

Supporting Information for:

Aqueous Solvation Free Energies of Ions and Ion–Water Clusters Based on an Accurate Value for the Absolute Aqueous Solvation Free Energy of the Proton

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TABLE S1: Slopes, Intercepts, and Y Values (kcal/mol), Computed Using All of the Conventional Aqueous Solvation Free Eneriges in Table 5

n	slope	intercept	Y^a
0	1.0000	0.0	-266.5
1	0.6841	-84.8	-266.1
2	0.4398	-149.2	-265.8
3	0.3131	-182.7	-266.0
4	0.2336	-203.9	-266.2
5	0.2049	-211.7	-266.3
6	0.1673	-221.6	-266.0
average			-266.1

aY is the average intersection ordinate of the n th straight line with all the others in this table.

TABLE S2: Slopes, Intercepts, and Y Values (kcal/mol), Computed Using the Monatomic Cation Subset

n	slope	intercept	Y^a
0	1.0000	0.0	-264.6
1	0.6345	-96.6	-264.6
2	0.3938	-160.2	-264.7
3	0.2600	-195.5	-265.0
4	0.1921	-213.8	-265.4
5	0.1649	-221.3	-265.7
6	0.1405	-227.9	-265.6
average			-265.1

aY is the average intersection ordinate of the n th straight line with all the others in this table.

TABLE S3: Slopes, Intercepts, and Y Values (kcal/mol), Computed Using the Oxonium Ion Subset

n	slope	intercept	Y^a
0	1.0000	0.0	-268.7
1	0.6781	-87.3	-267.9
2	0.4586	-145.3	-267.8
3	0.3493	-174.5	-267.9
4	0.2839	-192.1	-267.9
5	0.2412	-203.6	-267.7
6	0.2054	-212.7	-266.9
average			-267.8

aY is the average intersection ordinate of the n th straight line with all the others in this table.

TABLE S4: Slopes, Intercepts, and Y Values (kcal/mol), Computed Using the Ammonium Ion Data Set

n	slope	intercept	Y^a
0	1.0000	0.0	-266.2
1	0.7027	-79.6	-265.7
2	0.4845	-137.2	-265.4
3	0.3667	-168.3	-265.4
4	0.2700	-193.8	-265.8
5	0.2421	-201.5	-266.2
average			-265.8

aY is the average intersection ordinate of the n th straight line with all the others in this table.

TABLE S5: Slopes, Intercepts, and Y Values (kcal/mol), Computed Using Experimental Gas-Phase Clustering Free Energies Only

<i>n</i>	slope	intercept	<i>Y</i> ^a
0	1.0000	0.0	-266.4
1	0.6767	-86.7	-266.0
2	0.4398	-149.2	-265.9
3	0.3131	-182.7	-266.0
4	0.2336	-203.9	-266.3
5	0.2049	-211.7	-266.4
6	0.1673	-221.6	-266.0
average			-266.1

^a*Y* is the average intersection ordinate of the *n*th straight line with all the others in this table.

TABLE S6: Slopes, Intercepts, and Y Values (kcal/mol), Computed Using the Conventional Aqueous Solvation Free Energies and Gas-Phase Clustering Free Energies Reported by Tissandier et al.^a

<i>n</i>	slope	Intercept	<i>Y</i> ^a
0	1.0000	0.0	-265.6
1	0.6671	-88.3	-265.8
2	0.4530	-145.3	-265.9
3	0.3171	-181.6	-265.9
4	0.2424	-201.6	-265.7
5	0.1984	-213.1	-265.3
6	0.1511	-225.2	-264.7
average			-265.6

^aTissandier, M. D.; Cowen, K. A.; Feng, W. Y.; Gundlach, E.; Cohen, M. J.; Earhart, A. D.; Coe, J. V. *J. Phys. Chem. A* **1998**, *102*, 7787. ^b*Y* is the average intersection ordinate of the *n*th straight line with all the others in this table.

