	2.321036	2.236719	-0.809125
10	8	0	-0.319439	2.993763	0.267568
11	1	0	-4.003749	0.950766	0.316152
12	1	0	-1.959134	-2.632769	-0.521232
13	1	0	0.564686	0.214633	-1.094843
14	1	0	0.611628	-1.512003	-0.723320
15	1	0	0.573384	0.719374	1.381968
16	1	0	0.739396	-1.020551	1.704791
17	1	0	2.615851	0.669628	0.166708
18	1	0	2.878331	0.055233	1.687691
19	1	0	2.781747	-0.999481	0.399560
20	1	0	-4.222504	-1.532834	-0.103272
21	1	0	-0.916264	2.226618	0.173486
22	1	0	0.499775	2.745674	-0.179379
23	1	0	2.907502	2.954997	-0.544492
24	1	0	2.409087	2.178044	-1.767434
25	8	0	2.959245	-2.652134	-0.271414
26	1	0	3.431524	-2.812422	-1.094573
27	1	0	3.173679	-3.396239	0.300250

molecule: **t1·$(H_2O)_3$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93465 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.573028	-0.363132	-0.457604
2	6	0	-2.677815	-1.145302	-0.652292
3	7	0	-3.623503	-0.667061	0.220990
4	6	0	-3.074221	0.362420	0.902136
5	7	0	-1.834524	0.574107	0.519237
6	6	0	-0.234573	-0.431287	-1.120422
7	6	0	0.834955	-0.861306	-0.121980
8	7	0	2.193199	-0.807151	-0.740417
9	8	0	3.940199	-1.616922	1.296936
10	8	0	0.301512	2.388062	1.119208
11	1	0	-3.611432	0.916976	1.655218
12	1	0	-2.869174	-1.970501	-1.316951
13	1	0	0.022292	0.552714	-1.526938
14	1	0	-0.273565	-1.134382	-1.955317
15	1	0	0.857876	-0.193164	0.739612
16	1	0	0.668438	-1.880655	0.224588
17	1	0	2.399829	0.163467	-1.027631
18	1	0	2.910100	-1.109731	-0.052223
19	1	0	2.259088	-1.411219	-1.560812
20	1	0	-4.563427	-1.017842	0.333237
21	1	0	3.776367	-2.445109	1.758901
22	1	0	4.212391	-0.990341	1.974688
23	1	0	-0.474978	1.824305	0.938415
24	1	0	0.860391	2.323863	0.334252
25	8	0	2.248850	2.027994	-1.062277
26	1	0	3.043231	2.466866	-0.736453
27	1	0	2.059970	2.444056	-1.911216

molecule: **t1·$(H_2O)_3$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93461 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554728	-1.003316	-0.027882
2	7	0	-2.593703	-0.105562	-0.056079
3	6	0	-2.060866	1.129153	-0.151895
4	7	0	-0.744849	1.081504	-0.188296
5	6	0	-0.412988	-0.255261	-0.113401
6	6	0	1.020989	-0.679660	-0.125414
7	6	0	1.779237	-0.161106	1.108007
8	7	0	3.099580	0.407224	0.700928
9	8	0	1.646845	2.476753	-0.431656
10	8	0	3.956119	-1.904123	-0.630650
11	1	0	-2.662813	2.023507	-0.192054
12	1	0	-1.712476	-2.066143	0.045451
13	1	0	1.491442	-0.277752	-1.029030
14	1	0	1.094932	-1.765371	-0.184802
15	1	0	1.232938	0.645954	1.594475
16	1	0	1.964153	-0.950584	1.833381
17	1	0	3.657916	0.682637	1.508883
18	1	0	3.627151	-0.294798	0.154819
19	1	0	2.905727	1.249499	0.129483
20	1	0	-3.589883	-0.331210	-0.009702
21	1	0	3.744636	-2.077938	-1.553445
22	1	0	4.776970	-2.376780	-0.460441
23	1	0	0.719367	2.142399	-0.403208
24	1	0	1.735841	2.976568	-1.247444
25	8	0	-5.363273	-0.827782	0.092751
26	1	0	-5.972622	-0.731595	-0.645327
27	1	0	-5.887875	-0.668199	0.883036

molecule: **t1·$(H_2O)_3$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93394 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.651690	-0.181184	-0.647371
2	6	0	-1.854054	-0.833349	-0.654335
3	7	0	-2.699181	-0.067919	0.111341
4	6	0	-1.997630	0.996690	0.549792
5	7	0	-0.755322	0.964442	0.113218
6	6	0	0.646037	-0.534621	-1.302341
7	6	0	1.746423	-0.820694	-0.267122
8	7	0	3.022331	-0.134541	-0.629112
9	8	0	4.820685	-0.940059	1.380058
10	8	0	1.719588	2.219824	0.012007
11	1	0	-2.428003	1.762005	1.176522
12	1	0	-2.171413	-1.748266	-1.125607
13	1	0	0.953264	0.309690	-1.928034
14	1	0	0.513392	-1.391709	-1.962726
15	1	0	1.471250	-0.429099	0.711777
16	1	0	1.953959	-1.884559	-0.171494
17	1	0	2.841958	0.884773	-0.581569
18	1	0	3.765672	-0.382529	0.050008
19	1	0	3.341297	-0.382645	-1.565880
20	1	0	-3.680723	-0.266934	0.317141
21	1	0	5.122606	-1.850722	1.453408
22	1	0	4.690174	-0.634907	2.283224
23	1	0	0.777546	1.944503	0.110657
24	1	0	1.713105	3.107206	-0.356232
25	8	0	-5.447922	-0.661342	0.669867
26	1	0	-5.740669	-0.939953	1.542738
27	1	0	-6.171526	-0.139153	0.310747

molecule: **t1·$(H_2O)_4$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.38360 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.827506	0.748351	0.306875
2	6	0	1.861821	-0.595395	-0.004323
3	6	0	3.080145	-0.910695	-0.538494
4	7	0	3.792979	0.263285	-0.544786
5	6	0	3.003611	1.230318	-0.030011
6	6	0	0.671619	-1.467560	0.237157
7	6	0	-0.476575	-1.067031	-0.683305
8	7	0	-1.745043	-1.753656	-0.299065
9	8	0	-3.418098	-0.083039	-1.680591
10	8	0	-1.966755	-0.650536	2.354566
11	8	0	-0.614580	1.703693	1.328698
12	1	0	3.327871	2.253124	0.078242
13	1	0	3.490075	-1.838587	-0.899736
14	1	0	0.353579	-1.360303	1.279383
15	1	0	0.937442	-2.514548	0.078190
16	1	0	-0.676808	0.002636	-0.616204
17	1	0	-0.263915	-1.317846	-1.722033
18	1	0	-1.950834	-1.567977	0.695437
19	1	0	-2.520177	-1.350465	-0.867269
20	1	0	-1.697072	-2.762305	-0.443193
21	1	0	4.739885	0.384348	-0.873260
22	1	0	-3.574258	-0.079362	-2.628799
23	1	0	-3.056485	0.797816	-1.448729
24	1	0	0.285861	1.443317	1.031295
25	1	0	-0.967406	0.946769	1.819281
26	1	0	-2.854642	-0.363396	2.598224
27	1	0	-1.632924	-1.121591	3.126774
28	8	0	-2.292880	2.219906	-0.754116
29	1	0	-1.674343	2.097001	-0.001180
30	1	0	-1.899163	2.887497	-1.322195

molecule: **t1·$(H_2O)_4$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37569 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.593692	0.733002	0.411989
2	7	0	3.526089	-0.268551	0.530487
3	6	0	3.213344	-1.226062	-0.371667
4	7	0	2.143081	-0.905457	-1.064092
5	6	0	1.745751	0.322975	-0.584993
6	6	0	0.541902	1.024427	-1.131787
7	6	0	-0.645768	0.070173	-1.183102
8	7	0	-1.907144	0.803814	-1.500509
9	8	0	-1.811432	2.306526	0.810332
10	8	0	-0.320242	0.479724	2.189377
11	8	0	-1.744147	-1.800512	1.572718
12	8	0	-3.440763	-1.472641	-0.687513
13	1	0	3.791476	-2.130965	-0.477127
14	1	0	2.626725	1.629311	1.009776
15	1	0	0.747076	1.403203	-2.138159
16	1	0	0.304778	1.883970	-0.499556
17	1	0	-0.505296	-0.703497	-1.935474
18	1	0	-0.805598	-0.408104	-0.217560
19	1	0	-1.868184	1.264759	-2.409752
20	1	0	-2.691724	0.138212	-1.487870
21	1	0	-2.070969	1.511653	-0.754983
22	1	0	4.301703	-0.288843	1.176168
23	1	0	-3.407010	-2.243826	-1.265785
24	1	0	-4.372874	-1.361175	-0.467141
25	1	0	-1.288472	1.733912	1.409146
26	1	0	-2.530586	2.672836	1.332241
27	1	0	-2.403920	-1.750811	0.861077
28	1	0	-0.785221	-0.369952	2.066056
29	1	0	-2.116042	-2.379061	2.244570
30	1	0	0.579102	0.337871	1.871226

molecule: **t1·$(H_2O)_4$–c**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37409 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.783557	0.460577	0.237262
2	7	0	-4.412760	-0.298285	-0.718488
3	6	0	-3.497244	-1.158114	-1.224294
4	7	0	-2.323739	-1.000616	-0.655402
5	6	0	-2.490792	0.010848	0.266368
6	6	0	-1.352741	0.488533	1.110791
7	6	0	-0.268314	1.111756	0.240600
8	7	0	0.916789	1.496936	1.060278
9	8	0	2.796305	2.275343	-0.812181
10	8	0	3.947322	-0.056862	-1.650098
11	8	0	3.578685	-2.251048	0.111661
12	8	0	1.669061	-1.065174	1.818412
13	1	0	-3.739528	-1.870490	-1.997660
14	1	0	-4.294001	1.227059	0.795747
15	1	0	-0.921164	-0.352137	1.662669
16	1	0	-1.717157	1.219115	1.837409
17	1	0	0.085294	0.398799	-0.504283
18	1	0	-0.629100	2.004702	-0.269303
19	1	0	1.299446	0.646907	1.517693
20	1	0	1.656974	1.896333	0.442793
21	1	0	0.673592	2.180986	1.776652
22	1	0	-5.381696	-0.232306	-0.992904
23	1	0	2.499320	2.769950	-1.581192
24	1	0	3.242518	1.474280	-1.155317
25	1	0	2.348210	-1.515175	1.287208
26	1	0	1.710946	-1.451414	2.697698
27	1	0	4.391533	-2.543727	0.539551
28	1	0	3.232070	-3.030313	-0.337768
29	1	0	3.859688	-0.824176	-1.060274
30	1	0	4.845933	-0.084312	-1.990149

molecule: **t1·$(H_2O)_4$–d**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37408 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.189472	-0.055436	0.245847
2	6	0	3.397822	-0.934007	0.898916
3	7	0	2.146780	-0.821994	0.510864
4	6	0	2.131791	0.176138	-0.440487
5	6	0	3.397275	0.664902	-0.614088
6	6	0	0.857450	0.589107	-1.103943
7	6	0	-0.091829	1.228844	-0.096446
8	7	0	-1.410322	1.523862	-0.730901
9	8	0	-2.940894	2.703907	1.307127
10	8	0	-2.141076	-1.158198	-1.099174
11	8	0	-4.562559	-1.698729	0.039330
12	8	0	-0.369589	-2.120514	1.004902
13	1	0	3.777072	-1.625408	1.634835
14	1	0	3.791106	1.433581	-1.256916
15	1	0	0.374335	-0.287817	-1.547696
16	1	0	1.075058	1.291933	-1.911516
17	1	0	-0.290591	0.554131	0.736848
18	1	0	0.311035	2.163532	0.291938
19	1	0	-1.840130	0.631782	-1.039425
20	1	0	-2.041988	1.980885	-0.046026
21	1	0	-1.309425	2.140843	-1.537722
22	1	0	5.186262	0.047932	0.367741
23	1	0	-2.597414	3.454594	1.801550
24	1	0	-3.396606	2.153294	1.951391
25	1	0	0.517196	-1.738749	0.863411
26	1	0	-0.898530	-1.847530	0.242339
27	1	0	-3.025235	-1.392243	-0.747177
28	1	0	-2.069863	-1.594731	-1.954365
29	1	0	-5.387933	-1.527851	-0.424663
30	1	0	-4.697971	-2.524840	0.513599

molecule: **t1·$(H_2O)_4$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37401 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.926522	-0.735806	-0.153968
2	6	0	2.753231	-1.581496	-0.839042
3	7	0	4.020228	-1.076628	-0.666686
4	6	0	3.923281	0.033203	0.096682
5	7	0	2.672797	0.271019	0.425072
6	6	0	0.441934	-0.766190	0.022196
7	6	0	-0.228920	0.459132	-0.618826
8	7	0	-1.314426	0.980888	0.257330
9	8	0	0.837871	1.851188	1.847456
10	8	0	-2.707915	-1.419393	0.519509
11	8	0	-2.405562	2.999231	-1.412861
12	1	0	4.780796	0.622026	0.382018
13	1	0	2.558137	-2.470568	-1.414107
14	1	0	0.224285	-0.768051	1.095449
15	1	0	0.026900	-1.685888	-0.390023
16	1	0	0.485533	1.271372	-0.748499
17	1	0	-0.667347	0.221188	-1.586607
18	1	0	-1.821248	1.744994	-0.217094
19	1	0	-1.971342	0.214285	0.489395
20	1	0	-0.869370	1.347063	1.111488
21	1	0	4.873653	-1.463488	-1.042455
22	1	0	-2.452015	-2.070198	1.179146
23	1	0	-3.657362	-1.565443	0.351735
24	1	0	1.616104	1.393289	1.459489
25	1	0	1.034312	1.984136	2.778392
26	1	0	-3.299477	2.989235	-1.768310
27	1	0	-2.177236	3.928560	-1.313821
28	8	0	-5.408955	-1.819461	0.055380
29	1	0	-5.715229	-2.635735	-0.351378
30	1	0	-6.039096	-1.629311	0.757031

molecule: **t1·$(H_2O)_4$–f**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37391 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.204432	0.704830	0.203928
2	6	0	-1.663500	-0.506661	-0.172960
3	6	0	-2.588271	-1.498032	0.007507
4	7	0	-3.707761	-0.871190	0.497759
5	6	0	-3.431653	0.447390	0.599135
6	6	0	-0.256040	-0.603799	-0.666895
7	6	0	0.731125	-0.278739	0.450003
8	7	0	2.126856	-0.274203	-0.073415
9	8	0	3.702273	0.314786	2.208674
10	8	0	1.734850	2.051406	-1.733314
11	8	0	-0.504168	2.998255	-0.074077
12	1	0	-4.148735	1.167382	0.960972
13	1	0	-2.550319	-2.559594	-0.168057
14	1	0	-0.110133	0.099168	-1.493969
15	1	0	-0.061917	-1.609587	-1.045346
16	1	0	0.537583	0.707796	0.872724
17	1	0	0.679246	-1.021486	1.246261
18	1	0	2.215971	0.452377	-0.797730
19	1	0	2.791650	-0.063705	0.690861
20	1	0	2.352768	-1.199175	-0.474763
21	1	0	-4.583052	-1.313285	0.737298
22	1	0	3.462231	-0.073919	3.055454
23	1	0	4.000989	1.207182	2.409011
24	1	0	-1.136543	2.259778	0.015657
25	1	0	0.180573	2.684696	-0.679171
26	1	0	2.415737	2.731629	-1.675423
27	1	0	1.541698	1.968414	-2.673979
28	8	0	2.217518	-2.965348	-0.952512
29	1	0	2.348640	-3.251823	-1.861820
30	1	0	2.607223	-3.655651	-0.406797

molecule: **t1·$(H_2O)_4$–g**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37197 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.120222	0.911246	0.451770
2	6	0	-0.929724	-0.018851	-0.546608
3	6	0	-2.112140	-0.656134	-0.810655
4	7	0	-3.033950	-0.099701	0.039723
5	6	0	-2.394529	0.832817	0.775718
6	6	0	0.417508	-0.228817	-1.160047
7	6	0	1.380617	-0.842354	-0.149861
8	7	0	2.754494	-0.943311	-0.726595
9	8	0	4.257203	-2.236168	1.254015
10	8	0	3.203006	1.870263	-0.850396
11	8	0	1.187790	2.410516	1.230349
12	1	0	-2.893257	1.425096	1.526924
13	1	0	-2.367795	-1.432313	-1.512247
14	1	0	0.817519	0.730829	-1.504623
15	1	0	0.327478	-0.882335	-2.030898
16	1	0	1.459653	-0.222680	0.743940
17	1	0	1.067367	-1.844886	0.139476
18	1	0	3.110137	0.005305	-0.928497
19	1	0	3.392284	-1.407404	-0.051326
20	1	0	2.757827	-1.482096	-1.593695
21	1	0	-4.024772	-0.344034	0.102895
22	1	0	3.986044	-3.104161	1.568669
23	1	0	4.583473	-1.767530	2.028498
24	1	0	0.358422	1.953993	0.988307
25	1	0	1.781911	2.291309	0.478537
26	1	0	4.028728	2.185852	-0.464858
27	1	0	3.116687	2.343405	-1.685817
28	8	0	-5.798785	-0.852435	0.167412
29	1	0	-6.162363	-1.293463	0.941081
30	1	0	-6.505700	-0.289905	-0.162974

molecule: **t1·$(H_2O)_5$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.82955 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.655280	0.712555	-0.046704
2	7	0	4.247184	-0.448341	0.387454
3	6	0	3.303910	-1.413789	0.404118
4	7	0	2.142039	-0.942907	0.006878
5	6	0	2.347763	0.390480	-0.282360
6	6	0	1.224393	1.256278	-0.756675
7	6	0	0.174310	1.408619	0.338155
8	7	0	-1.044259	2.101026	-0.173693
9	8	0	-2.683870	1.261590	1.886165
10	8	0	-1.819307	0.088218	-1.983080
11	8	0	-4.049737	-0.809220	-0.748974
12	8	0	-0.453452	-1.880589	-0.441427
13	1	0	3.510590	-2.428197	0.706548
14	1	0	4.199061	1.636084	-0.149468
15	1	0	0.759880	0.802591	-1.638797
16	1	0	1.611328	2.234176	-1.050569
17	1	0	-0.158420	0.433890	0.696591
18	1	0	0.554974	1.980359	1.183700
19	1	0	-1.409648	1.580897	-0.992410
20	1	0	-1.771810	2.069334	0.566587
21	1	0	-0.858999	3.067993	-0.439904
22	1	0	5.215847	-0.562913	0.647547
23	1	0	-2.572520	1.514691	2.806668
24	1	0	-2.582850	0.291806	1.850292
25	1	0	0.487850	-1.644043	-0.273438
26	1	0	-0.755589	-1.301474	-1.159179
27	1	0	-2.703497	-0.228972	-1.692234
28	1	0	-1.849364	0.163601	-2.942183
29	1	0	-4.600569	-1.513841	-1.101571
30	1	0	-3.650246	-1.157340	0.068557
31	1	0	-1.595030	-1.678599	0.798490
32	8	0	-2.370141	-1.437981	1.363114
33	1	0	-2.467617	-2.129503	2.024714

