

A Blind Challenge for Computational Solvation Free Energies: Introduction and Overview.

Supporting Information

J. Peter Guthrie

Department of Chemistry

University of Western Ontario

London, Ont., Canada N6A 5B7

Cartesian coordinates for the 63 compounds in the SAMPL1 challenge set.

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14
CUP08001.xyz      0.0000000
C      -2.1310      -1.5690      -1.4740
C      -1.0270      -2.1020      -0.5670
H      -0.4180      -1.2620      -0.2100
H      -1.4830      -2.5990       0.3000
O      -0.2340      -3.0190      -1.3150
H      -2.7410      -2.4090      -1.8310
H      -1.6760      -1.0720      -2.3410
O      -2.9240      -0.6520      -0.7260
N       0.8270      -3.5760      -0.5570
O       0.9340      -3.2140       0.6160
O       1.5110      -4.3670      -1.2040
N      -3.9860      -0.0950      -1.4840
O      -4.0930      -0.4570      -2.6570
O      -4.6700       0.6960      -0.8370
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17
CUP08002.xyz      0.0000000
C      -0.0820       0.6590      -0.2820
C       0.3320      -0.8230      -0.3060
H       0.3540      -1.1920      -1.3390
O       1.5970      -1.0050       0.3430
C      -0.6710      -1.6910       0.4550
H      -1.6800      -1.5850       0.0450
H      -0.6940      -1.4400       1.5220
H      -0.3800      -2.7450       0.3920
H       0.6780       1.2670      -0.7850
O      -0.2050       1.0960       1.0740
H      -1.0440       0.7670      -0.7990
N      -0.6140       2.4490       1.1840
O      -0.7200       2.8210       2.3510
O      -0.8080       3.0670       0.1360
N       2.7210      -0.7680      -0.4880
O       3.7900      -0.9740       0.0850
O       2.5050      -0.3840      -1.6380
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17
CUP08003.xyz      0.0000000
C       0.6550       0.6610      -1.2740
H       0.2680      -0.0620      -0.5460
H       1.7200       0.4720      -1.4600
O      -0.0790       0.5690      -2.4940
C       0.4780       2.0760      -0.7280
H       0.8240       2.7990      -1.4780
C       1.2320       2.2740       0.5840
H       2.3000       2.0800       0.4330
H       0.8740       1.5550       1.3310
C       1.0520       3.6840       1.1230
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H	-0.0040	3.8990	1.3160
H	1.4300	4.4270	0.4130
H	1.6000	3.8030	2.0630
H	-0.5910	2.2790	-0.5870
N	0.0130	-0.7110	-3.0970
O	-0.6210	-0.7890	-4.1490
O	0.6900	-1.5630	-2.5190

17			
CUP08004.xyz		0.0000000	
C	0.6790	0.8530	-1.2420
H	0.2220	0.8850	-2.2370
H	0.1740	0.0820	-0.6520
H	1.7240	0.5570	-1.3850
C	0.5800	2.2220	-0.5700
O	1.2930	3.1350	-1.4090
C	1.2470	2.1740	0.8130
H	2.3140	1.9430	0.7040
H	0.7970	1.3740	1.4120
C	1.1230	3.4850	1.5780
H	0.0730	3.7690	1.7010
H	1.6460	4.2980	1.0650
H	1.5640	3.3810	2.5740
H	-0.4860	2.4480	-0.4600
N	0.6140	4.3430	-1.7080
O	1.2510	5.0660	-2.4730
O	-0.4830	4.5320	-1.1830

17			
CUP08005.xyz		0.0000000	
C	-0.2910	0.4890	0.2240
C	0.0980	-0.9610	0.5060
C	1.4280	-1.2960	-0.1740
H	2.2160	-0.6110	0.1570
H	1.3470	-1.2180	-1.2640
H	1.7520	-2.3130	0.0690
H	0.2430	-1.0820	1.5870
C	-1.0180	-1.9140	0.0530
H	-1.1330	-1.8580	-1.0370
H	-1.9590	-1.6210	0.5370
O	-0.6760	-3.2440	0.4450
H	-0.4400	0.6600	-0.8480
H	0.4880	1.1760	0.5720
H	-1.2200	0.7500	0.7420
N	-1.6490	-4.2000	0.0610
O	-1.3490	-5.3460	0.3960
O	-2.6430	-3.7890	-0.5390

12

CUP08006.xyz	0.0000000		
C	-2.0770	-1.6820	-1.0800
C	-0.8710	-2.2920	-0.3770
H	-0.2510	-1.4870	0.0370
H	-1.2190	-2.9270	0.4480
O	-0.1380	-3.0560	-1.3290
H	-2.7150	-2.4670	-1.4990
H	-1.7540	-1.0390	-1.9060
O	-2.8310	-0.9120	-0.1570
H	-3.5890	-0.5410	-0.6420
N	1.0120	-3.6710	-0.7740
O	1.2360	-3.4810	0.4220
O	1.6440	-4.3310	-1.5980