TABLE S7: y_{ij} values (kcal/mol) Computed Using Experimental Clustering Free Energies, by Subset^a

i	j	all ions	monatomic cations	oxonium ions	ammonium ions	all ions (expt. clustering free energies only)	Tissandier et al. Data
1	0	-268.4	-264.4	-271.3	-267.7	-268.0	-265.1
2	0	-266.3	-264.3	-268.4	-266.2	-266.3	-265.6
2	1	-265.1	-264.2	-266.5	-265.2	-265.2	-265.9
3	0	-266.0	-264.2	-268.2	-265.7	-266.0	-266.0
3	1	-265.3	-264.2	-267.2	-265.1	-265.4	-266.2
3	2	-265.5	-264.2	-267.9	-265.0	-265.7	-266.5
4	0	-266.0	-264.6	-268.3	-265.5	-266.0	-266.0
4	1	-265.7	-264.6	-267.6	-265.1	-265.6	-266.2
4	2	-265.9	-264.8	-268.2	-265.1	-265.8	-266.3
4	3	-266.2	-265.3	-268.5	-265.2	-266.0	-266.2
5	0	-266.3	-265.0	-268.3	-265.8	-266.3	-265.8
5	1	-266.0	-265.1	-267.8	-265.6	-266.0	-265.9
5	2	-266.2	-265.3	-268.2	-265.7	-266.3	-265.9
5	3	-266.6	-265.9	-268.4	-266.0	-266.7	-265.6
5	4	-267.4	-266.9	-268.3	-267.8	-267.9	-265.0
6	0	-266.1	-265.1	-267.7		-266.1	-265.2
6	1	-265.9	-265.2	-267.2		-265.9	-265.2
6	2	-266.0	-265.4	-267.4		-266.0	-265.1
6	3	-266.2	-265.9	-267.2		-266.1	-264.8
6	4	-266.3	-266.3	-266.6		-266.2	-264.2
6	5	-265.6	-265.8	-265.2		-265.3	-263.7
s.d. ^d		0.71	0.77	1.15	0.86	0.70	0.71

^a y_{ij} is the ordinate of the intersection between the i th and j th straight lines, where i and j refer to the number of clustering water molecules.

Cartesian coordinates of ion-water clusters used to test the continuum models.
 Bare ion listed first, followed by the name of the corresponding neutral species.

H3O+ water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.194495	-.038211	.057508
2	8	0	-1.194495	-.038211	-.057508
3	1	0	.000000	.019876	.000000
4	1	0	1.683991	.740849	.351170
5	1	0	1.649604	-.445097	-.691628
6	1	0	-1.683991	.740849	-.351171
7	1	0	-1.649604	-.445096	.691628

CH3OH2+ methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.546734	-.447608	.004361
2	8	0	-.522740	.617890	-.074485
3	8	0	1.787416	-.194856	-.001970
4	1	0	-1.230155	-1.206403	-.704870
5	1	0	-2.486754	.001109	-.303419
6	1	0	-1.589669	-.835494	1.019541
7	1	0	-.718191	1.374623	.494489
8	1	0	.487556	.292606	.008674
9	1	0	2.310460	-.356012	.790371
10	1	0	2.389748	.030949	-.719306

CH3CH2OH2+ ethanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.878238	-.538815	.061514
2	8	0	.123501	.583756	-.027865
3	8	0	2.486387	-.155095	-.036659
4	6	0	-2.264748	.035616	-.064719
5	1	0	-.700101	-1.046126	1.009417
6	1	0	-.600224	-1.181397	-.771113
7	1	0	-.074504	1.301226	.590450
8	1	0	1.129627	.292486	.018221
9	1	0	3.066024	.096770	-.763224
10	1	0	3.037582	-.349352	.728073
11	1	0	-2.979014	-.789870	-.025513
12	1	0	-2.397587	.556722	-1.013232
13	1	0	-2.502994	.709445	.762343