molecule: **t1·$(H_2O)_5$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.82470 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.304911	0.879821	0.204997
2	7	0	4.168436	-0.109580	0.607991
3	6	0	3.517798	-1.288629	0.522428
4	7	0	2.288244	-1.114758	0.088834
5	6	0	2.139711	0.241063	-0.117791
6	6	0	0.844570	0.812555	-0.596879
7	6	0	-0.235978	0.679134	0.472382
8	7	0	-1.541785	1.173346	-0.045887
9	8	0	0.092195	-2.641137	-0.512238
10	8	0	-1.933014	-1.221009	-1.518854
11	8	0	-3.479477	0.453436	1.844450
12	8	0	-0.806556	3.827725	-0.741032
13	1	0	3.975585	-2.230421	0.780178
14	1	0	3.586668	1.918824	0.181123
15	1	0	0.522886	0.284356	-1.500959
16	1	0	0.976333	1.866081	-0.852239
17	1	0	-0.375774	-0.363177	0.764932
18	1	0	0.014936	1.262975	1.357827
19	1	0	-1.830563	0.569756	-0.829466
20	1	0	-2.272509	1.090991	0.687913
21	1	0	-1.457153	2.154027	-0.358173
22	1	0	5.122891	0.017898	0.911312
23	1	0	-2.036422	-1.340000	-2.468047
24	1	0	-1.170543	-1.783167	-1.241836
25	1	0	-0.695447	4.116948	-1.652205
26	1	0	-1.130425	4.598904	-0.265066
27	1	0	-3.207802	0.207964	2.733201
28	1	0	-3.779234	-0.369191	1.409000
29	1	0	0.946065	-2.186067	-0.297009
30	1	0	0.318811	-3.503212	-0.871831
31	1	0	-3.377265	-1.613819	-0.473865
32	8	0	-4.093461	-1.635256	0.187411
33	1	0	-4.198870	-2.556470	0.439921

molecule: **t1·$(H_2O)_5$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.82304 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.443897	-0.265629	0.575513
2	6	0	2.682196	-0.847843	0.558822
3	7	0	3.489235	0.006999	-0.149214
4	6	0	2.733924	1.054864	-0.533218
5	7	0	1.490844	0.925755	-0.115336
6	6	0	0.170690	-0.755909	1.186331
7	6	0	-0.840677	-1.126818	0.107101
8	7	0	-2.144983	-1.511816	0.719460
9	8	0	-0.838602	2.348601	-0.203677
10	8	0	-2.826863	1.182657	1.130401
11	8	0	-4.815880	0.754984	-0.781698
12	8	0	-3.980386	-1.783306	-1.321242
13	1	0	3.125303	1.880311	-1.106781
14	1	0	3.046703	-1.769372	0.980856
15	1	0	-0.256044	0.024024	1.826240
16	1	0	0.378112	-1.625446	1.814546
17	1	0	-1.045221	-0.279831	-0.550038
18	1	0	-0.491784	-1.964543	-0.495431
19	1	0	-2.531530	-0.684970	1.202790
20	1	0	-2.829488	-1.780081	-0.023231
21	1	0	-2.043748	-2.280573	1.382403
22	1	0	4.484216	-0.123179	-0.347680
23	1	0	-3.035559	1.628113	1.957445
24	1	0	-2.084509	1.684492	0.713308
25	1	0	-3.694064	-1.953528	-2.222975
26	1	0	-4.356440	-0.879854	-1.310251
27	1	0	0.058536	1.921918	-0.203543
28	1	0	-0.694989	3.296543	-0.133877
29	1	0	-4.178565	1.040728	-0.101818
30	1	0	-4.882731	1.480962	-1.408009
31	8	0	6.272046	-0.424276	-0.664307
32	1	0	6.959700	0.117643	-0.265899
33	1	0	6.603721	-0.661204	-1.535535

molecule: **t1·$(H_2O)_5$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.82281 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.988435	1.097748	-0.369429
2	7	0	-3.887697	0.081915	-0.585587
3	6	0	-3.292949	-1.078787	-0.236551
4	7	0	-2.067153	-0.869842	0.191204
5	6	0	-1.862139	0.492783	0.115466
6	6	0	-0.553799	1.095611	0.514583
7	6	0	0.550858	0.677305	-0.450771
8	7	0	1.885423	1.098584	0.060839
9	8	0	1.353827	3.863554	-0.152703
10	8	0	3.210325	-0.551223	-1.721840
11	8	0	1.646260	-2.731289	-1.210776
12	8	0	0.142951	-2.392822	1.024002
13	8	0	1.837407	-0.538991	2.465951
14	1	0	-3.787479	-2.034445	-0.310418
15	1	0	-3.222383	2.129609	-0.569647
16	1	0	-0.295951	0.758417	1.524199
17	1	0	-0.629632	2.184491	0.536546
18	1	0	0.579253	-0.405987	-0.571419
19	1	0	0.413830	1.135008	-1.430524
20	1	0	2.028465	0.714154	1.005221
21	1	0	2.615428	0.701075	-0.557701
22	1	0	1.941595	2.128208	0.085221
23	1	0	-4.827414	0.181695	-0.940696
24	1	0	2.745324	-1.400642	-1.577574
25	1	0	4.140842	-0.764182	-1.830833
26	1	0	-0.691314	-1.931036	0.781707
27	1	0	0.611984	-1.803858	1.633607
28	1	0	2.666697	-0.998130	2.643148
29	1	0	1.556216	-0.188797	3.319011
30	1	0	1.611759	4.362329	-0.934368
31	1	0	1.346313	4.501289	0.567839
32	1	0	1.115153	-2.701183	-0.385047
33	1	0	1.919924	-3.644415	-1.330334

molecule: **t1·$(H_2O)_5$–e**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81904 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.876700	0.690607	0.366714
2	7	0	-4.567417	-0.047551	-0.562572
3	6	0	-3.712286	-0.949959	-1.091812
4	7	0	-2.515749	-0.836210	-0.559107
5	6	0	-2.604684	0.187735	0.360154
6	6	0	-1.413463	0.616907	1.155305
7	6	0	-0.362356	1.247917	0.248079
8	7	0	0.873139	1.577575	1.015358
9	8	0	2.702243	2.453356	-0.844826
10	8	0	4.219084	0.277499	-1.491814
11	8	0	0.044284	-2.119192	-0.765631
12	8	0	4.130715	-1.745364	0.501128
13	8	0	1.593470	-1.110626	1.488642
14	1	0	-4.008010	-1.658163	-1.849704
15	1	0	-4.336567	1.481399	0.934756
16	1	0	-0.978482	-0.250871	1.662343
17	1	0	-1.722805	1.330212	1.923006
18	1	0	-0.063533	0.558376	-0.542479
19	1	0	-0.731440	2.167373	-0.205211
20	1	0	1.264593	0.704702	1.409176
21	1	0	1.589508	1.994273	0.377008
22	1	0	0.683643	2.230789	1.775731
23	1	0	-5.541063	0.059238	-0.806590
24	1	0	2.373726	2.866532	-1.648314
25	1	0	3.274619	1.710743	-1.128161
26	1	0	-0.855747	-1.743871	-0.725980
27	1	0	0.486845	-1.825206	0.042317
28	1	0	2.496752	-1.354751	1.211023
29	1	0	1.449666	-1.546592	2.335169
30	1	0	4.855281	-1.695934	1.135301
31	1	0	4.170332	-2.636595	0.135194
32	1	0	4.235938	-0.428275	-0.824280
33	1	0	5.125492	0.375299	-1.796684

molecule: **t1·$(H_2O)_5$–f**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81537 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.256541	-1.637609	0.169697
2	7	0	3.363779	-1.497388	-0.631183
3	6	0	3.530761	-0.180256	-0.878577
4	7	0	2.598948	0.533072	-0.285364
5	6	0	1.792574	-0.368033	0.378293
6	6	0	0.606219	0.089802	1.164553
7	6	0	-0.428262	0.730966	0.246379
8	7	0	-1.574928	1.262128	1.043533
9	8	0	-2.336195	-1.117003	2.205114
10	8	0	-1.832167	-2.513267	-0.063206
11	8	0	-2.485658	-0.822547	-2.126333
12	8	0	-3.277917	1.734874	-1.218926
13	8	0	1.781821	3.195817	0.193742
14	1	0	4.335410	0.201784	-1.486686
15	1	0	1.913046	-2.597000	0.517882
16	1	0	0.926087	0.822162	1.913648
17	1	0	0.162176	-0.757703	1.691424
18	1	0	0.001188	1.565330	-0.306104
19	1	0	-0.836802	0.002461	-0.454354
20	1	0	-1.276495	2.010916	1.669633
21	1	0	-2.297397	1.628975	0.406639
22	1	0	-1.990932	0.489128	1.608117
23	1	0	3.951274	-2.243501	-0.973516
24	1	0	-2.994302	2.446311	-1.804906
25	1	0	-4.222607	1.874573	-1.085152
26	1	0	2.187012	2.326270	-0.003291
27	1	0	2.326679	3.580956	0.884423
28	1	0	-2.196333	-1.732249	1.455527
29	1	0	-3.183392	-1.345296	2.597640
30	1	0	-2.860802	0.046487	-1.906534
31	1	0	-2.069604	-1.982568	-0.848116
32	1	0	-2.947869	-1.126674	-2.912547
33	1	0	-0.987003	-2.927255	-0.257840

molecule: **t1·$(H_2O)_5$–g**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81481 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.746603	0.023006	0.832719
2	7	0	3.769306	-0.251133	-0.042545
3	6	0	3.377836	0.162726	-1.268946
4	7	0	2.172670	0.686980	-1.239712
5	6	0	1.765636	0.608681	0.073835
6	6	0	0.427804	1.113971	0.514631
7	6	0	-0.672986	0.587960	-0.399849
8	7	0	-2.015361	0.929891	0.150451
9	8	0	-1.631409	-0.608633	2.455775
10	8	0	0.227105	-2.246471	1.277271
11	8	0	-1.152503	-2.848261	-1.033396
12	8	0	-3.246687	-1.018434	-1.588922
13	8	0	-1.743161	3.736006	-0.048707
14	1	0	4.004119	0.057039	-2.141251
15	1	0	2.814158	-0.191734	1.886779
16	1	0	0.406453	2.208031	0.501163
17	1	0	0.243804	0.793552	1.543441
18	1	0	-0.598259	1.021663	-1.396195
19	1	0	-0.628463	-0.496959	-0.488805
20	1	0	-2.132762	1.954620	0.189820
21	1	0	-2.739723	0.511876	-0.445490
22	1	0	-2.101929	0.512742	1.094799
23	1	0	4.651674	-0.684509	0.186342
24	1	0	-3.279106	-0.797644	-2.526994
25	1	0	-4.129768	-1.340194	-1.374097
26	1	0	-2.092985	4.223360	-0.801046
27	1	0	-1.732968	4.362315	0.681767
28	1	0	-0.967512	-1.257497	2.145000
29	1	0	-2.269807	-1.097975	2.981681
30	1	0	-1.934432	-2.313787	-1.251945
31	1	0	-0.200893	-2.552226	0.454898
32	1	0	-1.343997	-3.741353	-1.332965
33	1	0	1.049975	-1.823208	1.005240

molecule: **t1·$(H_2O)_5$–h**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81320 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.413886	0.608939	-0.248423
2	7	0	4.257060	-0.340206	0.276278
3	6	0	3.516207	-1.429795	0.575452
4	7	0	2.250757	-1.238318	0.274886
5	6	0	2.171587	0.036517	-0.245642
6	6	0	0.864145	0.608086	-0.690222
7	6	0	-0.077747	0.792574	0.495543
8	7	0	-1.411772	1.262634	0.027088
9	8	0	-2.957624	1.480801	2.404861
10	8	0	-2.056325	-1.149815	-1.320208
11	8	0	-4.481794	-2.106524	-0.487284
12	8	0	-0.211468	-2.726706	0.282772
13	1	0	3.941147	-2.324774	1.001879
14	1	0	3.761169	1.575334	-0.572299
15	1	0	0.398395	-0.066934	-1.416483
16	1	0	1.024717	1.569645	-1.182408
17	1	0	-0.230954	-0.148495	1.025109
18	1	0	0.310599	1.533591	1.194407
19	1	0	-1.816517	0.548660	-0.600387
20	1	0	-2.046389	1.391799	0.833122
21	1	0	-1.310094	2.159800	-0.473270
22	1	0	5.253020	-0.246039	0.411249
23	1	0	-2.584559	1.914611	3.178450
24	1	0	-3.419499	0.706702	2.741532
25	1	0	0.657164	-2.282425	0.285630
26	1	0	-0.769785	-2.212630	-0.317546
27	1	0	-2.935542	-1.512647	-1.087432
28	1	0	-1.970518	-1.252439	-2.273565
29	1	0	-5.304473	-1.841261	-0.909672
30	1	0	-4.585318	-3.040972	-0.282720
31	8	0	-0.556344	3.699049	-1.152525
32	1	0	-0.653903	3.940057	-2.078998
33	1	0	-0.611000	4.527277	-0.665536

molecule: **t1·$(H_2O)_5$–i**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81295 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.443693	0.333613	-0.803066
2	7	0	4.252053	-0.021766	0.249060
3	6	0	3.456697	-0.446761	1.255157
4	7	0	2.188774	-0.386655	0.913412
5	6	0	2.165187	0.099254	-0.377149
6	6	0	0.872084	0.310361	-1.097285
7	6	0	0.064924	1.425976	-0.440952
8	7	0	-1.296387	1.513238	-1.045504
9	8	0	-2.491720	3.705365	0.266454
10	8	0	-2.124593	-0.954887	-0.127760
11	8	0	-4.724630	-1.365474	0.711207
12	8	0	-0.356022	-0.907576	2.164921
13	1	0	3.845703	-0.787760	2.201726
14	1	0	3.836591	0.706342	-1.733905
15	1	0	0.292297	-0.618744	-1.084161
16	1	0	1.070889	0.560461	-2.142324
17	1	0	-0.079675	1.230685	0.622024
18	1	0	0.550816	2.393720	-0.561487
19	1	0	-1.800540	0.623440	-0.847585
20	1	0	-1.821073	2.303878	-0.629254
21	1	0	-1.250124	1.652802	-2.055393
22	1	0	5.260232	0.023154	0.269140
23	1	0	-1.989116	4.516905	0.387054
24	1	0	-2.979615	3.577847	1.085962
25	1	0	0.531901	-0.783140	1.780579
26	1	0	-0.962171	-0.949995	1.410494
27	1	0	-3.043183	-1.150494	0.137799
28	1	0	-1.799453	-1.714425	-0.645789
29	1	0	-5.421264	-1.636314	0.105613
30	1	0	-4.887693	-1.852146	1.524949
31	8	0	-0.789527	-2.890110	-1.556400
32	1	0	-1.047362	-3.199559	-2.430204
33	1	0	-0.441810	-3.663573	-1.101612

molecule: **t1·$(H_2O)_5$–j**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81136 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.742723	0.579115	0.767622
2	7	0	-3.553983	-0.145178	-0.069283
3	6	0	-2.768393	-1.005622	-0.749345
4	7	0	-1.504073	-0.880633	-0.402203
5	6	0	-1.474054	0.111578	0.553529
6	6	0	-0.185411	0.543425	1.176654
7	6	0	0.713871	1.211077	0.141849
8	7	0	2.047614	1.532590	0.730308
9	8	0	3.477870	2.762765	-1.349840
10	8	0	2.854829	-1.136009	1.029827
11	8	0	5.248925	-1.627297	-0.188288
12	8	0	1.005972	-2.131109	-0.996083
13	1	0	-3.158170	-1.699204	-1.478112
14	1	0	-3.125355	1.338939	1.428145
15	1	0	0.331090	-0.327085	1.595157
16	1	0	-0.387956	1.235288	1.997610
17	1	0	0.898016	0.546310	-0.702731
18	1	0	0.276568	2.138767	-0.225756
19	1	0	2.509535	0.648114	1.012897
20	1	0	2.642676	2.011235	0.027750
21	1	0	1.961607	2.138972	1.546788
22	1	0	-4.568016	-0.051959	-0.161547
23	1	0	3.180165	3.585604	-1.750127
24	1	0	3.832026	2.234098	-2.071630
25	1	0	0.119998	-1.760664	-0.817822
26	1	0	1.565415	-1.842858	-0.261624
27	1	0	3.730872	-1.349779	0.646105
28	1	0	2.820741	-1.582207	1.882232
29	1	0	6.083950	-1.442721	0.252617
30	1	0	5.384707	-2.451208	-0.666252
31	8	0	-6.397800	0.178100	-0.285881
32	1	0	-6.791181	0.588098	-1.062094
33	1	0	-7.011698	-0.514223	-0.023101

molecule: **t1·$(H_2O)_6$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.26610 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.036686	0.013089	-0.913198
2	7	0	-4.727621	-0.103910	0.268176
3	6	0	-3.854319	0.090876	1.279558
4	7	0	-2.645308	0.326526	0.819531
5	6	0	-2.744769	0.282639	-0.556026
6	6	0	-1.541763	0.499292	-1.416931
7	6	0	-0.552341	-0.650584	-1.257105
8	7	0	0.756998	-0.328933	-1.893806
9	8	0	2.366704	-2.071904	-0.584138
10	8	0	0.933982	-1.912350	1.769423
11	8	0	-0.045985	0.622094	1.882927
12	8	0	4.761478	-0.798941	-0.032362
13	8	0	4.152171	1.938507	0.438195
14	8	0	1.431353	1.893316	-0.234690
15	1	0	-4.144679	0.053906	2.317674
16	1	0	-4.510089	-0.098793	-1.873831
17	1	0	-1.054984	1.434093	-1.119812
18	1	0	-1.841632	0.598935	-2.462105
19	1	0	-0.343603	-0.838836	-0.203781
20	1	0	-0.928405	-1.569653	-1.705387
21	1	0	1.092849	0.581818	-1.539276
22	1	0	1.462638	-1.046683	-1.590118
23	1	0	0.694666	-0.293191	-2.910644
24	1	0	-5.713247	-0.298856	0.366206
25	1	0	1.929507	-2.104891	0.288733
26	1	0	3.247355	-1.685261	-0.421301
27	1	0	-0.984413	0.588403	1.593621
28	1	0	0.421382	1.159708	1.224082
29	1	0	2.377424	1.931638	0.004161
30	1	0	1.182218	2.798694	-0.449987
31	1	0	4.658054	2.568697	-0.087750
32	1	0	4.310839	2.186652	1.356363
33	1	0	4.639797	0.155051	0.101311
34	1	0	5.580105	-0.899299	-0.525439