38

CUP08007.xyz	0.0000000		
C	0.5360	1.0310	0.8760
C	1.6750	1.9590	1.2430
H	2.6310	1.4270	1.2700
H	1.7880	2.7110	0.4510
C	1.4490	2.6590	2.5750
H	1.3540	1.9400	3.3940
H	0.5390	3.2690	2.5580
H	2.2920	3.3200	2.8010
C	-0.6400	1.6070	0.3700
H	-0.7130	2.6850	0.2440
C	-1.7330	0.8150	0.0370
H	-2.6430	1.2750	-0.3400
C	-1.6660	-0.5680	0.1910
H	-2.5460	-1.1540	-0.0640
C	-0.5000	-1.1940	0.6660
C	-0.4790	-2.7020	0.8250
H	-1.0140	-2.9610	1.7460
H	0.5470	-3.0630	0.9410
C	-1.0730	-3.4800	-0.3460
H	-0.6150	-3.1820	-1.2950
H	-2.1540	-3.3320	-0.4280
H	-0.9020	-4.5530	-0.2070
C	0.5960	-0.3760	1.0320
N	1.7690	-0.9550	1.5830
C	1.7920	-1.1430	3.0280
H	1.1090	-0.4350	3.5120
H	2.8070	-0.9680	3.4000
O	1.3920	-2.4770	3.3280
C	1.4560	-2.7400	4.7210
H	0.7890	-2.0690	5.2700
H	2.4830	-2.6330	5.0850
H	1.1320	-3.7700	4.8920
C	2.8750	-1.3330	0.8270
O	3.9030	-1.7840	1.3470
C	2.8100	-1.1740	-0.6820
Cl	2.6740	-2.7840	-1.4170
H	3.7420	-0.7160	-1.0250

H	1.9840	-0.5620	-1.0410
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26			
CUP08008.xyz	0.0000000		
C	1.6640	-0.4310	0.3400
S	1.5070	-2.2320	0.4770
C	-0.3380	-2.4920	0.2770
C	-0.8340	-1.7880	-0.9880
H	-0.2840	-2.1200	-1.8760
H	-0.7510	-0.6990	-0.9140
H	-1.8910	-1.9960	-1.1820
C	-1.0320	-1.9820	1.5430
H	-2.1210	-2.0620	1.4720
H	-0.8240	-0.9260	1.7380
H	-0.7310	-2.5590	2.4260
C	-0.5070	-4.0130	0.1350
H	0.4180	-4.6150	0.0950
N	-1.6010	-4.7150	0.0380
O	-2.7550	-3.9080	0.0740
C	-3.9120	-4.6570	-0.0250
N	-3.6870	-6.0050	-0.1340
C	-4.7150	-7.0030	-0.2500
H	-5.7100	-6.5540	-0.2400
H	-4.6140	-7.6980	0.5880
H	-4.5620	-7.5440	-1.1870
H	-2.6980	-6.2440	-0.1240
O	-5.0190	-4.1300	-0.0130
H	1.4430	-0.0980	-0.6760
H	2.7000	-0.1580	0.5600
H	1.0230	0.0870	1.0560

32			
CUP08009.xyz	0.0000000		
C	0.8760	1.0070	0.3610
N	2.0140	1.7690	0.4550
H	1.8700	2.7670	0.4990
C	3.3260	1.1740	0.4880
H	3.5030	0.5890	-0.4220
H	3.4180	0.5010	1.3490
C	4.3840	2.2600	0.5930
H	4.2490	2.8540	1.5030
H	4.3330	2.9420	-0.2630
H	5.3850	1.8170	0.6190
N	-0.2720	1.6740	0.3380
C	-1.3660	0.9210	0.2450
S	-2.9160	1.8010	0.2120
C	-4.0860	0.4220	0.1270
H	-3.9900	-0.2230	1.0040
H	-3.9300	-0.1650	-0.7830
H	-5.1040	0.8210	0.1050
N	-1.3780	-0.4090	0.1760

C	-0.1850	-0.9900	0.2070
N	-0.1850	-2.3610	0.1330
H	-1.0960	-2.7880	0.0540
C	1.0250	-3.1570	0.1470
H	1.7760	-2.7140	0.8130
C	1.5960	-3.2620	-1.2650
H	0.8700	-3.7030	-1.9570
H	2.4970	-3.8840	-1.2750
H	1.8670	-2.2760	-1.6570
C	0.6930	-4.5460	0.6920
H	-0.0500	-5.0540	0.0680
H	0.2830	-4.4770	1.7050
H	1.5900	-5.1730	0.7320
N	0.9610	-0.3200	0.2990