(CH3)2OH+ dimethyl ether

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.024068	1.251350	.093700
2	8	0	.383667	-.001816	-.316922
3	6	0	1.054100	-1.239514	.090828
4	8	0	-2.089865	.002969	.044935
5	1	0	.386158	2.052104	-.270877
6	1	0	1.996265	1.281252	-.391553
7	1	0	1.117031	1.273142	1.179126
8	1	0	-.629037	-.012530	-.129825
9	1	0	.439336	-2.055243	-.280427
10	1	0	1.143630	-1.263953	1.176525
11	1	0	2.028809	-1.242467	-.390288
12	1	0	-2.587941	-.084173	.863092
13	1	0	-2.713672	-.028373	-.687050

(C2H5)2OH+ diethyl ether

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.264505	-.947135	.333632
2	8	0	-.000038	-.326813	-.152441
3	6	0	1.264241	-.947534	.333545
4	8	0	.000731	2.223839	.156510
5	6	0	2.437517	-.294543	-.356163
6	6	0	-2.437757	-.294174	-.356204
7	1	0	-1.281858	-.834528	1.419442
8	1	0	-1.161323	-1.999601	.074450
9	1	0	.000238	.676466	-.008338
10	1	0	1.160849	-1.999921	.074124
11	1	0	1.281622	-.835181	1.419380
12	1	0	-.001155	2.749820	.961530
13	1	0	-.000131	2.836204	-.585431
14	1	0	3.349154	-.788478	-.013088
15	1	0	2.519617	.764398	-.106373
16	1	0	2.375723	-.411067	-1.438696
17	1	0	-3.349484	-.787640	-.012699
18	1	0	-2.376174	-.411277	-1.438684
19	1	0	-2.519589	.764918	-.107033

CH3C(OH)CH3+ acetone

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.152366	-.520022	.009327
2	6	0	-.759474	-.027050	-.007449
3	6	0	-.459612	1.424160	.003855
4	8	0	.151678	-.899338	-.031909
5	8	0	2.556515	-.069103	.018622
6	1	0	-2.211734	-1.567853	-.277253
7	1	0	-2.792587	.106461	-.615196
8	1	0	-2.524251	-.411397	1.037928
9	1	0	.584461	1.642601	.219787
10	1	0	-1.122068	1.936584	.705641
11	1	0	-.711383	1.817131	-.990459
12	1	0	1.124063	-.563637	-.011473
13	1	0	3.104206	-.172361	-.767290
14	1	0	3.112462	-.302526	.770207

CH3C(OH)C6H5+ acetophenone

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.505827	1.057496	.000461
2	6	0	2.707180	.370469	.000546
3	6	0	2.708131	-1.026012	.000036
4	6	0	1.504742	-1.738168	-.000548
5	6	0	.298294	-1.061467	-.000596
6	6	0	.278008	.353705	-.000082
7	6	0	-.953886	1.102314	-.000142
8	6	0	-.996677	2.593698	-.000269
9	8	0	-2.120011	.570016	-.000101
10	8	0	-2.882818	-1.941006	.000440
11	1	0	1.517000	2.139148	.000863
12	1	0	3.642169	.915962	.000997
13	1	0	3.649476	-1.562911	.000078
14	1	0	1.515537	-2.820701	-.000982
15	1	0	-.618606	-1.636316	-.001118
16	1	0	-.482441	2.987572	-.880658
17	1	0	-.483093	2.987633	.880485
18	1	0	-2.029357	2.933234	-.000618
19	1	0	-2.231555	-.424874	.000195
20	1	0	-3.382379	-2.231798	.770232
21	1	0	-3.383830	-2.231238	-.768623

NH4+ ammonia

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-1.340000	-.000077	.000131
2	8	0	1.357387	.000247	.000286
3	1	0	-.279397	.000272	-.003354
4	1	0	-1.690805	.901986	-.323239
5	1	0	-1.691149	-.730789	-.619641
6	1	0	-1.684769	-.170559	.945370
7	1	0	1.935506	.769443	-.001189
8	1	0	1.931514	-.771795	-.001149

F- hydrofluoric acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-.893482	-1.381749	.000000
2	8	0	.047793	-1.203159	.000000
3	1	0	.080996	-.142061	.000000
4	9	0	.047793	1.238786	.000000