35	1	0	0.608670	-0.999119	1.923994
36	1	0	1.208718	-2.256437	2.623336

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molecule: **t1·$(H_2O)_6$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.26009 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.490016	0.949699	0.075999
2	7	0	-3.370344	-0.095597	-0.052349
3	6	0	-2.689944	-1.231965	0.199759
4	7	0	-1.427458	-0.982557	0.482534
5	6	0	-1.287863	0.387428	0.410224
6	6	0	0.033184	1.039897	0.663324
7	6	0	1.027471	0.697782	-0.441768
8	7	0	2.394059	1.176696	-0.088916
9	8	0	1.703979	3.913469	-0.194770
10	8	0	3.590521	-0.410736	-2.014711
11	8	0	2.180132	-2.654466	-1.361563
12	8	0	0.923146	-2.403534	1.026162
13	8	0	2.694704	-0.480225	2.282426
14	1	0	-3.149660	-2.207354	0.166778
15	1	0	-2.785041	1.974789	-0.072532
16	1	0	0.428914	0.689969	1.622854
17	1	0	-0.086016	2.123373	0.726908
18	1	0	1.092742	-0.380037	-0.593032
19	1	0	0.747207	1.167387	-1.384682
20	1	0	2.667641	0.790193	0.825485
21	1	0	3.061725	0.819782	-0.795859
22	1	0	2.404999	2.207486	-0.056060
23	1	0	-4.361791	-0.027691	-0.293255
24	1	0	3.181302	-1.280571	-1.828529
25	1	0	4.513385	-0.580275	-2.221625
26	1	0	0.046360	-1.976865	0.884424
27	1	0	1.432302	-1.798040	1.585180
28	1	0	3.553463	-0.912373	2.358562
29	1	0	2.504590	-0.140360	3.164279
30	1	0	1.832072	4.435346	-0.992973
31	1	0	1.745612	4.542058	0.532674
32	1	0	1.740726	-2.650430	-0.482360
33	1	0	2.473524	-3.555612	-1.519239
34	8	0	-6.146857	0.175458	-0.713238

35	1	0	-6.838270	-0.042673	-0.081030
36	1	0	-6.501583	-0.064682	-1.574520

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molecule: **t1·$(H_2O)_6$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25841 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.204308	-1.864467	0.608096
2	7	0	3.311473	-1.999950	-0.193602
3	6	0	3.497955	-0.829084	-0.840974
4	7	0	2.579328	0.048950	-0.503771
5	6	0	1.761205	-0.586049	0.406655
6	6	0	0.583665	0.112706	1.006439
7	6	0	-0.446134	0.448427	-0.067633
8	7	0	-1.574676	1.228399	0.517663
9	8	0	-2.381504	-0.689316	2.361082
10	8	0	-1.890470	-2.715334	0.617532
11	8	0	-2.454037	-1.755934	-1.895628
12	8	0	-3.172565	0.978190	-1.875243
13	8	0	2.003469	2.812272	-1.013705
14	8	0	0.028504	3.561802	1.038279
15	1	0	4.306086	-0.669767	-1.537242
16	1	0	1.847993	-2.660812	1.239236
17	1	0	0.913041	1.036933	1.493797
18	1	0	0.127519	-0.520575	1.770658
19	1	0	-0.005855	1.052877	-0.861615
20	1	0	-0.862402	-0.460032	-0.503420
21	1	0	-1.225246	2.133430	0.862718
22	1	0	-2.287822	1.389825	-0.205751
23	1	0	-2.004588	0.687290	1.293862
24	1	0	3.886029	-2.825033	-0.284251
25	1	0	-2.831770	1.462925	-2.635900
26	1	0	-4.118511	1.163840	-1.857200
27	1	0	2.263006	1.883035	-0.863797
28	1	0	1.428486	3.046488	-0.273607
29	1	0	-0.329949	4.404385	0.736029
30	1	0	0.366614	3.735942	1.924049
31	1	0	-2.260163	-1.501201	1.827442
32	1	0	-3.221366	-0.780806	2.819299
33	1	0	-2.789546	-0.846774	-1.970255
34	1	0	-2.099286	-2.451735	-0.299561

35	1	0	-2.945669	-2.277854	-2.536090
36	1	0	-1.042653	-3.166813	0.585541

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molecule: **t1·$(H_2O)_6$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25789 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.541830	-1.382041	0.262000
2	6	0	2.619212	-0.065705	-0.142287
3	6	0	3.891657	0.398688	0.049455
4	7	0	4.593506	-0.658759	0.575009
5	6	0	3.744369	-1.703804	0.684620
6	6	0	1.419064	0.651196	-0.671745
7	6	0	0.373740	0.840541	0.423289
8	7	0	-0.857518	1.464771	-0.135418
9	8	0	-2.735509	1.483135	1.926320
10	8	0	-4.594063	-0.450877	1.386792
11	8	0	-4.200870	-1.707696	-1.130892
12	8	0	-1.590695	-0.824389	-1.667013
13	8	0	-0.017651	-2.649962	-0.031369
14	1	0	4.048724	-2.664082	1.070233
15	1	0	4.345244	1.357227	-0.137718
16	1	0	0.979364	0.072796	-1.491680
17	1	0	1.712182	1.625315	-1.068949
18	1	0	0.084825	-0.116551	0.859697
19	1	0	0.748371	1.491500	1.213334
20	1	0	-1.247403	0.842800	-0.860028
21	1	0	-1.574095	1.572787	0.611163
22	1	0	-0.631139	2.386126	-0.540349
23	1	0	5.569755	-0.659233	0.832043
24	1	0	-2.429699	1.375791	2.831171
25	1	0	-3.421714	0.799989	1.784525
26	1	0	0.879678	-2.279086	0.068238
27	1	0	-0.485282	-2.049269	-0.628147
28	1	0	-2.507263	-1.130842	-1.534784
29	1	0	-1.421903	-0.900750	-2.611916
30	1	0	-4.852682	-1.454383	-1.794644
31	1	0	-4.258519	-2.668314	-1.069222
32	1	0	-4.508456	-0.888808	0.523715
33	1	0	-5.530591	-0.264889	1.498084
34	8	0	0.336091	3.896794	-0.998002

35	1	0	0.241152	4.713703	-0.498380
36	1	0	0.448051	4.168846	-1.914187

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molecule: **t1·$(H_2O)_6$–e**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25630 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.946250	-0.872272	-0.372852
2	6	0	-1.978356	0.117903	0.585024
3	6	0	-3.252215	0.607053	0.694976
4	7	0	-4.003848	-0.101685	-0.207813
5	6	0	-3.179842	-0.974883	-0.823337
6	6	0	-0.738443	0.530271	1.311969
7	6	0	0.246700	1.197574	0.358361
8	7	0	1.530633	1.508516	1.050906
9	8	0	3.238790	2.504048	-0.864972
10	8	0	5.006811	0.523056	-1.489835
11	8	0	4.741815	-1.790491	0.138989
12	8	0	2.308736	-1.182914	1.382608
13	8	0	0.586560	-2.147593	-0.768999
14	1	0	-3.520634	-1.660457	-1.583492
15	1	0	-3.674335	1.373121	1.323413
16	1	0	-0.265144	-0.349017	1.762098
17	1	0	-0.999208	1.216754	2.121152
18	1	0	0.493129	0.537049	-0.473809
19	1	0	-0.155060	2.129586	-0.037961
20	1	0	1.955411	0.624703	1.381437
21	1	0	2.198406	1.959142	0.383649
22	1	0	1.389279	2.129300	1.848064
23	1	0	-5.005048	0.007725	-0.382988
24	1	0	2.858385	2.855894	-1.674781
25	1	0	3.893421	1.827627	-1.135893
26	1	0	-0.307459	-1.768089	-0.663828
27	1	0	1.084132	-1.868286	0.011637
28	1	0	3.184360	-1.414844	1.019280
29	1	0	2.241487	-1.641681	2.226559
30	1	0	5.493878	-1.934142	0.725058
31	1	0	4.667082	-2.597977	-0.382903
32	1	0	4.960062	-0.277584	-0.941224
33	1	0	5.941991	0.717463	-1.597728
34	8	0	-6.815909	0.253400	-0.660301

35	1	0	-7.156353	0.665106	-1.460226
36	1	0	-7.463029	-0.416865	-0.421080

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molecule: **t1·$(H_2O)_7$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.70835 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.322367	-2.192236	0.090531
2	7	0	3.386313	-1.980276	-0.752251
3	6	0	3.500324	-0.649276	-0.948299
4	7	0	2.574733	0.005956	-0.282446
5	6	0	1.828585	-0.949637	0.376499
6	6	0	0.664014	-0.561456	1.229283
7	6	0	-0.455439	0.017960	0.371074
8	7	0	-1.547476	0.565517	1.224383
9	8	0	-2.296160	-1.952748	2.095478
10	8	0	-2.299062	-3.001677	-0.419377
11	8	0	-2.574096	-0.960338	-2.230562
12	8	0	-2.589600	1.615317	-1.179378
13	8	0	-0.309801	2.871053	-1.879639
14	8	0	1.668486	2.655169	-0.045328
15	8	0	0.084028	2.674208	2.374812
16	1	0	4.263104	-0.214318	-1.574465
17	1	0	2.021388	-3.176563	0.406497
18	1	0	0.985547	0.188698	1.959547
19	1	0	0.294176	-1.427889	1.781545
20	1	0	-0.091485	0.832765	-0.254615
21	1	0	-0.892737	-0.747647	-0.270627
22	1	0	-1.167880	1.281679	1.858228
23	1	0	-2.245034	1.008847	0.609544
24	1	0	-1.983414	-0.210257	1.756097
25	1	0	3.981203	-2.690373	-1.153431
26	1	0	-1.818750	2.151266	-1.476519
27	1	0	-3.373615	2.155966	-1.316807
28	1	0	2.087628	1.768853	-0.129984
29	1	0	1.279315	2.686688	0.841643
30	1	0	-0.355165	3.531634	2.418380
31	1	0	0.519778	2.571562	3.228756
32	1	0	-2.342995	-2.429751	1.241685
33	1	0	-3.035291	-2.263347	2.625229
34	1	0	-2.643414	-0.033615	-1.934216

35	1	0	-2.430105	-2.316798	-1.104670
36	1	0	-3.158404	-1.045593	-2.989040
37	1	0	-1.568870	-3.548723	-0.722057
38	1	0	0.436881	2.869995	-1.239181
39	1	0	-0.286323	3.718527	-2.331928

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molecule: **t1·$(H_2O)_7$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.70727 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.610757	-1.825334	-0.668320
2	7	0	-2.497106	-1.355654	-0.150266
3	6	0	-2.705287	-0.006702	0.049443
4	6	0	-3.966155	0.325941	-0.363121
5	7	0	-4.526381	-0.843949	-0.815056
6	6	0	-1.629831	0.868051	0.608370
7	6	0	-0.485422	1.025097	-0.389188
8	7	0	0.615623	1.832426	0.204355
9	8	0	2.611503	2.093814	-1.726549
10	8	0	4.624935	0.371115	-1.096264
11	8	0	3.612678	-1.474111	0.721875
12	8	0	1.455423	-0.254184	1.942282
13	8	0	-0.839405	4.203155	0.821006
14	8	0	-0.105420	-2.392911	0.864752
15	1	0	-3.802321	-2.849929	-0.945489
16	1	0	-4.498016	1.262054	-0.371409
17	1	0	-1.243382	0.432676	1.536515
18	1	0	-2.039497	1.851658	0.848061
19	1	0	-0.068190	0.055695	-0.667405
20	1	0	-0.823775	1.533674	-1.292102
21	1	0	1.018443	1.313067	0.999537
22	1	0	1.369036	1.987803	-0.497253
23	1	0	0.252841	2.744835	0.522024
24	1	0	-5.457986	-0.954551	-1.188051
25	1	0	2.381110	1.982325	-2.652943
26	1	0	3.367199	1.494562	-1.554519
27	1	0	-0.961644	-2.093931	0.483787
28	1	0	0.264054	-1.636965	1.347835
29	1	0	2.298560	-0.635696	1.620812
30	1	0	1.541491	-0.171173	2.897566
31	1	0	4.249709	-1.926725	1.283956
32	1	0	3.130878	-2.175671	0.221097
33	1	0	4.351025	-0.282940	-0.426271
34	1	0	5.486280	0.696282	-0.820910

35	1	0	-0.725686	5.015932	0.318520
36	1	0	-1.078490	4.482904	1.710209
37	1	0	1.159651	-2.977522	-0.144348
38	8	0	2.008013	-3.146901	-0.613279
39	1	0	2.126644	-4.100265	-0.636131

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molecule: **t1·$(H_2O)_7$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.70479 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.021197	0.444683	-0.107579
2	7	0	4.682457	-0.731028	0.153132
3	6	0	3.782521	-1.735377	0.086398
4	7	0	2.584545	-1.276347	-0.201905
5	6	0	2.718852	0.091562	-0.328644
6	6	0	1.538061	0.951054	-0.646569
7	6	0	0.540737	0.952537	0.508041
8	7	0	-0.730269	1.615908	0.107720
9	8	0	0.488800	4.164005	-0.048619
10	8	0	-2.400837	0.525949	2.002378
11	8	0	-1.052269	-1.893854	2.066828
12	8	0	-0.031736	-2.305539	-0.420664
13	8	0	-4.831935	-0.033797	0.773192
14	8	0	-4.189521	-0.963023	-1.838822
15	8	0	-1.460493	-0.302653	-1.908031
16	1	0	4.045840	-2.768100	0.251910
17	1	0	4.520354	1.398579	-0.116723
18	1	0	1.044326	0.562890	-1.543980
19	1	0	1.859280	1.973111	-0.857290
20	1	0	0.290540	-0.064489	0.811003
21	1	0	0.936905	1.487557	1.371320
22	1	0	-1.083116	1.179257	-0.756868
23	1	0	-1.446004	1.439615	0.845680
24	1	0	-0.569370	2.622747	-0.034339
25	1	0	5.666027	-0.830171	0.357402
26	1	0	-1.990964	-0.353733	2.106016
27	1	0	-3.285365	0.360152	1.628380
28	1	0	0.911602	-2.030302	-0.396618
29	1	0	-0.477109	-1.691478	-1.026190
30	1	0	-2.408808	-0.533644	-1.907004
31	1	0	-1.220755	-0.201289	-2.835302
32	1	0	-4.694469	-0.561411	-2.555380
33	1	0	-4.350375	-1.910775	-1.914160
34	1	0	-4.691397	-0.318207	-0.144433

35	1	0	-5.569661	0.581752	0.750906
36	1	0	0.454888	4.804567	0.668606
37	1	0	0.620329	4.682186	-0.848591
38	1	0	-0.714672	-2.147218	1.180395
39	1	0	-1.389451	-2.696791	2.472657

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molecule: **t1·$(H_2O)_7$–d**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.70139 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.007864	0.549258	-0.529697
2	6	0	-4.538210	-0.688675	-0.799178
3	7	0	-3.303182	-0.829228	-0.371387
4	6	0	-2.960219	0.376054	0.204272
5	6	0	-4.011861	1.245624	0.110598
6	6	0	-1.601799	0.588159	0.790242
7	6	0	-0.532176	0.576540	-0.296957
8	7	0	0.821339	0.653186	0.317710
9	8	0	1.168326	3.238209	1.325068
10	8	0	3.007038	0.876253	-1.521665
11	8	0	4.505501	-1.281256	-0.912631
12	8	0	3.315835	3.406094	-0.374088
13	8	0	3.154007	-3.276934	0.596978
14	8	0	0.801124	-1.968888	1.410961
15	8	0	-1.301744	-2.894932	-0.383107
16	1	0	-5.127981	-1.439923	-1.300245
17	1	0	-4.135919	2.264122	0.437001
18	1	0	-1.388689	-0.207655	1.512525
19	1	0	-1.573082	1.539163	1.327524
20	1	0	-0.576832	-0.344031	-0.879798
21	1	0	-0.645096	1.427281	-0.968846
22	1	0	0.973269	-0.182830	0.903899
23	1	0	1.562302	0.678412	-0.404938
24	1	0	0.919564	1.518079	0.883343
25	1	0	-5.928429	0.895719	-0.756753
26	1	0	2.840842	0.869195	-2.469675
27	1	0	3.601863	0.115425	-1.335782
28	1	0	-2.023431	-2.238121	-0.373679
29	1	0	-0.655969	-2.590394	0.269515
30	1	0	1.612173	-2.457702	1.176462
31	1	0	0.639785	-2.155996	2.341628
32	1	0	3.682377	-3.608577	1.332348
33	1	0	2.966292	-4.049561	0.051156
34	1	0	4.076589	-1.970335	-0.377872

35	1	0	5.405015	-1.204568	-0.582365
36	1	0	1.983060	3.454761	0.830545
37	1	0	1.308635	3.532578	2.229039
38	1	0	3.357876	2.539890	-0.817009
39	1	0	4.218631	3.627972	-0.130405

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molecule: **t1·$(H_2O)_7$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.69606 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.980548	-1.791255	0.722875
2	7	0	2.755152	-1.601254	0.286050
3	6	0	2.699639	-0.288925	-0.135196
4	6	0	3.915003	0.307206	0.060994
5	7	0	4.717601	-0.665126	0.606508
6	6	0	1.436257	0.291973	-0.683285
7	6	0	0.371812	0.402738	0.404259
8	7	0	-0.910365	0.888318	-0.175338
9	8	0	-2.810076	0.823172	1.879283
10	8	0	-4.516391	-1.251289	1.351826
11	8	0	-3.883024	-2.683895	-1.019426
12	8	0	-1.416998	-1.501367	-1.658284
13	8	0	-0.063114	3.362628	-1.185095
14	8	0	0.336130	-3.122262	0.006642
15	1	0	4.378682	-2.710051	1.124008
16	1	0	4.268849	1.304764	-0.136677
17	1	0	1.059665	-0.348211	-1.488423
18	1	0	1.630324	1.280521	-1.105106
19	1	0	0.179756	-0.567693	0.863975
20	1	0	0.676622	1.107063	1.178584
21	1	0	-1.237579	0.207771	-0.877501
22	1	0	-1.636710	0.956056	0.564970
23	1	0	-0.766941	1.814515	-0.616890
24	1	0	5.686360	-0.561890	0.870544
25	1	0	-2.504203	0.750471	2.787573
26	1	0	-3.441897	0.088661	1.742614
27	1	0	1.192743	-2.664030	0.101264
28	1	0	-0.183003	-2.584676	-0.607568
29	1	0	-2.289685	-1.906582	-1.498541
30	1	0	-1.262171	-1.573894	-2.605805
31	1	0	-4.557850	-2.629383	-1.705949
32	1	0	-3.782233	-3.624859	-0.834394
33	1	0	-4.346782	-1.742860	0.531224
34	1	0	-5.466991	-1.112906	1.386703