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CUP08010.xyz 0.0000000

C	0.7910	0.0800	0.2460
H	1.5490	-0.0680	1.0110
C	-0.3990	0.7340	0.5560
H	-0.5730	1.0960	1.5670
C	-1.3620	0.9140	-0.4410
C	-1.1670	0.4590	-1.7360
C	0.0340	-0.1940	-2.0360
H	0.2170	-0.5590	-3.0440
C	1.0080	-0.3840	-1.0510
H	1.9360	-0.8940	-1.2970
C	-2.6240	1.5880	-0.1710
O	-2.8620	2.0280	0.9500
N	-3.4860	1.6760	-1.2490
C	-4.7850	2.3020	-1.0870
H	-5.0680	2.7980	-2.0210
H	-4.7270	3.0610	-0.3020
S	-6.0420	1.0790	-0.6390
N	-3.2030	1.1930	-2.4950
N	-2.1180	0.6270	-2.7480
P	-7.6480	2.2610	0.0710
O	-7.3650	3.8100	-0.3650
C	-8.2580	4.8340	0.0360
H	-8.6100	4.6780	1.0600
H	-9.1090	4.8720	-0.6490
H	-7.7310	5.7900	-0.0090
S	-9.4350	1.6610	-0.4590
O	-7.5570	2.4020	1.6940
C	-6.3400	2.7830	2.3080
H	-5.9080	3.6540	1.8110
H	-5.6340	1.9490	2.2870
H	-6.5430	3.0410	3.3500

39

CUP08011.xyz 0.0000000

C	0.8840	0.9560	0.0380
N	2.0480	1.6900	0.2080
C	3.1940	1.0620	0.8790
H	3.3300	1.5420	1.8560
C	4.4870	1.1800	0.0690
H	4.7800	2.2330	-0.0210
H	4.3340	0.8110	-0.9510
C	5.6250	0.3990	0.7280
H	5.3520	-0.6590	0.8100
H	5.7930	0.7720	1.7450
C	6.9160	0.5190	-0.0680
H	7.2360	1.5630	-0.1420
H	6.7900	0.1240	-1.0810
H	7.7150	-0.0480	0.4200
H	2.9880	0.0040	1.0860
C	2.0950	3.1040	-0.1790
H	2.9270	3.6030	0.3310
H	1.1910	3.6300	0.1460
C	2.2530	3.2770	-1.6800
H	1.3820	2.8900	-2.2170
H	3.1420	2.7610	-2.0540
H	2.3500	4.3390	-1.9280
C	-0.2540	1.1510	0.8440
C	-1.4620	0.4460	0.6740
H	-2.3110	0.6480	1.3280
C	-1.5670	-0.5270	-0.3250
C	-2.8590	-1.2760	-0.5390
F	-3.5670	-1.4490	0.6110
F	-2.6710	-2.5210	-1.0540
F	-3.6890	-0.6310	-1.4010
C	-0.4550	-0.7700	-1.1390
H	-0.5120	-1.5230	-1.9250
C	0.7340	-0.0420	-0.9400
N	1.8320	-0.3690	-1.8200
O	1.8720	0.2130	-2.9110
O	2.6080	-1.2550	-1.4380
N	-0.2030	2.0790	1.9560
O	0.5020	1.7690	2.9250
O	-0.9110	3.0920	1.8670

46			
CUP08012.xyz			
		0.0000000	
C	0.4060	1.3390	-0.7760
H	0.9090	2.3040	-0.7740
C	-0.8660	1.1900	-0.1950
C	-1.5010	2.3740	0.4190
O	-2.7050	2.5790	0.4350
O	-0.5480	3.1720	0.9700
C	-1.0580	4.3310	1.6320
H	-1.7170	4.0410	2.4560
H	-1.5840	4.9760	0.9220
H	-0.2100	4.8860	2.0440
C	-1.5070	-0.0670	-0.2300
C	-2.8630	-0.3400	0.3730

H	-3.3220	-1.2210	-0.0890
H	-3.5590	0.4870	0.2400
C	-0.8320	-1.1490	-0.8300
H	-1.2910	-2.1370	-0.8540
C	0.4320	-0.9880	-1.3960
H	0.9330	-1.8380	-1.8530
C	1.0510	0.2560	-1.3730
H	2.0350	0.3840	-1.8160
S	-2.6660	-0.6870	2.1240
N	-4.2510	-0.5290	2.6620
H	-4.4070	0.3110	3.2140
C	-5.3220	-1.3570	2.2730
O	-5.1570	-2.2810	1.4950
N	-6.4950	-0.9510	2.8320
H	-6.5190	-0.1560	3.4480
C	-7.7470	-1.5280	2.6470
O	-2.2350	-2.0580	2.2990
O	-1.9390	0.4000	2.7520
N	-8.7260	-0.8890	3.2970
C	-9.9730	-1.3810	3.1790
O	-10.8920	-0.6480	3.8760
C	-12.2520	-1.0550	3.8070
H	-12.3870	-2.0550	4.2340
H	-12.6270	-1.0100	2.7790
H	-12.8420	-0.3560	4.4070
C	-10.2570	-2.5040	2.4330
H	-11.2590	-2.8930	2.3440
C	-9.1840	-3.1000	1.8030
O	-9.2660	-4.2220	1.0220
C	-10.5090	-4.9120	0.9820
H	-11.2800	-4.3050	0.4970
H	-10.8230	-5.2250	1.9840
H	-10.3700	-5.8160	0.3800
N	-7.9300	-2.6180	1.8960