Cl- hydrochloric acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-.942416	2.602191	.000000
2	8	0	.016900	2.610061	.000000
3	1	0	.215706	1.648072	.000000
4	35	0	.016900	-.718022	.000000

Br- hydrobromic acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-.942416	2.602191	.000000
2	8	0	.016900	2.610061	.000000
3	1	0	.215706	1.648072	.000000
4	35	0	.016900	-.718022	.000000

OH- water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	1.516884	-.616439	.511395
2	8	0	1.222710	.095911	-.060855
3	1	0	-.057777	-.014292	-.068292
4	8	0	-1.219484	-.097348	-.056261
5	1	0	-1.484918	.642225	.493823

HO2- hydrogen peroxide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	.836773	.759305	.008693
2	8	0	.980453	-.698460	.010997
3	1	0	.002986	-.891692	-.029708
4	1	0	-.191840	.744042	-.028212
5	8	0	-1.550199	-.037591	-.108182
6	1	0	-1.947363	-.038380	.765857

O2- hydroperoxyl radical

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.268674	-.568987	-.000186
2	8	0	-.779467	.671729	.000228
3	1	0	.807656	.345126	-.000518
4	8	0	1.751427	-.025082	-.000228
5	1	0	1.566061	-.966409	.002006

HS- hydrogen sulfide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	2.129163	-.010620	.864986
2	8	0	2.061389	.010004	-.091827
3	1	0	1.075622	-.011307	-.213379
4	16	0	-1.149351	-.082080	.004209
5	1	0	-1.306280	1.255183	.015656

C2H- acetylene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.225583	1.993400	.000000
2	1	0	.410948	3.045261	.000000
3	6	0	.000000	.778419	.000000
4	1	0	-.248897	-1.033514	.000000
5	8	0	-.272149	-2.047145	.000000
6	1	0	.661639	-2.265504	.000000

CN- hydrogen cyanide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.647920	-2.109079	.000000
2	8	0	-.284765	-1.888463	.000000
3	1	0	-.267789	-.894197	.000000
4	7	0	.000000	.871858	.000000
5	6	0	.316331	2.001329	.000000

CH3O- methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	.498187	-.668148	.000856
2	6	0	1.422267	.327601	.008533
3	1	0	2.190906	.228376	.819820
4	1	0	2.026128	.405690	-.934963
5	1	0	.990705	1.350986	.150089
6	1	0	-.841427	-.181395	-.088689
7	8	0	-1.847782	.180281	-.102985
8	1	0	-2.103159	.133675	.819572

C2H5O- ethanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	.167331	-.628481	-.495552
2	6	0	-.799362	-.387321	.420644
3	6	0	-1.936646	.527674	-.107262
4	1	0	-1.305551	-1.321738	.786282
5	1	0	-.414029	.099765	1.353688
6	1	0	1.497077	-.129499	-.108057
7	8	0	2.437705	.270097	.140273
8	1	0	2.438299	1.110050	-.321108
9	1	0	-2.719068	.693619	.650065
10	1	0	-2.395791	.074083	-.993114
11	1	0	-1.525176	1.498675	-.405812

CH3CH2CH2O- 1-propanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	.926398	.852404	.048119
2	6	0	-.167804	.253647	-.473692
3	6	0	-1.368638	.170363	.509146
4	1	0	-.568497	.771938	-1.390116
5	1	0	.019715	-.798719	-.818433
6	1	0	2.162403	.042624	-.027326
7	8	0	3.032660	-.542729	-.018546
8	1	0	3.048090	-.883416	.877008
9	6	0	-2.612539	-.493599	-.092433
10	1	0	-1.602754	1.190199	.839480
11	1	0	-1.037673	-.377437	1.400309
12	1	0	-2.398010	-1.524415	-.396918
13	1	0	-2.947125	.043621	-.987635
14	1	0	-3.454729	-.524256	.608926