35	1	0	-0.338792	4.205433	-0.779097
36	1	0	0.050497	3.542630	-2.122538
37	8	0	-0.856477	5.736572	-0.002560
38	1	0	-1.724799	5.785893	0.408734
39	1	0	-0.260533	6.190797	0.600768

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molecule: **t1·$(H_2O)_7$–f**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.69505 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.278694	-1.510271	0.397965
2	7	0	2.033617	-1.245969	0.059352
3	6	0	2.028896	0.067066	-0.360331
4	6	0	3.293790	0.581742	-0.262620
5	7	0	4.076466	-0.437013	0.220492
6	6	0	0.766644	0.728579	-0.812079
7	6	0	-0.211526	0.883972	0.348273
8	7	0	-1.503396	1.448118	-0.132813
9	8	0	-3.297655	1.432148	2.004411
10	8	0	-5.146812	-0.528888	1.533483
11	8	0	-4.696932	-1.962685	-0.879417
12	8	0	-2.230019	-0.860387	-1.638785
13	8	0	-0.453828	3.935129	-1.025306
14	8	0	-0.475111	-2.614459	-0.109038
15	1	0	3.646237	-2.454047	0.770061
16	1	0	3.691365	1.556139	-0.492107
17	1	0	0.297001	0.125223	-1.596875
18	1	0	0.990290	1.710663	-1.234561
19	1	0	-0.427145	-0.080471	0.810044
20	1	0	0.184853	1.559528	1.106435
21	1	0	-1.908854	0.807115	-0.831890
22	1	0	-2.179024	1.529159	0.654460
23	1	0	-1.343362	2.376936	-0.550887
24	1	0	5.080555	-0.395878	0.406999
25	1	0	-2.970424	1.343674	2.903784
26	1	0	-3.978260	0.738703	1.888809
27	1	0	0.410575	-2.206650	-0.047405
28	1	0	-0.993279	-2.031527	-0.681106
29	1	0	-3.108681	-1.232796	-1.437003
30	1	0	-2.134986	-0.912371	-2.595572
31	1	0	-5.408590	-1.879979	-1.524702
32	1	0	-4.616275	-2.908075	-0.707506
33	1	0	-5.046045	-1.020384	0.701622
34	1	0	-6.085698	-0.342109	1.620356

35	1	0	-0.569626	4.746004	-0.520353
36	1	0	-0.362254	4.215032	-1.941371
37	8	0	6.903388	-0.284864	0.698674
38	1	0	7.288733	-0.271766	1.579870
39	1	0	7.532855	-0.762550	0.150258

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molecule: **t1·$(H_2O)_8$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -972.14580 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.588402	0.560022	-0.692855
2	7	0	3.515986	-0.142373	0.035657
3	6	0	2.957590	-1.321988	0.373360
4	7	0	1.729401	-1.422319	-0.092936
5	6	0	1.484655	-0.245369	-0.768791
6	6	0	0.162560	0.006167	-1.419866
7	6	0	-0.930357	0.149793	-0.365653
8	7	0	-2.275757	0.219983	-1.003657
9	8	0	-1.756416	2.700176	-2.122121
10	8	0	-0.800778	3.728846	0.212699
11	8	0	-1.788275	2.248564	2.300665
12	8	0	-3.279674	-0.000256	1.624381
13	8	0	-1.886959	-2.226724	2.229341
14	8	0	-0.429999	-3.183971	0.160420
15	8	0	-2.183462	-2.490389	-2.043036
16	1	0	3.477404	-2.070354	0.950804
17	1	0	2.786775	1.542236	-1.087938
18	1	0	-0.083074	-0.833136	-2.079245
19	1	0	0.205415	0.909594	-2.031782
20	1	0	-0.935356	-0.703675	0.311940
21	1	0	-0.794641	1.060758	0.217960
22	1	0	-2.429707	-0.619081	-1.579316
23	1	0	-2.986557	0.240150	-0.258095
24	1	0	-2.335781	1.081362	-1.577264
25	1	0	4.460056	0.167495	0.276669
26	1	0	-2.852742	-0.843952	1.900525
27	1	0	-4.190817	-0.038208	1.931806
28	1	0	0.392617	-2.649072	0.065353
29	1	0	-0.928979	-3.057924	-0.660422
30	1	0	-3.004627	-2.982504	-1.928096
31	1	0	-1.896776	-2.686763	-2.942344
32	1	0	-1.403781	3.174698	-1.341589
33	1	0	-2.317923	3.322854	-2.591529
34	1	0	-2.361056	1.474874	2.143035

35	1	0	-1.148294	3.256793	0.995008
36	1	0	-2.122019	2.672920	3.095943
37	1	0	0.143310	3.834878	0.359306
38	1	0	-1.368918	-2.651308	1.508536
39	1	0	-2.244378	-2.937263	2.768552
40	8	0	6.154560	0.775518	0.679930
41	1	0	6.946150	0.360622	0.324218
42	1	0	6.397215	1.081098	1.559111

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molecule: **t1·$(H_2O)_8$–b**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -972.14194 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.768293	0.216100	-0.897133
2	7	0	3.584587	0.523988	-0.414914
3	6	0	3.069734	-0.644790	0.105691
4	6	0	3.965574	-1.662188	-0.076531
5	7	0	5.041096	-1.094440	-0.715044
6	6	0	1.712750	-0.678765	0.730761
7	6	0	0.625054	-0.444369	-0.313627
8	7	0	-0.707167	-0.372689	0.347531
9	8	0	-2.728855	0.140462	-1.627332
10	8	0	-3.453402	2.697685	-1.168666
11	8	0	-2.240097	3.980477	1.048127
12	8	0	-0.222616	2.120009	1.642234
13	8	0	-0.935448	-2.933703	1.416846
14	8	0	1.913903	2.853832	-0.199762
15	1	0	5.456892	0.894048	-1.376365
16	1	0	3.934738	-2.705755	0.187354
17	1	0	1.644502	0.099157	1.499082
18	1	0	1.551292	-1.643266	1.217692
19	1	0	0.785121	0.496711	-0.841271
20	1	0	0.595945	-1.258222	-1.038175
21	1	0	-0.716424	0.430127	0.995505
22	1	0	-1.457538	-0.230377	-0.350113
23	1	0	-0.889034	-1.256009	0.864388
24	1	0	5.887364	-1.567921	-0.995528
25	1	0	-2.422959	0.083096	-2.538431
26	1	0	-3.027401	1.068247	-1.493858
27	1	0	2.532509	2.102691	-0.273309
28	1	0	1.262672	2.596304	0.467435
29	1	0	-0.921211	2.783081	1.487950
30	1	0	0.006767	2.191823	2.574600
31	1	0	-2.845550	4.154266	1.778211
32	1	0	-1.881097	4.841400	0.803675
33	1	0	-3.076869	3.154651	-0.397966
34	1	0	-4.364820	2.994592	-1.240047

35	1	0	-1.763303	-3.373914	1.130284
36	1	0	-0.815160	-3.156022	2.344147
37	1	0	-3.917026	-1.169592	-1.195798
38	8	0	-4.470348	-1.933333	-0.949874
39	8	0	-3.292286	-3.934581	0.501889
40	1	0	-3.746243	-3.249479	-0.028700
41	1	0	-5.324508	-1.575142	-0.694002
42	1	0	-3.333515	-4.745240	-0.012446

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molecule: **t1·$(H_2O)_8$–c**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -972.14107 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.693781	-2.256594	-0.551353
2	7	0	2.482236	-1.746545	-0.540981
3	6	0	2.571290	-0.567412	0.169292
4	6	0	3.860003	-0.380773	0.588563
5	7	0	4.560010	-1.465691	0.119031
6	6	0	1.365821	0.285863	0.399328
7	6	0	0.356774	-0.428142	1.295901
8	7	0	-0.906551	0.354738	1.377911
9	8	0	-2.924216	-1.120271	2.661171
10	8	0	-4.694357	-1.619851	0.619062
11	8	0	-4.296994	-0.309309	-1.873053
12	8	0	-1.554633	0.137480	-1.344342
13	8	0	0.088310	2.913411	2.034168
14	8	0	-0.122117	-2.343483	-1.633092
15	1	0	3.993139	-3.178856	-1.023977
16	1	0	4.326166	0.405570	1.157682
17	1	0	0.894907	0.515869	-0.562947
18	1	0	1.663779	1.230856	0.859006
19	1	0	0.105854	-1.409404	0.891035
20	1	0	0.748548	-0.550982	2.305446
21	1	0	-1.308951	0.419420	0.424520
22	1	0	-1.605705	-0.123206	1.976979
23	1	0	-0.716027	1.308869	1.727676
24	1	0	5.545515	-1.642328	0.247261
25	1	0	-2.727423	-1.946636	3.110701
26	1	0	-3.580076	-1.335275	1.968680
27	1	0	0.783275	-2.180360	-1.309780
28	1	0	-0.580308	-1.491313	-1.578222
29	1	0	-2.483309	0.059213	-1.619236
30	1	0	-1.158896	0.892750	-1.821994
31	1	0	-4.840463	0.475761	-2.004036
32	1	0	-4.473774	-0.873068	-2.634654
33	1	0	-4.587760	-1.168964	-0.234964
34	1	0	-5.640392	-1.646642	0.787113

35	1	0	-0.244800	3.582560	2.638729
36	1	0	0.364163	3.384855	1.229800
37	8	0	0.942523	4.010870	-0.431545
38	1	0	0.648936	4.916712	-0.583720
39	1	0	1.905037	4.045447	-0.480524
40	1	0	0.251758	2.850594	-1.729604
41	8	0	-0.076297	2.191296	-2.363997
42	1	0	-0.216819	2.662232	-3.190052

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molecule: **g1·$(H_2O)_1$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -437.05769 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.953454	-0.287099	-0.270118
2	6	0	-2.146725	-1.256548	0.210476
3	7	0	-0.895167	-0.853962	0.244329
4	6	0	-0.897215	0.441536	-0.236354
5	6	0	-2.174937	0.807840	-0.557093
6	6	0	0.374622	1.227749	-0.339540
7	6	0	1.230630	1.103830	0.916721
8	7	0	1.698392	-0.310671	1.070285
9	1	0	-2.513707	-2.222048	0.520488
10	1	0	-2.586111	1.722148	-0.949904
11	1	0	0.143926	2.282525	-0.494066
12	1	0	0.958225	0.900142	-1.206658
13	1	0	2.113714	1.737899	0.865067
14	1	0	0.657872	1.356202	1.808322
15	1	0	2.146799	-0.464695	1.973116
16	1	0	0.873435	-0.934418	0.978854
17	1	0	2.379684	-0.545926	0.324370
18	1	0	-3.953537	-0.354996	-0.390350
19	8	0	3.612810	-0.676130	-0.972703
20	1	0	4.124680	-1.487433	-1.050020
21	1	0	3.485884	-0.364684	-1.874319

molecule: **g1·$(H_2O)_1$–b**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -437.05746 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.915086	-0.674309	-0.372625
2	6	0	1.988143	-1.438102	0.242742
3	7	0	0.907023	-0.740076	0.513529
4	6	0	1.149681	0.537614	0.045906
5	6	0	2.396955	0.590256	-0.512419
6	6	0	0.119114	1.617284	0.184535
7	6	0	-1.272820	1.136330	-0.210987
8	7	0	-1.740434	0.064608	0.723901
9	1	0	2.145589	-2.481368	0.466006
10	1	0	2.942984	1.389749	-0.983554
11	1	0	0.384146	2.462429	-0.451982
12	1	0	0.090495	1.991425	1.213686
13	1	0	-2.002074	1.943762	-0.178425
14	1	0	-1.268882	0.698706	-1.209166
15	1	0	-2.609190	-0.375000	0.368420
16	1	0	-0.982332	-0.639517	0.809946
17	1	0	-1.923337	0.441002	1.655028
18	1	0	3.825897	-0.982830	-0.679945
19	1	0	-4.056789	-1.663062	-1.113361
20	8	0	-4.078641	-0.955002	-0.462386
21	1	0	-4.775548	-0.357141	-0.749872

molecule: **g1·$(H_2O)_1$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -437.057044 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709525	-0.552606	0.251712
2	6	0	-1.961248	-1.078391	0.089411
3	7	0	-2.775989	-0.012555	-0.204160
4	6	0	-2.014498	1.100533	-0.214282
5	7	0	-0.759909	0.812356	0.057419
6	6	0	0.561812	-1.272838	0.578485
7	6	0	1.619373	-1.219208	-0.538671
8	7	0	2.757386	-0.311864	-0.183686
9	8	0	1.613848	2.079427	0.284351
10	1	0	-2.412514	2.081929	-0.417967
11	1	0	-2.331561	-2.087082	0.157677
12	1	0	0.322112	-2.316832	0.781122
13	1	0	0.983696	-0.871543	1.505940
14	1	0	2.048302	-2.201390	-0.723652
15	1	0	1.198296	-0.840261	-1.468601
16	1	0	3.450199	-0.287619	-0.933403
17	1	0	2.416026	0.676259	-0.015080
18	1	0	3.237825	-0.636061	0.657101
19	1	0	-3.769025	-0.050742	-0.382115
20	1	0	0.667580	1.790718	0.181967
21	1	0	1.752374	2.826711	-0.304744

molecule: **g1·$(H_2O)_1$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -437.05558 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.670155	-0.052191	-0.047713
2	6	0	-0.932683	-1.176640	-0.125731
3	7	0	0.351629	-0.899185	-0.227150
4	6	0	0.444236	0.479028	-0.209117
5	6	0	-0.808958	1.015755	-0.094746
6	6	0	1.776672	1.160160	-0.307239
7	6	0	2.831670	0.474529	0.553226
8	7	0	3.060339	-0.920651	0.048479
9	1	0	-1.366211	-2.163975	-0.102740
10	1	0	-1.150985	2.035523	-0.041997
11	1	0	1.688443	2.195784	0.023215
12	1	0	2.122070	1.186559	-1.346517
13	1	0	3.784521	0.998767	0.526130
14	1	0	2.497847	0.380889	1.585769
15	1	0	3.640121	-1.468218	0.684716
16	1	0	2.121022	-1.370246	-0.061606
17	1	0	3.519569	-0.913801	-0.863871
18	1	0	-2.688392	-0.007838	0.038920
19	8	0	-4.518609	0.102095	0.211770
20	1	0	-5.117851	-0.179233	-0.486133
21	1	0	-4.959595	-0.123768	1.036281

molecule: **g1·$(H_2O)_2$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49718 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.183729	-0.777013	0.004689
2	6	0	-2.874569	0.531035	-0.121345
3	7	0	-1.572059	0.704051	-0.167456
4	6	0	-1.014309	-0.554606	-0.067842
5	6	0	-2.007311	-1.487024	0.042174
6	6	0	0.470994	-0.727118	-0.088785
7	6	0	1.142871	-0.051184	1.119062
8	7	0	2.329008	0.740744	0.673740
9	8	0	3.590670	-1.366048	-0.674751
10	1	0	-3.622588	1.306008	-0.178084
11	1	0	-1.982090	-2.559033	0.138638
12	1	0	0.855732	-0.277982	-1.010396
13	1	0	0.728689	-1.785358	-0.121242
14	1	0	0.465392	0.652393	1.601240
15	1	0	1.483450	-0.776744	1.854770
16	1	0	2.840571	1.130337	1.465469
17	1	0	2.968476	0.138603	0.127477
18	1	0	1.973587	1.522330	0.092759
19	1	0	-4.115224	-1.162048	0.061167
20	1	0	3.465496	-1.541413	-1.612820
21	1	0	4.457113	-1.724323	-0.457738
22	8	0	0.529166	2.507576	-0.465167
23	1	0	-0.323456	2.015888	-0.420908
24	1	0	0.527580	2.988028	-1.297383

molecule: **g1·$(H_2O)_2$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49659 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.690103	0.234102	0.795173
2	7	0	-3.347132	-0.476057	-0.180499
3	6	0	-2.447167	-0.802403	-1.132448
4	7	0	-1.253058	-0.340163	-0.832667
5	6	0	-1.390581	0.315285	0.376508
6	6	0	-0.218975	0.975580	1.037589
7	6	0	1.002635	0.063478	1.092597
8	7	0	1.504405	-0.210112	-0.288395
9	8	0	3.451687	-2.258307	0.031671
10	1	0	-2.707898	-1.370923	-2.011234
11	1	0	-3.189524	0.607055	1.673069
12	1	0	-0.486067	1.257286	2.057132
13	1	0	0.054651	1.894002	0.507973
14	1	0	1.817540	0.525711	1.648200
15	1	0	0.759543	-0.896410	1.548469
16	1	0	2.231963	-0.943510	-0.273876
17	1	0	0.706660	-0.506318	-0.874891
18	1	0	1.896971	0.660240	-0.680900
19	1	0	-4.327223	-0.718090	-0.184760
20	1	0	3.185029	-3.133821	0.328265
21	1	0	4.289418	-2.080445	0.470195
22	8	0	2.361618	2.443134	-0.786666
23	1	0	2.176020	2.943273	-1.587617
24	1	0	3.222125	2.751413	-0.485642

molecule: **g1·$(H_2O)_2$–c**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49603 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.447828	-1.206873	0.109124
2	7	0	3.234343	-0.250506	0.703643
3	6	0	2.575612	0.924528	0.640308
4	7	0	1.414693	0.779974	0.038352
5	6	0	1.319084	-0.553534	-0.302391
6	6	0	0.124674	-1.123346	-1.002437
7	6	0	-1.175069	-1.058086	-0.179777
8	7	0	-2.125564	-0.026656	-0.695277
9	8	0	-4.284571	-0.278079	1.108894
10	1	0	2.975878	1.843928	1.037416
11	1	0	2.750629	-2.237179	0.031450
12	1	0	0.335360	-2.166021	-1.241792
13	1	0	-0.020064	-0.612936	-1.960255
14	1	0	-1.704486	-2.008627	-0.203897
15	1	0	-0.974464	-0.802597	0.860184
16	1	0	-2.977873	-0.023872	-0.107360
17	1	0	-1.694458	0.929216	-0.676045
18	1	0	-2.405651	-0.232663	-1.654561
19	1	0	4.144262	-0.396429	1.116276
20	1	0	-4.226998	0.068610	2.004618
21	1	0	-4.761749	-1.110362	1.182021
22	8	0	-0.722201	2.327341	-0.609958
23	1	0	0.136816	1.924311	-0.321427
24	1	0	-0.940097	3.014707	0.025908