27			
CUP08013.xyz			
	0.0000000		
C	0.8980	0.3090	-0.6420
O	1.5060	0.4830	-1.6960
N	-0.1230	1.1620	-0.3180
H	-0.2970	1.8910	-1.0030
C	-0.8900	1.1010	0.8160
C	-1.9440	2.1730	0.9020
H	-1.4750	3.1630	0.8820
H	-2.5550	2.1240	1.8060
H	-2.6250	2.1000	0.0470
C	-0.6650	0.1420	1.7270
Br	-1.6330	-0.0610	3.3180
C	0.4320	-0.8420	1.4710
O	0.6650	-1.7280	2.2930
N	1.1570	-0.7000	0.2780
C	2.2440	-1.6700	0.0070
C	1.9690	-2.4890	-1.2600
H	2.0920	-1.8980	-2.1710

H	0.9460	-2.8820	-1.2510
H	2.6480	-3.3450	-1.3280
H	2.2640	-2.3950	0.8290
C	3.6250	-0.9810	-0.0020
H	3.7290	-0.3220	-0.8710
C	4.7870	-1.9650	0.0020
H	4.8190	-2.5520	-0.9200
H	4.7190	-2.6520	0.8510
H	5.7360	-1.4230	0.0830
H	3.7100	-0.3420	0.8860

24
cup0814a.xyz 0.0000000

C	0.00000	0.00000	0.00000
C	1.53408	0.00000	0.00000
C	2.05973	1.40826	0.00000
C	1.49639	2.33132	0.79080
C	0.34061	1.95560	1.67538
C	-0.65097	1.06667	0.91383
C	-1.47940	1.87224	-0.07541
O	-2.16063	2.82703	0.21125
N	-1.37015	1.36609	-1.50449
S	-2.15391	2.03450	-2.84301
C	-0.55973	0.36535	-1.36640
O	-0.30449	-0.21433	-2.39435
H	-0.38457	-1.02206	0.23600
H	1.92333	-0.51443	0.90973
H	1.91950	-0.55826	-0.88526
H	2.92224	1.66132	-0.64009
H	1.88277	3.36457	0.81911
H	-0.17322	2.87084	2.05249
H	0.74574	1.41516	2.56283
H	-1.37462	0.60022	1.62583
C	-3.75015	1.14794	-2.77989
Cl	-4.68855	1.56685	-1.31795
Cl	-3.54838	-0.62524	-2.84990
Cl	-4.72332	1.64387	-4.21188

26
CUP08015.xyz 0.0000000

C	1.5230	0.6530	0.1990
C	0.3920	1.4960	0.2290
H	0.4770	2.5210	0.5830
C	-0.8570	1.0360	-0.1890
H	-1.7180	1.6980	-0.1600
C	-0.9990	-0.2720	-0.6420
H	-1.9720	-0.6320	-0.9670
C	0.1060	-1.1230	-0.6740
H	-0.0290	-2.1430	-1.0280
C	1.3720	-0.6780	-0.2570
C	2.4880	-1.5340	-0.2830
H	2.3830	-2.5610	-0.6290

C	3.7470	-1.0960	0.1390
H	4.5930	-1.7780	0.1190
C	3.9130	0.2090	0.5880
H	4.8860	0.5550	0.9230
C	2.8110	1.0650	0.5990
O	3.0210	2.3840	1.0620
C	3.4330	3.4210	0.2080
O	3.6540	4.5420	0.6580
N	3.5560	3.0970	-1.1270
H	3.3470	2.1600	-1.4430
C	3.9730	4.0740	-2.0980
H	4.9480	4.4780	-1.8100
H	3.2390	4.8840	-2.1310
H	4.0420	3.5920	-3.0760