(CH3)2CHO- 2-propanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-.340597	-.164173	1.052517
2	6	0	.856561	.015821	.447491
3	1	0	1.694032	.074945	1.194798
4	6	0	1.233411	-1.161048	-.497937
5	6	0	.933315	1.348208	-.355145
6	1	0	-1.576293	-.192455	.165055
7	8	0	-2.439681	-.148546	-.410489
8	1	0	-2.758339	.739595	-.242115
9	1	0	.484709	-1.244727	-1.294205
10	1	0	.175802	1.341538	-1.147413
11	1	0	1.222585	-2.095639	.071386
12	1	0	2.226513	-1.038353	-.955774
13	1	0	1.921004	1.514524	-.810518
14	1	0	.712491	2.184439	.316110

CH3CH2CHOCH3- 2-butanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-.831954	-.852970	-.329499
2	6	0	-.036499	-.672797	.749904
3	6	0	1.269555	.136488	.452260
4	1	0	-.543105	-.129737	1.590726
5	1	0	.312397	-1.638802	1.208149
6	1	0	-2.111179	-.107310	-.277969
7	8	0	-3.039604	.374875	-.227360
8	1	0	-3.631835	-.330586	.036866
9	1	0	1.839540	.207457	1.393811
10	6	0	.921775	1.550511	-.027293
11	6	0	2.122340	-.599176	-.588644
12	1	0	.270175	1.482222	-.902722
13	1	0	1.523913	-.760207	-1.489703
14	1	0	1.816471	2.127870	-.294011
15	1	0	.375507	2.102151	.745170
16	1	0	2.432015	-1.582262	-.215608
17	1	0	3.025535	-.036187	-.857194

C(CH3)3O- t-butanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-.434055	-.017033	-.966299
2	6	0	.572069	-.002292	-.053363
3	6	0	1.951615	-.096454	-.770022
4	6	0	.558326	1.310560	.790844
5	6	0	.466191	-1.205515	.937454
6	1	0	-1.844183	.086384	-.428140
7	8	0	-2.825202	.098337	-.080845
8	1	0	-3.102525	-.811599	-.198042
9	1	0	-.405088	1.397226	1.302046
10	1	0	-.494448	-1.155483	1.459192
11	1	0	.659431	2.167803	.117275
12	1	0	1.362386	1.353940	1.539818
13	1	0	1.272920	-1.225920	1.684355
14	1	0	.493484	-2.139702	.366364
15	1	0	2.803654	-.090752	-.074915
16	1	0	2.053990	.747670	-1.459598
17	1	0	1.985238	-1.017794	-1.360676

H2C=CHCH2O- allyl alcohol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.440795	-.456773	.040460
2	6	0	-.240439	.431204	.325047
3	8	0	.689350	.369447	-.663582
4	1	0	-.643505	1.460734	.509841
5	1	0	.155060	.104516	1.323104
6	1	0	-1.177762	-1.484529	-.212066
7	6	0	-2.722355	-.079862	.014379
8	1	0	-3.528138	-.768240	-.228335
9	1	0	-3.006028	.948666	.227820
10	1	0	2.014067	-.093658	-.186269
11	8	0	2.960810	-.370352	.166469
12	1	0	3.406563	.472341	.263488

CH3OCH2CH2O- 2-methoxyethanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.758702	-.080483	.341817
2	6	0	.467956	-.684863	-.370414
3	8	0	1.530403	-.757056	.472061
4	1	0	.136568	-1.677028	-.768331
5	1	0	.649074	-.058505	-1.277477
6	1	0	-.982093	-.683162	1.236330
7	1	0	-.513936	.940107	.676376
8	8	0	-1.912323	-.040482	-.508743
9	6	0	-3.027618	.504697	.126566
10	1	0	-3.862778	.498595	-.581219
11	1	0	-3.319372	-.075927	1.018363
12	1	0	-2.850906	1.544250	.451236
13	1	0	2.675096	.094402	.068570
14	8	0	3.465627	.732996	-.186032
15	1	0	3.308873	1.497493	.370054