molecule: **g1·$(H_2O)_2$–d**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49543 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.375847	0.902698	0.419989
2	7	0	2.213611	-0.119839	0.049118
3	6	0	1.448846	-1.115560	-0.440323
4	7	0	0.169660	-0.801442	-0.402397
5	6	0	0.108900	0.467934	0.138845
6	6	0	-1.205803	1.160621	0.337537
7	6	0	-2.111898	1.036002	-0.882849
8	7	0	-2.484926	-0.401028	-1.081522
9	8	0	-3.969163	-0.729219	1.280698
10	1	0	1.861410	-2.040905	-0.810986
11	1	0	1.742515	1.825429	0.837463
12	1	0	-1.037100	2.220451	0.532914
13	1	0	-1.731712	0.751265	1.206476
14	1	0	-3.035046	1.598701	-0.755575
15	1	0	-1.605876	1.370178	-1.787901
16	1	0	-2.977284	-0.550602	-1.961468
17	1	0	-1.612134	-0.964200	-1.063832
18	1	0	-3.093049	-0.707091	-0.301109
19	1	0	3.232985	-0.125391	0.127693
20	1	0	-4.905649	-0.521922	1.358844
21	1	0	-3.804315	-1.431233	1.918265
22	8	0	5.067059	-0.058361	0.315503
23	1	0	5.664025	0.008132	-0.435914
24	1	0	5.534299	-0.586177	0.969936

molecule: **g1·$(H_2O)_2$–e**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -513.49479 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.609717	0.980766	-0.330389
2	7	0	2.278730	-0.161243	0.034136
3	6	0	1.401212	-0.961911	0.670540
4	7	0	0.209510	-0.404702	0.744797
5	6	0	0.326823	0.820857	0.118744
6	6	0	-0.846651	1.747401	0.009601
7	6	0	-2.114969	1.018246	-0.419104
8	7	0	-2.523558	0.029709	0.628787
9	8	0	-4.551876	-1.538497	-0.537174
10	1	0	1.670909	-1.932203	1.057082
11	1	0	2.089023	1.785451	-0.862258
12	1	0	-0.634371	2.526356	-0.723963
13	1	0	-1.028843	2.250847	0.965222
14	1	0	-2.945779	1.705186	-0.568277
15	1	0	-1.950933	0.451185	-1.335382
16	1	0	-3.281721	-0.585068	0.280139
17	1	0	-1.685270	-0.531033	0.880682
18	1	0	-2.849233	0.502242	1.473055
19	1	0	3.262471	-0.373194	-0.147531
20	1	0	-4.350627	-2.370160	-0.977313
21	1	0	-5.240045	-1.123341	-1.066218
22	8	0	5.042252	-0.717850	-0.492499
23	1	0	5.696350	-0.723037	0.212714
24	1	0	5.315485	-1.410953	-1.100959

molecule: **g1·$(H_2O)_3$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93953 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.008461	-0.386376	0.329750
2	6	0	3.295215	-0.504112	0.778352
3	7	0	4.056306	0.243087	-0.087871
4	6	0	3.228051	0.783007	-1.007164
5	7	0	1.981927	0.424255	-0.789341
6	6	0	0.751616	-0.989695	0.880434
7	6	0	-0.381602	0.025591	0.979594
8	7	0	-0.790346	0.466200	-0.388591
9	8	0	-3.142882	2.041603	0.255439
10	8	0	-2.246401	-1.840313	-0.912802
11	1	0	3.576647	1.422586	-1.802534
12	1	0	3.723475	-1.034938	1.611477
13	1	0	0.944454	-1.392443	1.875720
14	1	0	0.418678	-1.824958	0.254915
15	1	0	-1.260643	-0.408372	1.455040
16	1	0	-0.073729	0.911945	1.534026
17	1	0	-1.492683	1.215157	-0.331980
18	1	0	0.050011	0.773976	-0.904722
19	1	0	-1.225196	-0.339768	-0.874515
20	1	0	5.056713	0.370574	-0.045069
21	1	0	-3.478534	2.718603	-0.343067
22	1	0	-3.124152	2.456401	1.125310
23	1	0	-2.391169	-2.345345	-1.717481
24	1	0	-3.122305	-1.522084	-0.620563
25	1	0	-4.114462	0.419900	0.196531
26	8	0	-4.402361	-0.506199	0.142756
27	1	0	-5.299608	-0.487258	-0.201409

molecule: **g1·$(H_2O)_3$–b**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93569 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.548572	0.476945	-0.141280
2	6	0	2.588197	1.036481	-0.829814
3	7	0	3.632447	0.151507	-0.702182
4	6	0	3.202384	-0.891747	0.039720
5	7	0	1.947315	-0.730862	0.395682
6	6	0	0.152508	0.968949	0.070928
7	6	0	-0.879185	0.058617	-0.615141
8	7	0	-2.058919	-0.160297	0.268673
9	8	0	-0.261245	-1.591613	1.889166
10	8	0	-3.855403	-1.677617	-1.332027
11	1	0	3.833256	-1.729788	0.290675
12	1	0	2.675471	1.957800	-1.380012
13	1	0	0.050245	1.993511	-0.286112
14	1	0	-0.045882	0.984119	1.147844
15	1	0	-1.237540	0.484331	-1.551032
16	1	0	-0.456703	-0.925620	-0.814198
17	1	0	-2.783783	-0.705892	-0.226239
18	1	0	-1.732420	-0.692900	1.089708
19	1	0	-2.448851	0.748631	0.561637
20	1	0	4.557367	0.258819	-1.092261
21	1	0	-3.599911	-2.564300	-1.604673
22	1	0	-4.265581	-1.278594	-2.105584
23	1	0	0.606549	-1.472890	1.443628
24	1	0	-0.267497	-2.479337	2.256160
25	8	0	-2.583111	2.591615	0.640413
26	1	0	-2.191827	3.092011	1.363479
27	1	0	-3.415572	3.033106	0.444879

molecule: **g1·$(H_2O)_3$–c**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93451 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.067791	1.127728	-0.148850
2	7	0	0.751909	1.088696	-0.192861
3	6	0	0.411235	-0.246229	-0.123976
4	6	0	1.547734	-1.001939	-0.034644
5	7	0	2.592440	-0.110729	-0.053562
6	6	0	-1.025533	-0.660739	-0.143642
7	6	0	-1.777669	-0.173336	1.106242
8	7	0	-3.099317	0.404199	0.717065
9	8	0	-1.662289	2.419397	-0.545729
10	8	0	-3.946854	-1.905806	-0.620402
11	1	0	2.675833	2.018185	-0.183717
12	1	0	1.698304	-2.066008	0.035981
13	1	0	-1.107995	-1.743691	-0.234199
14	1	0	-1.495837	-0.230312	-1.034471
15	1	0	-1.960513	-0.980518	1.812435
16	1	0	-1.229327	0.622429	1.608205
17	1	0	-3.650897	0.670740	1.532598
18	1	0	-2.907993	1.252552	0.153865
19	1	0	-3.632315	-0.290257	0.166818
20	1	0	3.587164	-0.341815	-0.003308
21	1	0	-0.723330	2.141327	-0.433411
22	1	0	-1.690169	3.371300	-0.418044
23	1	0	-4.763938	-2.383464	-0.445920
24	1	0	-3.747223	-2.066854	-1.548171
25	8	0	5.363248	-0.829352	0.104388
26	1	0	5.887201	-0.665121	0.894161
27	1	0	5.971627	-0.730484	-0.634146

molecule: **g1·$(H_2O)_3$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93376 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.640692	-0.509384	0.412223
2	6	0	1.939296	-0.558275	0.842378
3	7	0	2.678351	0.079187	-0.123169
4	6	0	1.824637	0.491047	-1.081787
5	7	0	0.582934	0.153542	-0.798213
6	6	0	-0.599171	-1.043413	1.063863
7	6	0	-1.723227	-0.012645	1.091926
8	7	0	-2.172467	0.294662	-0.299979
9	8	0	-3.884593	2.548002	-0.000522
10	8	0	-3.256073	-2.270330	-0.832942
11	1	0	2.148299	1.029413	-1.958925
12	1	0	2.386533	-0.979034	1.727160
13	1	0	-0.374259	-1.338123	2.089981
14	1	0	-0.957742	-1.936230	0.540763
15	1	0	-2.589285	-0.381750	1.639858
16	1	0	-1.389505	0.923426	1.540123
17	1	0	-2.819300	1.099469	-0.304890
18	1	0	-1.335515	0.499853	-0.872730
19	1	0	-2.644700	-0.534987	-0.692880
20	1	0	3.690865	0.219396	-0.116501
21	1	0	-3.529397	3.441792	0.022611
22	1	0	-4.603268	2.538412	0.638918
23	1	0	-3.112488	-2.775361	-1.639280
24	1	0	-4.127999	-2.529655	-0.519284
25	8	0	5.525910	0.421662	-0.041882
26	1	0	6.111950	-0.033384	-0.654023
27	1	0	5.948766	1.266365	0.139782

molecule: **g1·$(H_2O)_3$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93342 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.603880	-0.416904	-0.652831
2	6	0	1.814170	-1.011678	-0.416427
3	7	0	2.617363	-0.037603	0.121027
4	6	0	1.888220	1.091829	0.196235
5	7	0	0.666410	0.903952	-0.262213
6	6	0	-0.628259	-1.042386	-1.230939
7	6	0	-1.819449	-1.124842	-0.263101
8	7	0	-2.825771	-0.043558	-0.491945
9	8	0	-1.579301	2.398489	-0.361425
10	8	0	-4.714306	-0.557788	1.546649
11	1	0	2.280398	2.018617	0.584968
12	1	0	2.161006	-2.017529	-0.583944
13	1	0	-0.374317	-2.055790	-1.544275
14	1	0	-0.929819	-0.508085	-2.138033
15	1	0	-2.351287	-2.067279	-0.380661
16	1	0	-1.495732	-1.039207	0.773642
17	1	0	-3.588421	-0.137869	0.201904
18	1	0	-2.411362	0.917021	-0.405372
19	1	0	-3.237252	-0.121615	-1.422534
20	1	0	3.592863	-0.144774	0.410224
21	1	0	-4.566666	-0.278915	2.455479
22	1	0	-5.172216	-1.402015	1.603331
23	1	0	-0.669061	2.004576	-0.289063
24	1	0	-1.700740	2.971006	0.401254
25	8	0	5.344492	-0.402799	0.909138
26	1	0	6.073144	-0.054269	0.386673
27	1	0	5.624991	-0.322749	1.825803

molecule: **g1·$(H_2O)_3$–e**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93342 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.603880	-0.416904	-0.652831
2	6	0	1.814170	-1.011678	-0.416427
3	7	0	2.617363	-0.037603	0.121027
4	6	0	1.888220	1.091829	0.196235
5	7	0	0.666410	0.903952	-0.262213
6	6	0	-0.628259	-1.042386	-1.230939
7	6	0	-1.819449	-1.124842	-0.263101
8	7	0	-2.825771	-0.043558	-0.491945
9	8	0	-1.579301	2.398489	-0.361425
10	8	0	-4.714306	-0.557788	1.546649
11	1	0	2.280398	2.018617	0.584968
12	1	0	2.161006	-2.017529	-0.583944
13	1	0	-0.374317	-2.055790	-1.544275
14	1	0	-0.929819	-0.508085	-2.138033
15	1	0	-2.351287	-2.067279	-0.380661
16	1	0	-1.495732	-1.039207	0.773642
17	1	0	-3.588421	-0.137869	0.201904
18	1	0	-2.411362	0.917021	-0.405372
19	1	0	-3.237252	-0.121615	-1.422534
20	1	0	3.592863	-0.144774	0.410224
21	1	0	-4.566666	-0.278915	2.455479
22	1	0	-5.172216	-1.402015	1.603331
23	1	0	-0.669061	2.004576	-0.289063
24	1	0	-1.700740	2.971006	0.401254
25	8	0	5.344492	-0.402799	0.909138
26	1	0	6.073144	-0.054269	0.386673
27	1	0	5.624991	-0.322749	1.825803

molecule: **g1·$(H_2O)_3$–f**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -589.93340 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.748339	-0.524581	-0.308618
2	6	0	3.029222	-0.910720	-0.029286
3	7	0	3.590801	0.145198	0.648050
4	6	0	2.653346	1.112011	0.756586
5	7	0	1.525920	0.742770	0.190644
6	6	0	0.656860	-1.253693	-1.025335
7	6	0	-0.526071	-1.563228	-0.093987
8	7	0	-1.825993	-1.271819	-0.767194
9	8	0	-1.084963	1.373458	-0.744468
10	8	0	-3.735129	-2.046045	1.159535
11	1	0	2.841126	2.053679	1.247896
12	1	0	3.574166	-1.813083	-0.248462
13	1	0	1.044535	-2.172344	-1.466016
14	1	0	0.308473	-0.621561	-1.848239
15	1	0	-0.537052	-2.603720	0.224864
16	1	0	-0.503170	-0.924838	0.788481
17	1	0	-2.614222	-1.535479	-0.148916
18	1	0	-1.847496	-0.247307	-0.942112
19	1	0	-1.921517	-1.775049	-1.649456
20	1	0	4.534393	0.192724	1.003386
21	1	0	-3.625757	-1.736067	2.063875
22	1	0	-4.059348	-2.949147	1.231296
23	1	0	-0.193941	1.369223	-0.340488
24	1	0	-1.538330	2.180525	-0.450162
25	8	0	-2.432930	3.686283	0.102467
26	1	0	-3.246392	3.591142	0.606931
27	1	0	-2.596577	4.409958	-0.509815

molecule: **g1·$(H_2O)_4$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.38330 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.228512	0.570922	0.169959
2	7	0	1.970784	0.396456	0.511051
3	6	0	1.431889	-0.458305	-0.429535
4	6	0	2.391979	-0.797520	-1.340627
5	7	0	3.527009	-0.131482	-0.943247
6	6	0	-0.001298	-0.873345	-0.332699
7	6	0	-0.266735	-1.685999	0.944909
8	7	0	-1.558863	-1.263536	1.562031
9	8	0	-0.166504	1.197224	2.020578
10	8	0	-1.369543	2.573494	-0.062297
11	8	0	-2.721515	1.018152	-1.863708
12	8	0	-3.133475	-1.381000	-0.672873
13	1	0	3.949581	1.185400	0.685084
14	1	0	2.368742	-1.431727	-2.210416
15	1	0	-0.293687	-1.444100	-1.214070
16	1	0	-0.622625	0.029126	-0.324544
17	1	0	-0.328298	-2.752784	0.740153
18	1	0	0.508358	-1.511352	1.689699
19	1	0	-1.810681	-1.852072	2.355915
20	1	0	-1.441857	-0.295940	1.896287
21	1	0	-2.319468	-1.304441	0.847362
22	1	0	4.427073	-0.160364	-1.399663
23	1	0	0.727225	1.005122	1.634979
24	1	0	-0.025073	1.614803	2.876047
25	1	0	-3.054221	-0.540358	-1.172837
26	1	0	-4.052553	-1.655714	-0.734857
27	1	0	-2.246609	1.056650	-2.698524
28	1	0	-2.247176	1.615246	-1.251331
29	1	0	-0.983081	2.193574	0.748808
30	1	0	-1.705950	3.441389	0.177420

molecule: **g1·$(H_2O)_4$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.38228 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.763023	0.618589	-0.416740
2	6	0	-2.056577	-0.392122	0.481431
3	6	0	-3.312846	-0.870326	0.230008
4	7	0	-3.783529	-0.135536	-0.830142
5	6	0	-2.825550	0.742703	-1.185996
6	6	0	-1.057192	-0.853606	1.494332
7	6	0	0.069438	-1.673601	0.868897
8	7	0	0.841362	-0.836659	-0.093839
9	8	0	2.010523	1.268821	1.184000
10	8	0	4.361720	0.688956	-0.149904
11	8	0	3.367598	-1.770256	-1.205406
12	1	0	-2.946351	1.447681	-1.993175
13	1	0	-3.895116	-1.644195	0.700488
14	1	0	-1.551711	-1.477424	2.240067
15	1	0	-0.630019	0.007096	2.018437
16	1	0	0.770568	-2.018844	1.627491
17	1	0	-0.324636	-2.533205	0.327933
18	1	0	1.595031	-1.360583	-0.560544
19	1	0	0.219659	-0.440661	-0.805155
20	1	0	1.295448	-0.028510	0.412317
21	1	0	-4.690495	-0.228022	-1.264705
22	1	0	3.429087	-1.908971	-2.157322
23	1	0	3.774262	-2.548733	-0.808229
24	1	0	1.475656	1.994247	0.810893
25	1	0	2.885408	1.295804	0.756584
26	1	0	4.142407	-0.142989	-0.599683
27	1	0	4.859351	1.212331	-0.783885
28	1	0	-0.604945	2.064390	-0.177134
29	8	0	0.024089	2.781232	0.052355
30	1	0	0.117649	3.317508	-0.739716

molecule: **g1·$(H_2O)_4$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.38164 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.531559	-0.412796	0.583269
2	6	0	-1.642250	0.150647	-0.674864
3	6	0	-2.947871	0.485507	-0.904694
4	7	0	-3.631524	0.115280	0.227483
5	6	0	-2.746371	-0.416582	1.092875
6	6	0	-0.450941	0.363793	-1.554101
7	6	0	0.479544	1.456134	-1.033219
8	7	0	1.140174	1.030929	0.235227
9	8	0	0.715840	-1.696369	1.592453
10	8	0	2.510082	3.348431	1.112968
11	8	0	2.712679	-0.838802	-1.085933
12	1	0	-3.027366	-0.791723	2.064137
13	1	0	-3.434420	0.939518	-1.751092
14	1	0	-0.787589	0.657678	-2.549316
15	1	0	0.117225	-0.565343	-1.662622
16	1	0	1.277740	1.658243	-1.746190
17	1	0	-0.065889	2.377895	-0.831871
18	1	0	1.673156	1.818680	0.642780
19	1	0	0.453090	0.703123	0.919646
20	1	0	1.789173	0.249632	0.020623
21	1	0	-4.623981	0.214470	0.385149
22	1	0	2.165395	3.929760	1.797728
23	1	0	2.925639	3.926179	0.465462
24	1	0	-0.154586	-1.339170	1.300682
25	1	0	0.630698	-1.897660	2.528814
26	1	0	2.584091	-1.784848	-0.872440
27	1	0	3.652018	-0.718432	-1.250242
28	8	0	2.044909	-3.305692	-0.149723
29	1	0	1.485048	-3.924260	-0.626194
30	1	0	1.480162	-2.885171	0.528991

molecule: **g1·$(H_2O)_4$–d**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37957 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.716005	0.550161	-1.195328
2	7	0	2.477934	0.274699	-0.848451
3	6	0	2.559097	-0.371550	0.370477
4	6	0	3.870132	-0.476337	0.746383
5	7	0	4.590840	0.111842	-0.264656
6	6	0	1.328643	-0.837820	1.087983
7	6	0	0.245980	0.235428	1.137531
8	7	0	-0.270333	0.510236	-0.235428
9	8	0	-1.673340	-1.893830	-0.576257
10	8	0	-2.223062	2.471881	0.119734
11	8	0	-4.625368	1.156758	0.051363
12	8	0	-4.475662	-1.663869	-0.247898
13	1	0	4.027231	1.058391	-2.094342
14	1	0	4.338368	-0.902923	1.617008
15	1	0	1.588073	-1.117265	2.110199
16	1	0	0.915401	-1.730409	0.605810
17	1	0	-0.600696	-0.085022	1.743192
18	1	0	0.635900	1.171501	1.537455
19	1	0	-0.938466	1.305168	-0.225455
20	1	0	0.529192	0.703797	-0.857001
21	1	0	-0.768754	-0.330260	-0.577896
22	1	0	5.595141	0.204846	-0.305391
23	1	0	-1.466233	-2.613767	-1.178636
24	1	0	-2.641988	-1.877819	-0.494502
25	1	0	-3.109524	2.058752	0.103116
26	1	0	-4.606088	0.188556	-0.029061
27	1	0	-2.298219	3.294564	-0.371180
28	1	0	-5.326483	1.357611	0.677403
29	1	0	-4.804848	-2.150652	0.516325
30	1	0	-4.996788	-1.979320	-0.995106