31			
CUP08016.xyz		0.0000000	
C	0.8380	0.7900	-0.1200
C	-0.3650	1.2690	-0.6050
O	-0.5670	2.6330	-0.8720
C	-1.3920	0.3750	-0.8990
H	-2.3330	0.7340	-1.3060
C	-1.2040	-0.9960	-0.6640
H	-2.0080	-1.6950	-0.8850
C	0.0070	-1.4720	-0.1460
H	0.1450	-2.5320	0.0430
C	1.0190	-0.5610	0.1130
C	2.3650	-0.7950	0.6850
H	2.2750	-1.0580	1.7440
H	2.9150	-1.5830	0.1620
C	2.9910	0.6050	0.4820
C	3.6990	1.0840	1.7510
H	4.1080	2.0910	1.6140
H	4.5160	0.4110	2.0340
H	2.9950	1.1490	2.5890
C	3.9680	0.6220	-0.7000
H	3.4690	0.3220	-1.6290
H	4.8150	-0.0500	-0.5310
H	4.3540	1.6340	-0.8710
O	1.9270	1.5560	0.1910
C	-0.5080	3.6270	0.1190
O	-0.4410	4.8130	-0.1930
N	-0.5850	3.1840	1.4230
H	-0.6720	2.1960	1.6110
C	-0.5420	4.1030	2.5300
H	-1.4150	4.7590	2.4850
H	0.3690	4.7040	2.4680
H	-0.5510	3.5320	3.4610

34			
CUP08017.xyz		0.0000000	

P	0.1120	-0.5530	-0.0950
S	0.4820	-2.4960	0.6750
C	0.3280	-3.5920	-0.7530
H	1.1560	-3.3970	-1.4380
H	-0.6160	-3.3840	-1.2630
S	0.3610	-5.3330	-0.2320
C	-0.1100	-6.1280	-1.7600
O	0.5610	0.5360	1.0360
C	1.9340	0.6860	1.3620
H	2.4030	1.3480	0.6270
H	2.4440	-0.2810	1.3400
C	2.0380	1.2940	2.7460
H	1.5540	0.6500	3.4870
H	1.5250	2.2620	2.7820
H	3.0830	1.4380	3.0320
O	-1.4920	-0.2560	-0.0340
C	-2.4020	-1.0780	-0.7460
H	-2.5130	-2.0290	-0.2160
H	-2.0310	-1.2760	-1.7550
C	-3.7380	-0.3690	-0.8170
H	-3.6370	0.5940	-1.3280
H	-4.1170	-0.1570	0.1890
H	-4.4750	-0.9760	-1.3510
S	0.8550	-0.0990	-1.8520
C	-1.1770	-7.0340	-1.7480
H	-1.7130	-7.2440	-0.8250
C	-1.5710	-7.6800	-2.9240
H	-2.4040	-8.3790	-2.9010
C	-0.8910	-7.4250	-4.1130
Cl	-1.3760	-8.2180	-5.5620
C	0.1820	-6.5360	-4.1350
H	0.7200	-6.3410	-5.0590
C	0.5750	-5.8920	-2.9580
H	1.4280	-5.2190	-2.9920

24

cup0818b.xyz	0.000000		
C	0.00000	0.00000	0.00000
C	1.54810	0.00000	0.00000
Cl	2.26808	1.63247	0.00000
C	1.88133	-0.89157	1.23193
Cl	3.63563	-1.26512	1.38008
Cl	1.29111	-0.24248	2.79886
C	2.01333	-0.94888	-1.07926
Cl	2.74138	-0.45991	-2.56643
C	1.71452	-2.18916	-0.67834
Cl	1.96677	-3.67002	-1.52923
C	1.04521	-2.08070	0.67174
Cl	1.02849	-3.55331	1.67864
C	-0.34936	-1.44305	0.46224
C	-1.27788	-2.01346	-0.62345
C	-1.93676	-0.75530	-1.21058
C	-0.75243	0.22008	-1.32264
H	-0.39520	0.73241	0.74617

H	-0.90764	-1.37851	1.42791
Cl	-2.43511	-3.21215	0.01915
H	-0.70148	-2.53720	-1.41830
Cl	-2.74561	-1.02541	-2.78080
H	-2.70547	-0.34343	-0.51386
H	-1.07395	1.27946	-1.46154
H	-0.11812	-0.06085	-2.19298

34
CUP08019.xyz 0.0000000

C	1.8720	0.6060	-1.4850
Cl	3.2710	1.1950	-2.2980
C	0.6070	1.0290	-1.8900
H	0.4960	1.7270	-2.7160
C	-0.5280	0.5550	-1.2270
H	-1.5100	0.8960	-1.5510
C	-0.4090	-0.3430	-0.1520
C	-1.6430	-0.7870	0.5150
O	-2.3040	-1.7730	-0.1900
P	-3.7680	-2.4010	0.0690
O	-3.7100	-2.9810	1.5770
C	-3.2570	-4.3090	1.7860
H	-3.6240	-4.9690	0.9940
H	-3.6890	-4.6560	2.7290
C	-1.7460	-4.3530	1.8720
H	-1.3830	-3.6570	2.6340
H	-1.2930	-4.0590	0.9200
H	-1.4010	-5.3610	2.1200
O	-4.7220	-1.1030	0.2140
C	-6.1070	-1.3340	0.4120
H	-6.2500	-1.9870	1.2790
H	-6.5210	-1.8240	-0.4740
C	-6.7910	-0.0030	0.6430
H	-6.6390	0.6630	-0.2130
H	-6.3670	0.5020	1.5180
H	-7.8650	-0.1370	0.7990
C	-2.0780	-0.2520	1.6640
Cl	-1.3000	1.0060	2.5370
H	-2.9860	-0.5530	2.1680
C	0.8750	-0.7640	0.2370
Cl	1.1170	-1.8810	1.5350
C	2.0110	-0.2900	-0.4280
H	3.0020	-0.6180	-0.1200
O	-4.2250	-3.3840	-0.9680

