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

Casey P. Kelly, Christopher J. Cramer, Donald G. Truhlar
Department of Chemistry and Supercomputing Institute, 207 Pleasant St. SE, University of Minnesota, Minneapolis, MN 55455-0431.

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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

[a]*Y* 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

[a]*Y* 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

[a]*Y* 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

[a]*Y* 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

n	slope	intercept	Y^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 Eneriges and Gas-Phase Clustering Free Energies Reported by Tissandier et al.[a]

n	slope	Intercept	Y^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

[a]Tissandier, 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

CH3OO- 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

CH3CH2OO- 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