molecule: **g1·$(H_2O)_4$–e**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37864 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.327681	0.436437	-1.563194
2	7	0	2.207512	0.158739	-0.932784
3	6	0	2.577433	-0.281227	0.323879
4	6	0	3.940562	-0.260029	0.433781
5	7	0	4.399670	0.195063	-0.778424
6	6	0	1.550779	-0.688072	1.336921
7	6	0	0.413387	0.322866	1.443228
8	7	0	-0.376498	0.337425	0.175580
9	8	0	-1.652220	-2.147875	0.152376
10	8	0	-2.395423	2.430606	0.491899
11	8	0	-4.553638	0.987550	-0.662544
12	1	0	3.415377	0.810290	-2.571045
13	1	0	4.602735	-0.518921	1.242269
14	1	0	2.021778	-0.785313	2.316044
15	1	0	1.132077	-1.668603	1.084355
16	1	0	-0.271254	0.065457	2.250350
17	1	0	0.795980	1.330200	1.607191
18	1	0	-1.077758	1.091387	0.185940
19	1	0	0.275051	0.462813	-0.615797
20	1	0	-0.867913	-0.574174	0.068545
21	1	0	5.365656	0.329876	-1.038479
22	1	0	-2.213914	3.266113	0.046457
23	1	0	-2.518065	2.658150	1.420629
24	1	0	-2.588181	-2.084515	-0.132481
25	1	0	-1.656806	-2.628095	0.985297
26	1	0	-3.858376	1.519470	-0.241839
27	1	0	-5.387316	1.401871	-0.424069
28	1	0	-4.392716	-0.781247	-0.700559
29	8	0	-4.186252	-1.734913	-0.754639
30	1	0	-4.949933	-2.196140	-0.397830

molecule: **g1·$(H_2O)_4$–f**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37805 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.863153	1.621839	-0.421199
2	7	0	-1.937330	0.894277	0.162964
3	6	0	-2.343182	-0.417780	0.028067
4	6	0	-3.529058	-0.464793	-0.650119
5	7	0	-3.844967	0.843933	-0.927122
6	6	0	-1.508445	-1.525707	0.586603
7	6	0	-0.149107	-1.633443	-0.123871
8	7	0	0.957097	-1.786911	0.864619
9	8	0	0.480236	0.807957	1.681217
10	8	0	2.638273	2.286122	0.726700
11	8	0	3.187482	-1.709564	-0.784348
12	8	0	4.221340	0.889276	-1.183835
13	1	0	-2.871659	2.697319	-0.502357
14	1	0	-4.156850	-1.287125	-0.948221
15	1	0	-2.046960	-2.471398	0.523429
16	1	0	-1.340848	-1.322936	1.649348
17	1	0	-0.108757	-2.476369	-0.810866
18	1	0	0.074356	-0.720347	-0.674764
19	1	0	1.869749	-1.854361	0.370786
20	1	0	0.956606	-0.921869	1.442448
21	1	0	0.833145	-2.606622	1.458199
22	1	0	-4.664251	1.169551	-1.418810
23	1	0	-0.327472	1.030014	1.175343
24	1	0	1.187892	1.387395	1.345597
25	1	0	3.898116	-2.354902	-0.834995
26	1	0	3.596121	-0.839822	-0.935291
27	1	0	3.178410	1.856167	0.043747
28	1	0	2.561255	3.206481	0.460891
29	1	0	5.160901	0.984569	-0.990240
30	1	0	4.115666	1.194138	-2.092237

molecule: **g1·$(H_2O)_4$–g**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37675 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.302295	0.195959	-0.838292
2	6	0	1.307116	-0.502687	0.353043
3	6	0	2.590330	-0.597104	0.820327
4	7	0	3.373737	0.048241	-0.103821
5	6	0	2.560011	0.508858	-1.075027
6	6	0	0.035420	-1.024189	0.951339
7	6	0	-1.067223	0.029015	0.965926
8	7	0	-1.460853	0.375407	-0.433421
9	8	0	-3.666743	2.149470	0.210968
10	8	0	-3.171070	-1.760579	-1.015520
11	8	0	6.225076	0.328484	0.054445
12	1	0	2.923570	1.062683	-1.926503
13	1	0	3.000166	-1.053412	1.705608
14	1	0	0.218688	-1.347657	1.976928
15	1	0	-0.318202	-1.901264	0.397756
16	1	0	-1.960736	-0.335362	1.472430
17	1	0	-0.729483	0.945659	1.449385
18	1	0	-2.115025	1.168387	-0.431847
19	1	0	-0.606979	0.590221	-0.975799
20	1	0	-1.951416	-0.436253	-0.853626
21	1	0	4.388787	0.162954	-0.063759
22	1	0	-3.973733	2.838624	-0.388974
23	1	0	-3.571343	2.581007	1.067740
24	1	0	-3.971630	-1.393859	-0.592665
25	1	0	-3.054033	-2.647545	-0.664186
26	1	0	6.813720	-0.131368	-0.551593
27	1	0	6.656169	1.166924	0.245446
28	1	0	-4.771776	0.617394	0.230504
29	8	0	-5.137342	-0.281882	0.196398
30	1	0	-6.036285	-0.191688	-0.132087

molecule: **g1·$(H_2O)_4$–h**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37320 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.057459	0.659991	0.750612
2	6	0	-0.907879	-0.400872	-0.121172
3	6	0	-2.140209	-0.812045	-0.553205
4	7	0	-3.048561	0.007972	0.069208
5	6	0	-2.354788	0.873787	0.835329
6	6	0	0.449528	-0.930461	-0.472570
7	6	0	1.429846	0.182724	-0.826421
8	7	0	1.708255	1.022589	0.378680
9	8	0	3.218257	3.227847	-0.613959
10	8	0	3.120279	-1.050700	1.626128
11	8	0	-5.900803	-0.148558	-0.223877
12	1	0	-2.832243	1.636269	1.430791
13	1	0	-2.439039	-1.594386	-1.230359
14	1	0	0.372623	-1.606071	-1.325911
15	1	0	0.863763	-1.512273	0.358025
16	1	0	2.379357	-0.230053	-1.164152
17	1	0	1.022754	0.839072	-1.595741
18	1	0	2.250405	1.861761	0.120653
19	1	0	0.806547	1.291708	0.806135
20	1	0	2.250137	0.454779	1.052394
21	1	0	-4.065450	-0.028430	-0.027992
22	1	0	2.811490	4.006953	-1.004957
23	1	0	4.029655	3.082408	-1.109639
24	1	0	3.922290	-1.038159	2.155803
25	1	0	3.280815	-1.674873	0.895092
26	1	0	-6.457708	-0.472462	0.490484
27	1	0	-6.416760	0.535257	-0.661454
28	8	0	3.231715	-2.608687	-0.656378
29	1	0	2.733638	-3.431626	-0.690030
30	1	0	4.057509	-2.791753	-1.115729

molecule: **g1·$(H_2O)_4$–i**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37239 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.933484	0.613217	0.090215
2	6	0	1.737755	-0.747613	-0.033665
3	6	0	2.895373	-1.407563	0.271797
4	7	0	3.806543	-0.426188	0.582014
5	6	0	3.185352	0.767483	0.459455
6	6	0	0.402283	-1.281723	-0.442713
7	6	0	-0.677519	-0.979409	0.608684
8	7	0	-1.942759	-0.549434	-0.050643
9	8	0	-0.531950	1.720622	-0.822894
10	8	0	-3.799158	-0.226678	2.089992
11	8	0	-2.141085	-2.822275	-1.731904
12	1	0	3.683817	1.705708	0.645772
13	1	0	3.144274	-2.454991	0.292548
14	1	0	0.461682	-2.354119	-0.628376
15	1	0	0.118709	-0.806306	-1.387531
16	1	0	-0.898779	-1.848617	1.225962
17	1	0	-0.371112	-0.156154	1.253172
18	1	0	-2.693086	-0.427228	0.647900
19	1	0	-1.748257	0.357073	-0.509730
20	1	0	-2.229236	-1.253235	-0.747566
21	1	0	4.768343	-0.568323	0.853337
22	1	0	-3.473473	0.067944	2.946086
23	1	0	-4.511249	-0.843969	2.283444
24	1	0	0.373355	1.559640	-0.491190
25	1	0	-0.698982	2.675399	-0.768543
26	1	0	-1.663802	-2.871571	-2.566191
27	1	0	-2.922648	-3.370630	-1.852068
28	8	0	-1.058829	4.483854	-0.679084
29	1	0	-1.749373	4.793618	-0.085330
30	1	0	-1.182344	4.981365	-1.493028

molecule: **g1·$(H_2O)_4$–j**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37230 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.138937	0.395027	0.863789
2	6	0	1.120065	0.433630	-0.516956
3	6	0	2.336323	0.032112	-1.000098
4	7	0	3.103844	-0.248841	0.103180
5	6	0	2.344898	-0.020505	1.193926
6	6	0	-0.105370	0.862496	-1.266224
7	6	0	-1.367895	0.181826	-0.747679
8	7	0	-1.655540	0.623972	0.649909
9	8	0	-3.762371	-1.074419	1.344827
10	8	0	-2.301956	3.296688	-0.059375
11	8	0	5.831112	-1.140211	0.022995
12	1	0	2.709625	-0.168971	2.198327
13	1	0	2.709951	-0.075464	-2.004504
14	1	0	0.010196	0.619453	-2.323548
15	1	0	-0.241961	1.946923	-1.197169
16	1	0	-2.235397	0.438052	-1.354812
17	1	0	-1.253440	-0.902438	-0.729363
18	1	0	-2.421939	0.053935	1.054581
19	1	0	-0.791465	0.522198	1.207478
20	1	0	-1.928947	1.618161	0.638030
21	1	0	4.073451	-0.572307	0.100670
22	1	0	-3.831043	-1.564123	2.168864
23	1	0	-3.966061	-1.706893	0.630862
24	1	0	-1.912388	4.093216	0.314496
25	1	0	-3.184636	3.551934	-0.344976
26	1	0	6.556650	-0.611037	0.367614
27	1	0	6.085505	-2.055092	0.176378
28	8	0	-4.237884	-2.710185	-0.825955
29	1	0	-5.096683	-3.107620	-0.999526
30	1	0	-3.591430	-3.383368	-1.059294

molecule: **g1·$(H_2O)_4$–k**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37225 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.064063	-0.458236	0.832368
2	6	0	0.883179	0.576773	-0.060649
3	6	0	2.086338	0.887937	-0.635303
4	7	0	3.004878	0.031798	-0.081285
5	6	0	2.347585	-0.756686	0.790137
6	6	0	-0.448819	1.209517	-0.321077
7	6	0	-1.491290	0.267692	-0.946101
8	7	0	-2.477214	-0.234152	0.055625
9	8	0	-1.089702	-1.482295	2.124560
10	8	0	-4.133063	-1.849821	-1.617726
11	8	0	-3.503874	2.329482	0.720989
12	1	0	2.835729	-1.526310	1.367343
13	1	0	2.357039	1.627561	-1.370004
14	1	0	-0.294315	2.048861	-1.000607
15	1	0	-0.855956	1.635353	0.601383
16	1	0	-2.071023	0.786669	-1.707988
17	1	0	-1.019564	-0.600796	-1.404892
18	1	0	-3.154004	-0.852917	-0.418488
19	1	0	-2.023460	-0.763765	0.830351
20	1	0	-2.985895	0.570050	0.453822
21	1	0	4.005091	-0.006010	-0.291163
22	1	0	-3.848428	-2.727452	-1.890401
23	1	0	-4.532667	-1.454581	-2.398633
24	1	0	-0.208804	-1.210061	1.756777
25	1	0	-1.067845	-2.437751	2.227122
26	1	0	-3.445920	2.753472	1.582862
27	1	0	-4.301616	2.682358	0.314707
28	8	0	5.796310	-0.052650	-0.723699
29	1	0	6.479885	0.243203	-0.114925
30	1	0	6.170342	-0.812887	-1.179252

molecule: **g1·$(H_2O)_4$–l**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -666.37171 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.094669	-0.226423	-0.671747
2	6	0	0.088490	0.340188	0.587914
3	6	0	-1.171900	0.258928	1.116471
4	7	0	-1.940788	-0.360085	0.162784
5	6	0	-1.140200	-0.634884	-0.886098
6	6	0	1.335321	0.920559	1.184504
7	6	0	2.533395	-0.011824	1.037232
8	7	0	2.885720	-0.167927	-0.406756
9	8	0	4.784946	-2.287840	-0.492088
10	8	0	3.762944	2.503636	-0.750965
11	8	0	-4.694543	-0.941498	0.437979
12	1	0	-1.495646	-1.129891	-1.776393
13	1	0	-1.573877	0.580171	2.062774
14	1	0	1.175807	1.114975	2.246079
15	1	0	1.580503	1.878048	0.713132
16	1	0	3.411481	0.384633	1.545244
17	1	0	2.312558	-1.005115	1.428388
18	1	0	3.588022	-0.914090	-0.534349
19	1	0	2.021466	-0.394948	-0.928548
20	1	0	3.260874	0.726112	-0.760001
21	1	0	-2.939983	-0.581158	0.235981
22	1	0	4.499107	-3.196458	-0.356576
23	1	0	5.633414	-2.214337	-0.044484
24	1	0	3.491143	3.110549	-1.446402
25	1	0	4.642796	2.790811	-0.487941
26	1	0	-5.398064	-0.413349	0.019367
27	1	0	-5.029550	-1.840528	0.490461
28	8	0	-6.685604	0.586819	-0.749552
29	1	0	-7.165155	1.227946	-0.216286
30	1	0	-6.504686	1.030936	-1.583545

molecule: **g1·$(H_2O)_5$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.82049 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.153640	-0.750679	0.829274
2	7	0	-1.897641	-0.460494	0.561157
3	6	0	-1.885751	0.083082	-0.707684
4	6	0	-3.163972	0.112583	-1.193626
5	7	0	-3.952648	-0.421853	-0.204576
6	6	0	-0.639605	0.562303	-1.385047
7	6	0	0.027173	1.769124	-0.710370
8	7	0	1.122992	1.364843	0.218129
9	8	0	0.316621	-0.712742	2.045821
10	8	0	1.749099	-2.953138	1.323151
11	8	0	2.817172	-2.576372	-1.159498
12	8	0	2.788815	0.100840	-1.614360
13	8	0	1.842569	3.946663	1.151954
14	1	0	-3.523431	-1.192117	1.741112
15	1	0	-3.566662	0.457145	-2.130989
16	1	0	-0.902539	0.846795	-2.404903
17	1	0	0.088524	-0.250815	-1.470908
18	1	0	0.489709	2.415833	-1.454621
19	1	0	-0.692887	2.357117	-0.142285
20	1	0	1.511298	2.206718	0.672816
21	1	0	0.813878	0.705124	0.951472
22	1	0	1.871654	0.901274	-0.334666
23	1	0	-4.953423	-0.549712	-0.241425
24	1	0	-0.576928	-0.697215	1.594149
25	1	0	0.169579	-0.520921	2.977316
26	1	0	2.849450	-0.872578	-1.508533
27	1	0	3.666997	0.405293	-1.858752
28	1	0	2.365095	-3.161131	-1.773564
29	1	0	2.439380	-2.762556	-0.275307
30	1	0	1.261704	-2.176061	1.660321
31	1	0	2.303828	-3.259000	2.045723
32	1	0	2.679481	4.375787	0.948940
33	1	0	1.576945	4.293066	2.009306

molecule: **g1·$(H_2O)_5$–b**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.82027 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.375117	0.107355	0.900361
2	6	0	-3.213625	0.252657	1.573918
3	7	0	-2.180343	0.055654	0.784970
4	6	0	-2.703440	-0.228355	-0.461894
5	6	0	-4.069744	-0.196032	-0.404390
6	6	0	-1.811612	-0.509343	-1.632775
7	6	0	-0.687043	0.512875	-1.764048
8	7	0	0.248771	0.397724	-0.608191
9	8	0	1.582709	-2.097939	-0.240366
10	8	0	4.226803	-1.535170	-0.345113
11	8	0	3.820759	0.858063	1.006215
12	8	0	2.315954	2.487889	-0.687627
13	1	0	-3.175846	0.500148	2.623111
14	1	0	-4.827205	-0.355254	-1.153016
15	1	0	-2.400340	-0.496295	-2.550994
16	1	0	-1.374349	-1.510457	-1.548069
17	1	0	-0.109500	0.349083	-2.672596
18	1	0	-1.078561	1.529920	-1.769553
19	1	0	0.964326	1.138523	-0.620993
20	1	0	-0.281575	0.451500	0.277437
21	1	0	0.729052	-0.519734	-0.603894
22	1	0	-5.301524	0.208604	1.288541
23	1	0	2.036875	3.344264	-0.343565
24	1	0	2.673710	2.667279	-1.564767
25	1	0	2.550953	-2.049468	-0.388303
26	1	0	1.292519	-2.975915	-0.502930
27	1	0	3.436998	1.548401	0.436431
28	1	0	4.505099	1.281874	1.533326
29	1	0	4.229270	-0.664515	0.093084
30	1	0	4.723121	-1.426538	-1.160970
31	1	0	2.267068	0.079628	1.832987
32	8	0	1.401173	-0.321147	2.002415
33	1	0	1.420334	-1.150553	1.505703

molecule: **g1·$(H_2O)_5$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81877 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.330385	-0.489733	0.937816
2	7	0	-2.085364	-0.450023	0.509080
3	6	0	-2.128837	0.119151	-0.750340
4	6	0	-3.425228	0.419864	-1.063967
5	7	0	-4.171312	0.024075	0.019113
6	6	0	-0.888750	0.375781	-1.546602
7	6	0	-0.028480	1.488990	-0.952909
8	7	0	0.583450	1.054143	0.335783
9	8	0	0.094976	-1.720848	1.671137
10	8	0	2.376879	-0.686202	-0.776045
11	8	0	1.647064	-3.222239	0.012059
12	8	0	1.809657	3.394827	1.382323
13	1	0	-3.664335	-0.879622	1.886333
14	1	0	-3.867529	0.866202	-1.938196
15	1	0	-1.167280	0.669232	-2.559766
16	1	0	-0.288328	-0.536401	-1.624720
17	1	0	0.796487	1.740207	-1.618368
18	1	0	-0.619506	2.384334	-0.760814
19	1	0	1.054227	1.850730	0.796700
20	1	0	-0.120838	0.669964	0.971040
21	1	0	1.290101	0.311992	0.125796
22	1	0	-5.174420	0.095324	0.111233
23	1	0	1.312937	4.215758	1.453579
24	1	0	2.692125	3.650922	1.096933
25	1	0	-0.749868	-1.366482	1.309819
26	1	0	-0.083326	-1.980009	2.579744
27	1	0	2.236292	-1.636813	-0.611037
28	1	0	3.329493	-0.516103	-0.680751
29	1	0	1.154522	-3.844835	-0.528970
30	1	0	1.005458	-2.830866	0.637530
31	8	0	5.088300	-0.044197	-0.490759
32	1	0	5.528513	-0.229642	0.344270
33	1	0	5.722921	-0.286304	-1.171891