42
CUP08020.xyz 0.0000000

C	1.6520	0.1700	-0.4130
Cl	2.9750	1.2370	-0.1750
N	0.4510	0.7140	-0.1600
C	-0.6040	-0.0920	-0.3330
N	-1.8240	0.5020	-0.0410

H	-1.7470	1.4610	0.2590
N	-0.5220	-1.3650	-0.7340
C	0.7090	-1.8510	-0.9720
O	0.8680	-3.1590	-1.3870
C	-0.3640	-3.8580	-1.5450
H	-0.9900	-3.3890	-2.3110
H	-0.9000	-3.9360	-0.5920
H	-0.1310	-4.8730	-1.8810
C	1.8570	-1.1190	-0.8250
H	2.8360	-1.5310	-1.0210
C	-3.0480	-0.0940	-0.1220
N	-4.0600	0.7850	0.3100
H	-3.7400	1.5770	0.8920
O	-3.2910	-1.2310	-0.4940
S	-5.5950	0.2500	0.7510
C	-6.4870	1.7700	1.0330
O	-6.2160	-0.3990	-0.3850
O	-5.5100	-0.3960	2.0440
C	-6.1030	2.6830	2.0240
C	-6.8970	3.8100	2.2780
H	-6.6020	4.5380	3.0310
C	-8.0700	4.0190	1.5510
H	-8.6840	4.8940	1.7500
C	-8.4520	3.1110	0.5650
H	-9.3680	3.2750	0.0030
C	-7.6660	1.9860	0.3060
H	-7.9970	1.2820	-0.4550
C	-4.8360	2.5640	2.7430
O	-5.0450	2.6710	4.0740
C	-3.8640	2.5290	4.8740
H	-3.1470	3.3160	4.6150
H	-3.4130	1.5460	4.6940
C	-4.2610	2.6540	6.3320
H	-4.9940	1.8860	6.5990
H	-4.7330	3.6240	6.5210
H	-3.3890	2.5530	6.9840
O	-3.7750	2.3840	2.1590

7			
CUP08021.xyz	0.0000000		
C	0.1270	0.0200	-0.0190
Cl	0.5890	-1.6840	-0.0200
Cl	0.6820	0.8660	-1.4720
Cl	0.6940	0.8680	1.4280
N	-1.4040	0.0180	-0.0140
O	-1.9970	-0.0150	-1.1050
O	-1.9890	-0.0070	1.0820

29			
CUP08022.xyz	0.0000000		
C	1.5530	0.1310	-0.7130

Cl	3.1760	0.6470	-0.9560
C	0.5050	1.0070	-0.4530
Cl	0.7080	2.7110	-0.3320
N	-0.7770	0.6170	-0.2570
C	-1.0300	-0.7040	-0.3270
O	-2.3200	-1.1200	-0.1370
P	-3.5940	-0.1370	-0.0060
O	-3.5840	0.3250	1.5480
C	-2.6720	1.2970	2.0250
H	-2.5230	2.0860	1.2850
H	-1.7160	0.8110	2.2390
C	-3.2320	1.8950	3.3000
H	-3.3970	1.1160	4.0530
H	-4.2030	2.3650	3.1110
H	-2.5510	2.6450	3.7120
O	-4.7850	-1.2460	0.0840
C	-5.0490	-2.0750	-1.0370
H	-4.1110	-2.4090	-1.4930
H	-5.6190	-1.5060	-1.7770
C	-5.8530	-3.2720	-0.5730
H	-6.7890	-2.9510	-0.1060
H	-5.2980	-3.8390	0.1830
H	-6.0860	-3.9350	-1.4110
C	-0.0490	-1.6590	-0.5780
Cl	-0.4100	-3.3400	-0.6600
C	1.2620	-1.2310	-0.7750
H	2.0510	-1.9530	-0.9750
S	-3.9200	1.2240	-1.3620