HOCH2CH2O- 1,2-ethanediol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.298787	-.123668	.464215
2	6	0	.215057	.520472	-.421634
3	8	0	-.879760	.857003	.309764
4	1	0	.706037	1.390728	-.925469
5	1	0	.006210	-.206077	-1.243907
6	1	0	1.531384	.571295	1.282798
7	1	0	.888662	-1.044808	.900881
8	8	0	2.494454	-.421047	-.294564
9	1	0	3.098294	-.888870	.284089
10	1	0	-2.071631	.041014	.014220
11	8	0	-2.911031	-.567396	-.157206
12	1	0	-2.871331	-1.192585	.567951

C6H5CH2O- benzyl alcohol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.251460	-.346876	-.184446
2	6	0	-.601736	1.004476	-.216822
3	6	0	-1.919081	1.408412	.009536
4	6	0	-2.912397	.464962	.273981
5	6	0	-2.572711	-.891094	.308624
6	6	0	-1.256214	-1.286035	.080026
7	1	0	.201552	1.703926	-.426549
8	1	0	-2.174863	2.464323	-.020125
9	1	0	-3.936945	.777827	.450580
10	1	0	-3.336852	-1.635907	.514083
11	1	0	-.997140	-2.342836	.105887
12	6	0	1.209007	-.760103	-.442830
13	8	0	2.050629	.257676	-.697124
14	1	0	1.497742	-1.376661	.448948
15	1	0	1.143985	-1.517116	-1.271569
16	1	0	3.356028	.189560	.085102
17	8	0	4.210834	.171510	.665130
18	1	0	3.982338	.740948	1.401169

CF3CH2O- 2,2,2-trifluoroethanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.252194	-.640006	.626639
2	8	0	1.198204	-.950760	-.266054
3	8	0	3.345227	.400759	.095408
4	6	0	-.976511	.063689	.020223
5	9	0	-1.919213	.360487	.971846
6	9	0	-.684162	1.240251	-.580142
7	9	0	-1.622165	-.679625	-.908016
8	1	0	.570243	.063661	1.437415
9	1	0	-.204492	-1.511932	1.163702
10	1	0	2.499830	-.169144	-.046611
11	1	0	3.162726	1.185317	-.423701

CH(CF3)2O- 1,1,1,3,3,3-hexafluoropropan-2-ol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.098275	-.063677	.828903
2	8	0	.520013	1.035898	1.205320
3	8	0	1.923862	2.709773	-.358624
4	6	0	.831491	-1.042505	.033384
5	9	0	.242631	-2.216276	-.328594
6	9	0	1.330350	-.509296	-1.101149
7	9	0	1.888515	-1.385561	.795203
8	6	0	-1.396083	.221740	-.002408
9	9	0	-1.166549	.869827	-1.160028
10	9	0	-2.233902	.994332	.716187
11	9	0	-2.112023	-.892716	-.326306
12	1	0	-.482531	-.717660	1.657209
13	1	0	1.405487	2.097396	.233169
14	1	0	1.962044	2.218744	-1.181035

CH300- methyl hydroperoxide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.548707	-.623556	-.204274
2	8	0	.856967	.282821	.587760
3	8	0	-.062713	.987561	-.300346
4	1	0	2.252699	-1.163200	.449901
5	1	0	2.117081	-.114602	-1.002678
6	1	0	.871331	-1.350060	-.682005
7	8	0	-2.167420	-.431415	-.067156
8	1	0	-1.304837	.150505	-.188032
9	1	0	-2.243188	-.493043	.886392

CH3CH200- ethyl hydroperoxide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.046865	.037822	.490502
2	8	0	-.259690	.551776	-.534135
3	8	0	.921023	1.140971	.089939
4	6	0	-2.290351	-.602671	-.129393
5	1	0	-1.337545	.841549	1.191347
6	1	0	-.481229	-.708044	1.073209
7	1	0	-2.942150	-1.013945	.649087
8	1	0	-2.007026	-1.413692	-.806634
9	1	0	-2.859918	.134682	-.703419
10	8	0	2.503657	-.855485	.088277
11	1	0	1.864220	-.025408	.108308
12	1	0	2.467022	-1.124153	-.831204

END OF SUPPORTING INFORMATION