molecule: **g1·$(H_2O)_5$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81809 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.574310	0.485196	-0.548305
2	6	0	3.499273	0.796909	-1.303751
3	7	0	2.412229	0.220178	-0.840475
4	6	0	2.806754	-0.497742	0.272438
5	6	0	4.151099	-0.337767	0.467246
6	6	0	1.819682	-1.292233	1.072424
7	6	0	0.559752	-0.494568	1.394248
8	7	0	-0.197556	-0.199449	0.141442
9	8	0	-1.279455	-2.665623	-0.620978
10	8	0	-3.997695	-2.457936	-0.581529
11	8	0	-4.413973	0.242279	-0.424061
12	8	0	-2.332253	1.598103	0.860725
13	1	0	3.559671	1.439612	-2.167830
14	1	0	4.822755	-0.724965	1.214499
15	1	0	2.279042	-1.608528	2.009937
16	1	0	1.536194	-2.202107	0.532128
17	1	0	-0.104557	-1.054034	2.051798
18	1	0	0.806282	0.457710	1.864037
19	1	0	-0.970252	0.460798	0.326594
20	1	0	0.455571	0.200887	-0.550737
21	1	0	-0.593577	-1.082807	-0.237580
22	1	0	5.519217	0.805161	-0.702619
23	1	0	-2.215889	2.514072	0.531705
24	1	0	-2.438351	1.668425	1.815287
25	1	0	-2.258677	-2.681938	-0.578893
26	1	0	-0.975313	-3.484015	-0.219297
27	1	0	-3.735601	0.753982	0.052452
28	1	0	-5.258693	0.641094	-0.198958
29	1	0	-4.222377	-1.510797	-0.485372
30	1	0	-4.522442	-2.925327	0.073883
31	8	0	-2.016876	4.138313	-0.091717
32	1	0	-1.190190	4.386970	-0.516521
33	1	0	-2.713028	4.515650	-0.638304

molecule: **g1·$(H_2O)_5$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81792 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.249440	0.344733	-0.046095
2	7	0	-2.990981	0.353324	0.337764
3	6	0	-2.396427	-0.739076	-0.259937
4	6	0	-3.326668	-1.402713	-1.012146
5	7	0	-4.497529	-0.700090	-0.861854
6	6	0	-0.949795	-1.078591	-0.077680
7	6	0	0.024115	-0.023206	-0.628891
8	7	0	0.628759	0.807630	0.451233
9	8	0	-1.469518	2.040288	1.850164
10	8	0	2.045266	-1.338244	1.574497
11	8	0	2.485631	2.220009	-1.085302
12	8	0	4.667231	0.572487	-1.257881
13	8	0	4.627598	-1.686055	0.463591
14	1	0	-5.005657	1.059723	0.237023
15	1	0	-3.259516	-2.288513	-1.620785
16	1	0	-0.759187	-2.025780	-0.583755
17	1	0	-0.732798	-1.249882	0.981452
18	1	0	0.856263	-0.500312	-1.144814
19	1	0	-0.470966	0.651997	-1.326391
20	1	0	1.299184	1.475030	0.026223
21	1	0	-0.085906	1.332399	0.993465
22	1	0	1.157737	0.184122	1.082599
23	1	0	-5.387224	-0.923760	-1.283219
24	1	0	-2.154401	1.521658	1.358185
25	1	0	-1.683499	2.969082	1.726231
26	1	0	2.014379	-1.703422	2.463053
27	1	0	2.949052	-1.490631	1.250855
28	1	0	3.293624	1.676523	-1.176740
29	1	0	4.671613	-0.224856	-0.702298
30	1	0	2.781105	3.127317	-0.972135
31	1	0	5.004441	0.300397	-2.115904
32	1	0	4.716238	-2.530680	0.007347
33	1	0	5.353387	-1.661222	1.097553

molecule: **g1·$(H_2O)_5$–f**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81674 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.808963	-2.153999	-0.060615
2	7	0	1.903767	-1.284029	0.328793
3	6	0	2.313320	-0.061785	-0.164976
4	6	0	3.479912	-0.215175	-0.860956
5	7	0	3.780821	-1.554230	-0.782504
6	6	0	1.498338	1.165199	0.091328
7	6	0	0.125429	1.089565	-0.595974
8	7	0	-0.944049	1.584582	0.313494
9	8	0	-0.488192	-0.738664	1.827549
10	8	0	-2.713857	-2.326653	1.264161
11	8	0	0.242234	4.133456	0.646322
12	8	0	-3.212478	1.089941	-1.251620
13	8	0	-4.196991	-1.553220	-1.037755
14	1	0	2.809429	-3.211560	0.151481
15	1	0	4.103512	0.487366	-1.387000
16	1	0	2.037211	2.055574	-0.232500
17	1	0	1.350441	1.257755	1.172700
18	1	0	0.094346	1.683746	-1.507683
19	1	0	-0.129623	0.058237	-0.838074
20	1	0	-1.863235	1.541783	-0.161668
21	1	0	-0.962500	0.944230	1.125412
22	1	0	-0.735546	2.549233	0.608324
23	1	0	4.583752	-2.010708	-1.189590
24	1	0	0.300833	-1.103466	1.380976
25	1	0	-1.217666	-1.357644	1.648058
26	1	0	0.860357	4.324451	1.358769
27	1	0	-0.162383	4.978093	0.425663
28	1	0	-3.915589	1.691243	-1.511740
29	1	0	-3.614133	0.206363	-1.196279
30	1	0	-3.216645	-2.121938	0.459119
31	1	0	-2.739688	-3.282822	1.356834
32	1	0	-5.145785	-1.632633	-0.886535
33	1	0	-4.022371	-2.063278	-1.836847

molecule: **g1·$(H_2O)_5$–g**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81590 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.791453	0.057131	-0.329179
2	6	0	2.792155	0.418843	-1.158751
3	7	0	1.613559	0.113684	-0.655407
4	6	0	1.868778	-0.474624	0.567844
5	6	0	3.220455	-0.511654	0.782093
6	6	0	0.753407	-0.958715	1.444461
7	6	0	-0.365078	0.070030	1.578300
8	7	0	-1.034051	0.270340	0.257906
9	8	0	-2.388037	-2.127531	-0.228674
10	8	0	-4.919501	-1.503167	-1.017273
11	8	0	-5.087353	1.231829	-0.828051
12	8	0	-2.966959	2.439216	0.624502
13	1	0	2.968207	0.897448	-2.109517
14	1	0	3.806561	-0.881545	1.606463
15	1	0	1.140809	-1.181102	2.439759
16	1	0	0.332824	-1.889950	1.048865
17	1	0	-1.126799	-0.261560	2.282884
18	1	0	0.024534	1.035269	1.901684
19	1	0	-1.705167	1.049827	0.298247
20	1	0	-0.305414	0.458781	-0.451197
21	1	0	-1.543205	-0.598217	-0.005990
22	1	0	4.790946	0.187748	-0.499694
23	1	0	-2.707289	3.299195	0.274683
24	1	0	-3.157028	2.589566	1.557689
25	1	0	-3.325116	-1.989108	-0.481194
26	1	0	-2.390139	-2.794245	0.463808
27	1	0	-4.406242	1.687048	-0.306199
28	1	0	-5.910287	1.697880	-0.656688
29	1	0	-5.054607	-0.539221	-0.928314
30	1	0	-5.694966	-1.919663	-0.631805
31	8	0	6.606329	0.400799	-0.780091
32	1	0	7.043225	0.033266	-1.554183
33	1	0	7.048283	1.238046	-0.609538

molecule: **g1·$(H_2O)_5$–h**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81589 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.059662	-0.777680	-0.448980
2	6	0	-4.035212	-1.020028	-1.294496
3	7	0	-2.926398	-0.456639	-0.867651
4	6	0	-3.253064	0.178779	0.315226
5	6	0	-4.578889	-0.016589	0.588815
6	6	0	-2.222298	0.931005	1.100794
7	6	0	-0.942414	0.123750	1.294884
8	7	0	-0.265112	-0.089837	-0.019317
9	8	0	0.790026	2.407796	-0.662086
10	8	0	3.475364	2.317613	-0.257464
11	8	0	4.016347	-0.326970	-0.486576
12	8	0	1.893394	-1.986219	0.503921
13	1	0	-4.147146	-1.604256	-2.194197
14	1	0	-5.202002	0.306719	1.405183
15	1	0	-2.623996	1.183788	2.082972
16	1	0	-1.976656	1.875130	0.602443
17	1	0	-0.239146	0.646085	1.942202
18	1	0	-1.157593	-0.856863	1.719517
19	1	0	0.508484	-0.763860	0.072001
20	1	0	-0.962696	-0.441656	-0.695139
21	1	0	0.114077	0.815968	-0.362489
22	1	0	-6.008907	-1.102455	-0.560655
23	1	0	1.820919	-2.830965	0.045329
24	1	0	1.968706	-2.209507	1.438549
25	1	0	1.752573	2.474354	-0.485125
26	1	0	0.398791	3.244225	-0.396602
27	1	0	3.353823	-0.935072	-0.126175
28	1	0	4.887028	-0.721370	-0.309967
29	1	0	3.735072	1.372022	-0.297341
30	1	0	3.866162	2.669542	0.546676
31	8	0	6.579959	-1.350911	-0.038376
32	1	0	6.966150	-1.336840	0.842408
33	1	0	6.855105	-2.187871	-0.424644

molecule: **g1·$(H_2O)_5$–i**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81311 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.836984	-2.122470	0.506871
2	7	0	1.866797	-1.287612	0.806558
3	6	0	1.663402	-0.516503	-0.320199
4	6	0	2.528746	-0.906769	-1.303794
5	7	0	3.268213	-1.929246	-0.758205
6	6	0	0.613106	0.547567	-0.322895
7	6	0	-0.799526	-0.044593	-0.190921
8	7	0	-1.631264	0.775917	0.732295
9	8	0	0.130067	-0.193550	2.718832
10	8	0	-1.123968	3.179208	-0.594455
11	8	0	1.523916	3.987506	-0.488827
12	8	0	-4.088445	-0.502186	0.348666
13	1	0	3.257781	-2.870758	1.159736
14	1	0	2.680191	-0.557661	-2.310932
15	1	0	0.687138	1.152628	-1.226912
16	1	0	0.800627	1.216900	0.523579
17	1	0	-1.310191	-0.086457	-1.152113
18	1	0	-0.763679	-1.048600	0.231119
19	1	0	-2.604040	0.417944	0.734662
20	1	0	-1.225206	0.684873	1.674769
21	1	0	-1.613136	1.762799	0.424118
22	1	0	4.004463	-2.444897	-1.217668
23	1	0	-4.685108	-0.793278	1.043604
24	1	0	-3.969090	-1.264502	-0.247838
25	1	0	0.794982	-0.707791	2.210217
26	1	0	-0.017862	-0.668731	3.540496
27	1	0	-0.203688	3.500265	-0.561116
28	1	0	-1.676633	3.958189	-0.701699
29	1	0	2.124046	3.700160	-1.183953
30	1	0	2.011823	3.876817	0.333069
31	8	0	-3.604259	-2.597546	-1.388970
32	1	0	-3.857263	-2.504771	-2.312514
33	1	0	-2.716137	-2.967391	-1.401510

molecule: **g1·$(H_2O)_5$–j**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -742.81192 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.642991	-1.010702	0.827127
2	7	0	1.341067	-0.841175	0.931083
3	6	0	1.004645	0.094285	-0.025375
4	6	0	2.129471	0.476826	-0.703381
5	7	0	3.163223	-0.235653	-0.146127
6	6	0	-0.417819	0.525029	-0.189599
7	6	0	-1.311544	-0.625246	-0.681731
8	7	0	-2.607089	-0.632934	0.054134
9	8	0	-1.046600	-1.380351	2.285987
10	8	0	-3.189822	2.049113	-0.453095
11	8	0	-1.323817	3.877569	0.469982
12	8	0	-4.132273	-2.655950	-1.253366
13	1	0	3.245165	-1.672401	1.430082
14	1	0	2.278407	1.176250	-1.508681
15	1	0	-0.480474	1.372578	-0.872594
16	1	0	-0.786895	0.873358	0.781224
17	1	0	-1.531043	-0.539597	-1.744717
18	1	0	-0.841466	-1.590189	-0.495625
19	1	0	-3.244847	-1.340903	-0.343831
20	1	0	-2.398311	-0.870838	1.035640
21	1	0	-3.039803	0.305272	-0.004192
22	1	0	4.147691	-0.190053	-0.417910
23	1	0	-3.797754	-3.557935	-1.268343
24	1	0	-4.483226	-2.496477	-2.134974
25	1	0	-0.126476	-1.325080	1.941819
26	1	0	-1.097846	-2.186852	2.805877
27	1	0	-2.552988	2.711648	-0.126214
28	1	0	-4.042048	2.491878	-0.491406
29	1	0	-0.629532	4.175895	-0.125786
30	1	0	-0.886245	3.713614	1.311245
31	8	0	5.911434	-0.071439	-0.955669
32	1	0	6.558515	0.435260	-0.455776
33	1	0	6.390928	-0.829795	-1.302440

molecule: **g1·$(H_2O)_6$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.26403 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.833454	-0.032059	0.888867
2	7	0	2.590824	0.169292	0.500311
3	6	0	2.468798	-0.439971	-0.735116
4	6	0	3.663724	-1.011507	-1.074860
5	7	0	4.515768	-0.739418	-0.032510
6	6	0	1.172766	-0.456606	-1.482052
7	6	0	0.120161	-1.340430	-0.817481
8	7	0	-0.301468	-0.771100	0.493618
9	8	0	0.733383	1.920959	1.605647
10	8	0	-1.727861	1.254942	-0.715428
11	8	0	-0.514146	3.647687	-0.095840
12	8	0	-2.234590	-2.588399	1.299369
13	8	0	-4.543042	-1.715698	0.121077
14	8	0	-4.577510	1.029181	-0.576735
15	1	0	4.274909	0.314003	1.810022
16	1	0	3.971582	-1.570514	-1.942148
17	1	0	1.343248	-0.837669	-2.490102
18	1	0	0.774290	0.558254	-1.578956
19	1	0	-0.777995	-1.399238	-1.431171
20	1	0	0.502597	-2.345551	-0.641200
21	1	0	-0.963498	-1.419033	0.966101
22	1	0	0.503170	-0.589390	1.098106
23	1	0	-0.797460	0.124728	0.310078
24	1	0	5.485619	-1.013181	0.032090
25	1	0	1.479290	1.375344	1.264700
26	1	0	0.973991	2.184099	2.498616
27	1	0	-1.431023	2.177620	-0.613978
28	1	0	-2.695986	1.255474	-0.666513
29	1	0	0.082188	4.114501	-0.687019
30	1	0	0.050295	3.153974	0.531453
31	1	0	-3.090016	-2.319040	0.907648
32	1	0	-4.584831	-0.783038	-0.150085
33	1	0	-2.426988	-2.897854	2.188511
34	1	0	-4.925644	-2.219877	-0.602399

35	1	0	-5.021982	1.241394	-1.405137
36	1	0	-5.004911	1.577642	0.090586

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molecule: **g1·$(H_2O)_6$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25941 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.918377	-0.104648	-0.976332
2	6	0	-3.344330	0.958616	-0.373160
3	7	0	-2.058834	0.756902	-0.186177
4	6	0	-1.791379	-0.499630	-0.691729
5	6	0	-2.940493	-1.047077	-1.189345
6	6	0	-0.400539	-1.046485	-0.644668
7	6	0	0.560912	-0.210846	-1.503905
8	7	0	1.877941	-0.063214	-0.823762
9	8	0	0.348539	1.495223	1.038420
10	8	0	0.332946	-0.452252	2.970116
11	8	0	0.814862	-3.002112	2.104835
12	8	0	2.299393	-2.730085	-0.160437
13	8	0	3.488141	1.291281	-2.742960
14	1	0	-3.898983	1.840507	-0.093842
15	1	0	-3.142432	-1.993995	-1.660307
16	1	0	-0.389335	-2.089563	-0.961841
17	1	0	-0.058619	-1.029130	0.395635
18	1	0	0.734522	-0.667764	-2.476846
19	1	0	0.172132	0.795877	-1.652487
20	1	0	2.552578	0.415074	-1.442471
21	1	0	1.723594	0.508850	0.018322
22	1	0	2.242272	-0.997288	-0.552503
23	1	0	-4.892620	-0.187333	-1.227335
24	1	0	3.228613	2.165498	-3.049492
25	1	0	3.836468	0.838925	-3.517270
26	1	0	-0.553064	1.452411	0.647065
27	1	0	0.523196	2.422935	1.280591
28	1	0	1.789911	-2.922291	0.654654
29	1	0	3.135726	-3.196049	-0.074995
30	1	0	-0.025969	-3.466545	2.070569
31	1	0	0.618923	-2.109667	2.454803
32	1	0	0.372094	0.312300	2.360141
33	1	0	0.725802	-0.160743	3.797450
34	8	0	0.961746	4.110922	1.756136

35	1	0	0.972809	4.804026	1.089250
36	1	0	0.557232	4.509400	2.532767

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molecule: **g1·$(H_2O)_6$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25877 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.043122	-2.900308	-0.270142
2	6	0	2.978755	-1.976161	0.707836
3	7	0	1.998871	-1.125022	0.484410
4	6	0	1.401330	-1.520381	-0.695495
5	6	0	2.044857	-2.628853	-1.173406
6	6	0	0.223683	-0.817501	-1.295891
7	6	0	-1.057038	-0.895621	-0.455022
8	7	0	-1.216426	0.277943	0.451906
9	8	0	1.155877	0.929863	1.985363
10	8	0	2.029979	3.353042	1.008961
11	8	0	0.812576	3.894365	-1.372225
12	8	0	-1.367629	2.277800	-1.483364
13	8	0	-3.669581	-0.356373	1.646870
14	1	0	3.653977	-1.960338	1.548511
15	1	0	1.883472	-3.227652	-2.053544
16	1	0	0.020197	-1.274644	-2.265335
17	1	0	0.460755	0.232967	-1.492997
18	1	0	-1.935586	-0.895639	-1.099068
19	1	0	-1.076914	-1.797128	0.156695
20	1	0	-2.079676	0.152751	1.012785
21	1	0	-0.417189	0.416078	1.090695
22	1	0	-1.314304	1.133623	-0.129680
23	1	0	3.711089	-3.655386	-0.325939
24	1	0	-3.754382	-0.827039	2.480388
25	1	0	-4.274031	-0.796758	1.020925
26	1	0	1.586269	0.162935	1.508315
27	1	0	1.220558	0.750492	2.928431
28	1	0	-0.608372	2.898378	-1.504150
29	1	0	-2.155313	2.805767	-1.639023
30	1	0	1.474252	3.868726	-2.068626
31	1	0	1.289650	3.733021	-0.532458
32	1	0	1.733076	2.519575	1.424537
33	1	0	2.031036	4.015766	1.704592
34	8	0	-5.308130	-1.584318	-0.214355