40

CUP08023.xyz 0.0000000

C	0.3590	0.5320	1.1070
C	-0.4500	0.8460	0.0230
C	-1.4340	-0.0060	-0.4230
H	-2.0610	0.2450	-1.2720
C	-1.5860	-1.2150	0.2620
H	-2.3470	-1.9240	-0.0590
C	-0.7630	-1.5340	1.3620
H	-0.8990	-2.4840	1.8740
C	0.2280	-0.6500	1.7990
H	0.8680	-0.8890	2.6410
C	1.2820	1.6350	1.2990
O	2.1060	1.6990	2.1950
N	1.0160	2.5480	0.3090
C	1.7600	3.7940	0.1570
S	2.6010	3.8920	-1.4550
P	4.0760	2.3770	-1.5720
O	5.3460	2.7650	-0.6270
C	5.2220	2.8220	0.7830
H	4.5300	2.0580	1.1420
H	4.8440	3.8090	1.0620
C	6.5900	2.6050	1.3960
H	7.2980	3.3600	1.0390
H	6.9920	1.6290	1.1060

H	6.5410	2.6550	2.4880
O	4.8480	2.5560	-3.0020
C	4.1050	2.5390	-4.2120
H	3.7170	3.5450	-4.4010
H	3.2610	1.8460	-4.1410
C	5.0260	2.1200	-5.3390
H	5.4360	1.1220	-5.1500
H	5.8770	2.8040	-5.4170
H	4.4950	2.1070	-6.2940
H	2.5360	3.8110	0.9270
C	0.8430	5.0090	0.3740
H	0.2350	4.8680	1.2740
H	0.1560	5.1720	-0.4630
Cl	1.7670	6.5160	0.6290
C	-0.0420	2.1500	-0.4700
O	-0.5910	2.7360	-1.3860
S	3.5430	0.5030	-1.3400

40

CUP08024.xyz	0.0000000		
C	0.8070	0.3440	-0.1780
C	1.9990	1.2660	-0.0640
C	2.4090	1.8000	-1.4360
H	2.7390	0.9950	-2.1030
H	3.2330	2.5150	-1.3430
H	1.5720	2.3130	-1.9230
H	1.7100	2.1250	0.5560
C	3.1680	0.5650	0.6270
H	3.5280	-0.2920	0.0460
H	2.8730	0.1950	1.6160
H	4.0070	1.2550	0.7630
N	-0.3200	0.7120	0.4570
C	-1.3720	-0.1190	0.3550
O	-2.4750	0.3360	1.0170
C	-1.3360	-1.2880	-0.3700
H	-2.1820	-1.9530	-0.4750
C	-0.1370	-1.5860	-0.9910
C	0.0010	-2.8380	-1.8020
H	-0.1840	-3.7170	-1.1770
H	1.0100	-2.9240	-2.2190
H	-0.7100	-2.8310	-2.6340
N	0.9410	-0.7830	-0.9040
P	-3.8140	-0.5090	1.3170
S	-3.6460	-2.1010	2.4170
O	-4.8130	0.6370	1.8870
C	-4.4940	1.2800	3.1120
H	-3.4470	1.5990	3.1060
H	-4.6480	0.5810	3.9390
C	-5.4000	2.4830	3.2740
H	-6.4520	2.1770	3.2690
H	-5.2670	3.1810	2.4400
H	-5.1900	3.0070	4.2100
O	-4.4290	-0.7610	-0.1640
C	-4.8030	0.3500	-0.9650

H	-4.0630	1.1520	-0.8760
H	-5.7730	0.7240	-0.6230
C	-4.8980	-0.1070	-2.4060
H	-5.6280	-0.9170	-2.5070
H	-3.9360	-0.5020	-2.7490
H	-5.1940	0.7190	-3.0590

19			
CUP08025.xyz			
	0.0000000		
C	0.8720	0.9270	0.1470
O	1.8350	1.8440	0.4920
C	2.5650	2.2720	-0.6600
H	1.9030	2.6080	-1.4650
H	3.2230	1.4780	-1.0260
H	3.1910	3.1180	-0.3610
C	-0.4450	1.3540	-0.0730
C	-1.4430	0.4310	-0.3980
Cl	-3.0700	0.9060	-0.7310
C	-1.1310	-0.9290	-0.4700
H	-1.8970	-1.6600	-0.7190
C	0.1710	-1.3650	-0.2090
H	0.3960	-2.4290	-0.2490
C	1.1690	-0.4410	0.1090
Cl	2.7470	-1.0400	0.4720
C	-0.7570	2.7660	0.0320
O	-0.5220	3.6170	-0.8070
O	-1.3440	3.0240	1.2140
H	-1.5140	3.9890	1.2200