35	1	0	-6.103494	-1.143713	-0.528693
36	1	0	-4.898311	-1.964011	-0.997703

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molecule: **g1·$(H_2O)_6$–d**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25785 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.417738	-0.105851	-0.081477
2	6	0	-2.595994	-0.531257	0.895036
3	7	0	-1.331848	-0.326601	0.577980
4	6	0	-1.338976	0.263304	-0.669118
5	6	0	-2.635267	0.405303	-1.086010
6	6	0	-0.095882	0.677045	-1.394256
7	6	0	0.684331	1.816096	-0.725708
8	7	0	1.756272	1.312787	0.182188
9	8	0	0.877577	-0.736189	2.015055
10	8	0	2.193026	-3.046589	1.305238
11	8	0	3.240813	-2.743529	-1.195183
12	8	0	3.280079	-0.072363	-1.688005
13	8	0	2.851501	3.716494	1.252472
14	1	0	-2.952178	-0.979493	1.809318
15	1	0	-3.052429	0.814043	-1.991036
16	1	0	-0.388246	1.011202	-2.390938
17	1	0	0.571701	-0.178590	-1.539955
18	1	0	1.190031	2.422664	-1.475901
19	1	0	0.026717	2.461170	-0.143816
20	1	0	2.227626	2.112391	0.634983
21	1	0	1.407047	0.677626	0.918903
22	1	0	2.451119	0.788296	-0.386322
23	1	0	-4.439447	-0.159279	-0.074452
24	1	0	2.363738	4.256847	1.881353
25	1	0	3.325474	4.337052	0.690624
26	1	0	-0.017940	-0.663001	1.566587
27	1	0	0.746548	-0.540150	2.947999
28	1	0	3.308003	-1.045686	-1.568731
29	1	0	4.160008	0.193795	-1.968430
30	1	0	2.773645	-3.331228	-1.794961
31	1	0	2.867850	-2.907040	-0.304375
32	1	0	1.742998	-2.241754	1.630559
33	1	0	2.753030	-3.351790	2.024024
34	8	0	-6.275200	-0.221896	-0.131015

35	1	0	-6.741756	-1.045004	-0.304802
36	1	0	-6.821967	0.255221	0.500373

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molecule: **g1·$(H_2O)_6$–e**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -819.25521 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.565123	0.726685	0.512578
2	7	0	-2.266066	0.628181	0.716841
3	6	0	-1.870844	-0.541971	0.103224
4	6	0	-2.962739	-1.136922	-0.470605
5	7	0	-4.029648	-0.318018	-0.198582
6	6	0	-0.454572	-1.028652	0.091023
7	6	0	0.529681	-0.123453	-0.663664
8	7	0	1.264736	0.804246	0.243480
9	8	0	-0.485595	2.376834	1.794699
10	8	0	2.681443	-1.230283	1.564482
11	8	0	3.094836	1.880932	-1.575168
12	8	0	5.254965	0.195061	-1.534809
13	8	0	5.304893	-1.676621	0.601568
14	1	0	-4.198686	1.528277	0.858705
15	1	0	-3.065301	-2.050976	-1.031050
16	1	0	-0.443906	-2.010383	-0.385166
17	1	0	-0.090918	-1.179507	1.112475
18	1	0	1.292856	-0.722106	-1.159726
19	1	0	0.020787	0.478897	-1.415725
20	1	0	1.931052	1.366890	-0.318265
21	1	0	0.641263	1.442290	0.775580
22	1	0	1.816477	0.237580	0.908816
23	1	0	-5.000316	-0.469489	-0.482877
24	1	0	-1.250942	1.831173	1.478796
25	1	0	-0.681197	3.287785	1.558282
26	1	0	2.606170	-1.531399	2.474180
27	1	0	3.596416	-1.414109	1.292728
28	1	0	3.892928	1.316218	-1.597799
29	1	0	5.290923	-0.472295	-0.829490
30	1	0	3.403279	2.788345	-1.644698
31	1	0	5.541404	-0.250051	-2.337133
32	1	0	5.456207	-2.586921	0.322663
33	1	0	6.009187	-1.481432	1.230227
34	8	0	-6.728193	-0.792000	-1.033895

35	1	0	-7.169932	-0.241649	-1.687493
36	1	0	-7.418115	-1.073511	-0.425555

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molecule: **g1·$(H_2O)_7$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.70363 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.125144	-2.982259	0.297823
2	7	0	1.394929	-1.889214	0.292211
3	6	0	1.992824	-1.033845	-0.611736
4	6	0	3.094696	-1.636314	-1.151397
5	7	0	3.163357	-2.875226	-0.559343
6	6	0	1.407518	0.318457	-0.865092
7	6	0	0.006314	0.219475	-1.488130
8	7	0	-0.901353	1.241994	-0.898826
9	8	0	-0.625382	-0.338219	1.476087
10	8	0	0.797890	1.591865	2.774984
11	8	0	2.169561	3.271812	1.105558
12	8	0	0.765571	3.447853	-1.225742
13	8	0	-3.142123	-1.312027	2.001328
14	8	0	-3.367806	0.506131	-2.000819
15	8	0	-4.910181	-1.064047	-0.214532
16	1	0	1.948686	-3.863675	0.893913
17	1	0	3.814611	-1.302466	-1.879129
18	1	0	2.068035	0.909286	-1.500092
19	1	0	1.336305	0.846482	0.092110
20	1	0	0.029662	0.372105	-2.565854
21	1	0	-0.442945	-0.751240	-1.281188
22	1	0	-1.843301	1.176238	-1.323184
23	1	0	-0.986014	1.024488	0.104408
24	1	0	-0.496281	2.188048	-1.021079
25	1	0	3.862524	-3.582301	-0.733500
26	1	0	-0.016194	-1.045067	1.167717
27	1	0	-1.478048	-0.752180	1.712145
28	1	0	1.320969	3.469493	-0.418833
29	1	0	0.547237	4.361062	-1.431314
30	1	0	3.080467	2.965715	1.081151
31	1	0	1.702857	2.684418	1.733837
32	1	0	0.224991	0.883454	2.417782
33	1	0	0.350852	1.940130	3.550949
34	1	0	-3.945157	0.978328	-2.606852

35	1	0	-3.948737	-0.012034	-1.418382
36	1	0	-3.762954	-1.276702	1.254846
37	1	0	-3.323895	-2.136873	2.459848
38	1	0	-5.738792	-0.651962	0.055802
39	1	0	-5.162618	-1.907666	-0.607125

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molecule: **g1·$(H_2O)_7$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.70247 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.592158	-1.426705	-1.357731
2	7	0	4.662622	-1.068122	-0.575972
3	6	0	4.206488	-0.267715	0.407120
4	7	0	2.906183	-0.088937	0.301078
5	6	0	2.503016	-0.811307	-0.804110
6	6	0	1.081235	-0.887105	-1.266554
7	6	0	0.136330	-1.618636	-0.306331
8	7	0	-0.503328	-0.696656	0.674483
9	8	0	1.265678	1.204062	1.990976
10	8	0	0.450832	3.693599	1.132869
11	8	0	-1.125565	3.472712	-1.092821
12	8	0	-1.959636	0.857649	-1.072115
13	8	0	-2.377722	-2.411468	1.834987
14	1	0	4.846648	0.156951	1.163992
15	1	0	3.693104	-2.068474	-2.216342
16	1	0	1.068581	-1.420504	-2.218420
17	1	0	0.685769	0.114233	-1.465647
18	1	0	-0.683031	-2.077339	-0.859081
19	1	0	0.657896	-2.398349	0.248008
20	1	0	-1.137615	-1.238567	1.290222
21	1	0	0.167182	-0.168007	1.251150
22	1	0	-1.087014	-0.012038	0.144576
23	1	0	5.622801	-1.349348	-0.711229
24	1	0	1.977566	0.800948	1.416666
25	1	0	1.552369	1.107486	2.904319
26	1	0	-1.722577	1.803190	-1.142125
27	1	0	-2.927368	0.801062	-1.077308
28	1	0	-0.646679	3.827858	-1.846229
29	1	0	-0.547106	3.603619	-0.314224
30	1	0	0.744690	2.834524	1.495298
31	1	0	0.127807	4.203094	1.880865
32	8	0	-4.790351	0.455848	-1.041043
33	8	0	-4.598422	-2.051094	0.269215
34	1	0	-3.203003	-2.315085	1.319322

35	1	0	-4.692878	-1.209646	-0.207866
36	1	0	-2.641404	-2.519931	2.752435
37	1	0	-4.858253	-2.738668	-0.350060
38	1	0	-5.185520	0.433169	-1.919714
39	1	0	-5.304179	1.104175	-0.546641

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molecule: **g1·$(H_2O)_7$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -895.69798 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.593671	0.323092	-0.308033
2	7	0	-3.363512	0.241145	0.147709
3	6	0	-2.939327	-1.042704	-0.131444
4	6	0	-3.937313	-1.728576	-0.765471
5	7	0	-4.983708	-0.842856	-0.868106
6	6	0	-1.562504	-1.480973	0.253938
7	6	0	-0.481786	-0.681904	-0.492087
8	7	0	0.628859	-0.316456	0.426170
9	8	0	-1.214432	1.448156	1.633905
10	8	0	-0.123491	3.865083	0.735161
11	8	0	1.774014	-2.811830	1.052230
12	8	0	2.481985	1.086226	-1.065934
13	8	0	4.839203	-0.355837	-0.941949
14	8	0	2.505118	3.853830	-0.376484
15	8	0	4.507085	-2.901714	0.301510
16	1	0	-5.235466	1.188645	-0.258271
17	1	0	-3.994992	-2.736425	-1.139789
18	1	0	-1.441700	-2.549655	0.074132
19	1	0	-1.441297	-1.320832	1.330549
20	1	0	-0.060871	-1.245180	-1.323797
21	1	0	-0.889597	0.253410	-0.874181
22	1	0	1.358961	0.230581	-0.082464
23	1	0	0.222814	0.279997	1.164234
24	1	0	1.066610	-1.164215	0.825218
25	1	0	-5.883330	-1.027053	-1.287270
26	1	0	-2.030564	1.211446	1.151880
27	1	0	-0.938460	2.321792	1.307934
28	1	0	1.633015	-3.319858	1.855948
29	1	0	2.718810	-2.898126	0.839943
30	1	0	3.358085	0.658142	-1.057555
31	1	0	4.747257	-1.237526	-0.544365
32	1	0	2.609048	2.020342	-0.839595
33	1	0	5.392499	-0.475133	-1.718765
34	1	0	4.701402	-3.640747	-0.286342

35	1	0	5.111719	-3.003602	1.045427
36	1	0	0.760936	3.885775	0.334950
37	1	0	-0.594728	4.621272	0.375609
38	1	0	3.173073	4.138286	0.257339
39	1	0	2.617051	4.430913	-1.140105

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molecule: **g1·$(H_2O)_8$–a**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -972.13989 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.217726	-1.445998	-0.885004
2	6	0	3.208931	-2.319249	-1.241685
3	7	0	4.374498	-1.780589	-0.754423
4	6	0	4.065457	-0.626768	-0.129442
5	7	0	2.771727	-0.391080	-0.188553
6	6	0	0.750849	-1.572380	-1.156534
7	6	0	-0.112721	-1.762979	0.096473
8	7	0	-0.621934	-0.471875	0.637934
9	8	0	1.317756	1.634180	0.919565
10	8	0	0.487785	3.544593	-0.854059
11	8	0	-1.399040	2.623853	-2.600879
12	8	0	-2.250954	0.275890	-1.462690
13	8	0	-2.347041	-1.405973	2.634873
14	8	0	-4.743602	-1.633486	1.322831
15	8	0	-5.055803	0.062919	-0.928044
16	1	0	4.804364	0.000028	0.344261
17	1	0	3.185288	-3.247864	-1.786179
18	1	0	0.604202	-2.439694	-1.802187
19	1	0	0.386144	-0.704527	-1.715986
20	1	0	-0.996004	-2.355391	-0.140321
21	1	0	0.440273	-2.269194	0.887214
22	1	0	-1.189923	-0.656892	1.485012
23	1	0	0.120180	0.210564	0.865106
24	1	0	-1.249350	-0.044735	-0.077394
25	1	0	5.299755	-2.173804	-0.847319
26	1	0	1.975009	0.999772	0.537672
27	1	0	1.662473	1.938566	1.777814
28	1	0	-2.022524	1.105568	-1.925647
29	1	0	-3.211199	0.273008	-1.330814
30	1	0	-1.015641	2.620435	-3.481871
31	1	0	-0.712654	2.991479	-2.006997
32	1	0	0.796684	2.897527	-0.185686
33	1	0	0.333263	4.366471	-0.380960
34	1	0	-3.229834	-1.499784	2.224945

35	1	0	-4.879810	-1.080937	0.534914
36	1	0	-2.494962	-1.076682	3.525329
37	1	0	-5.082103	-2.504441	1.097747
38	1	0	-5.554719	-0.312102	-1.662375
39	1	0	-5.501849	0.889702	-0.712620
40	8	0	2.223823	2.617487	3.368335
41	1	0	2.150969	2.109633	4.182018
42	1	0	3.067089	3.076643	3.427304

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molecule: **g1·$(H_2O)_8$–b**
(PCM)/M06–2X/6–311+G(d,p) OPT energy: -972.13989 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.082087	-0.483640	-0.633153
2	6	0	3.279942	-0.929300	-1.124249
3	7	0	4.242462	-0.465266	-0.263146
4	6	0	3.618113	0.229510	0.704825
5	7	0	2.312264	0.242444	0.517245
6	6	0	0.716717	-0.722802	-1.198880
7	6	0	-0.203834	-1.569134	-0.312018
8	7	0	-1.017120	-0.735966	0.618454
9	8	0	0.431944	1.307758	2.093526
10	8	0	-0.458072	3.733852	1.145667
11	8	0	-1.856108	3.364708	-1.176558
12	8	0	-2.530429	0.702315	-1.182520
13	8	0	-2.781930	-2.617130	1.701294
14	8	0	-5.054018	-2.323456	0.195753
15	8	0	-5.338708	0.163837	-1.135704
16	1	0	4.142283	0.708248	1.517152
17	1	0	3.519858	-1.518719	-1.993372
18	1	0	0.836874	-1.242691	-2.150673
19	1	0	0.220923	0.227018	-1.425571
20	1	0	-0.919847	-2.117103	-0.923631
21	1	0	0.364257	-2.285289	0.281225
22	1	0	-1.630708	-1.349546	1.186620
23	1	0	-0.453990	-0.142835	1.245460
24	1	0	-1.633339	-0.112512	0.050999
25	1	0	5.252002	-0.611251	-0.342943
26	1	0	1.223074	0.983642	1.570122
27	1	0	0.653508	1.219521	3.025563
28	1	0	-2.345669	1.660263	-1.240900
29	1	0	-3.493813	0.594030	-1.189005
30	1	0	-1.344185	3.734459	-1.900671
31	1	0	-1.348353	3.549696	-0.360612
32	1	0	-0.147638	2.900324	1.551953
33	1	0	-0.834493	4.256921	1.858354

34	1	0	-3.620638	-2.549632	1.203007
35	1	0	-5.179674	-1.490102	-0.288295
36	1	0	-3.023968	-2.751121	2.621482
37	1	0	-5.329068	-3.023090	-0.403135
38	1	0	-5.740866	0.119370	-2.010424
39	1	0	-5.871327	0.797454	-0.642107
40	8	0	7.058800	-0.886472	-0.543506
41	1	0	7.634584	-0.181129	-0.853950
42	1	0	7.576997	-1.375498	0.102706

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molecule: **g1·$(H_2O)_8$–c**

(PCM)/M06–2X/6–311+G(d,p) OPT energy: -972.13945 a.u.

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.783260	-0.485185	-1.063554
2	6	0	3.891662	-0.959761	-1.710037
3	7	0	4.813864	-1.224334	-0.727503
4	6	0	4.254528	-0.914494	0.458129
5	7	0	3.028049	-0.463457	0.295011
6	6	0	1.483738	-0.062891	-1.674827
7	6	0	0.294853	-0.964750	-1.327392
8	7	0	-0.396885	-0.540241	-0.078511
9	8	0	1.264865	0.178549	2.227059
10	8	0	0.916299	2.884349	2.619189
11	8	0	-0.305708	4.031445	0.458130
12	8	0	-1.376951	1.903803	-0.911288
13	8	0	-2.557964	-2.244402	0.038004
14	8	0	-4.641317	-0.798975	-1.085332
15	8	0	-4.206813	1.997484	-1.340136
16	1	0	4.768438	-1.029077	1.399346
17	1	0	4.096942	-1.124723	-2.754107
18	1	0	1.606154	-0.074930	-2.759105
19	1	0	1.244169	0.969605	-1.399729
20	1	0	-0.457094	-0.915113	-2.114616
21	1	0	0.605185	-2.002792	-1.210175
22	1	0	-1.188774	-1.191334	0.118160
23	1	0	0.218115	-0.493012	0.744960
24	1	0	-0.798537	0.409015	-0.235934
25	1	0	5.746791	-1.585364	-0.864298
26	1	0	2.015892	-0.034452	1.605033
27	1	0	1.374042	-0.381675	3.001482
28	1	0	-1.045729	2.711280	-0.472097
29	1	0	-2.331608	2.014886	-1.037708
30	1	0	0.328818	4.606205	0.021986
31	1	0	0.149223	3.672367	1.246736
32	1	0	1.038033	1.917130	2.544160
33	1	0	0.581348	3.045950	3.505176
34	1	0	-3.331582	-1.789168	-0.341468

35	1	0	-4.512328	0.156264	-1.208013
36	1	0	-2.868970	-2.736398	0.816110
37	1	0	-5.087928	-1.108725	-1.877938
38	1	0	-4.447040	2.370603	-2.195596
39	1	0	-4.708707	2.503714	-0.691529
40	8	0	-3.322555	-3.721852	2.292900
41	1	0	-3.697062	-3.297018	3.070364
42	1	0	-3.820086	-4.537725	2.183706