13			
CUP08026.xyz			
	0.0000000		
C	1.2060	0.6970	0.0000
Cl	2.7430	1.4930	0.0000
C	-0.0010	1.4120	0.0000
C	-1.2080	0.6970	0.0000
Cl	-2.7440	1.4930	0.0000
C	-1.2060	-0.7020	0.0000
H	-2.1430	-1.2560	0.0000
C	-0.0010	-1.4000	0.0000
H	-0.0010	-2.4880	0.0000
C	1.2050	-0.7020	0.0000
H	2.1410	-1.2560	0.0000
C	-0.0010	2.8460	0.0000
N	-0.0010	4.0070	0.0000

35			
CUP08027.xyz			
	0.0000000		
C	0.1790	0.8320	-0.2840

C	-0.8640	1.7810	-0.4480
N	-0.6540	3.0170	-1.0490
H	-1.4290	3.6700	-1.1680
H	0.2500	3.3260	-1.3860
C	-2.1450	1.4320	0.0230
C	-3.3420	2.3480	-0.0890
F	-3.8470	2.6830	1.1300
F	-4.3690	1.7710	-0.7730
F	-3.0930	3.5300	-0.7240
C	-2.3410	0.1800	0.6340
H	-3.3330	-0.0950	0.9970
C	-1.2700	-0.7130	0.7730
C	0.0250	-0.4340	0.3210
N	1.0710	-1.3350	0.4550
C	1.5130	-2.0890	-0.7220
H	2.5450	-1.8180	-0.9710
H	0.9030	-1.8340	-1.5980
C	1.4170	-3.5910	-0.5030
H	0.3990	-3.8890	-0.2350
H	2.0870	-3.9260	0.2950
H	1.6970	-4.1230	-1.4170
C	1.6940	-1.5090	1.7710
H	1.4900	-2.5180	2.1470
H	1.2620	-0.8110	2.4990
C	3.1960	-1.2730	1.7290
H	3.4330	-0.2820	1.3320
H	3.7030	-2.0160	1.1060
H	3.6160	-1.3450	2.7370
N	1.4990	1.2020	-0.7400
O	1.8060	0.8860	-1.8980
O	2.2040	1.8520	0.0440
N	-1.5630	-1.9900	1.3830
O	-2.0580	-2.8580	0.6520
O	-1.3470	-2.0960	2.5970

29			
CUP08028.xyz			
		0.0000000	
C	0.9730	0.5570	-0.9820
C	2.2150	1.1690	-1.6300
C	1.9800	1.3260	-3.1360
H	1.8920	0.3520	-3.6310
H	2.7990	1.8730	-3.6120
H	1.0570	1.8820	-3.3350
H	2.3700	2.1680	-1.2050
C	3.5100	0.3810	-1.3210
H	3.5240	-0.5740	-1.8600
H	3.5450	0.1420	-0.2510
C	4.7780	1.1490	-1.6740
H	4.8070	2.1170	-1.1640
H	4.8580	1.3210	-2.7510
H	5.6590	0.5780	-1.3640
C	-0.0110	1.3440	-0.3550
O	0.0700	2.7070	-0.3110
H	0.5850	3.0350	-1.0660

C	-1.1080	0.7290	0.2610
C	-1.2900	-0.6550	0.2630
H	-2.1550	-1.0980	0.7510
C	-0.3370	-1.4360	-0.3910
C	0.7770	-0.8430	-1.0120
H	1.5040	-1.4730	-1.5230
N	-2.1110	1.5420	0.9110
O	-2.1640	1.4780	2.1470
O	-2.8710	2.1940	0.1830
N	-0.4990	-2.8930	-0.4320
O	-1.5130	-3.3730	0.0940
O	0.3860	-3.5570	-0.9890

25
CUP08029.xyz 0.0000000

C	1.4670	1.0640	0.5350
H	2.2380	1.2990	-0.2130
C	0.0600	1.0210	-0.1610
Cl	-0.2840	2.4150	-1.1670
C	-0.9630	0.6930	0.9100
Cl	-2.0640	1.8020	1.5600
C	-0.7820	-0.5870	1.2570
Cl	-1.5990	-1.4690	2.4470
C	0.3640	-1.1240	0.4210
Cl	0.4650	-2.8680	0.2670
C	1.6820	-0.4500	0.9460
H	2.5380	-0.8160	0.3610
C	0.0910	-0.3510	-0.9090
Cl	-1.4570	-0.7930	-1.7290
Cl	1.3790	-0.5040	-2.1490
C	2.0170	-0.7270	2.4150
H	1.2490	-0.3680	3.1090
H	2.0960	-1.8080	2.5730
O	3.2970	-0.1820	2.7230
S	3.2870	1.2740	3.4100
O	2.9670	2.1430	2.0930
C	1.6150	2.1100	1.6450
H	1.3990	3.1040	1.2400
H	0.9190	1.9570	2.4780
O	4.6980	1.5830	3.8100

27
CUP08030.xyz 0.0000000

Cl	-4.3920	-2.7680	-3.7110
C	-5.2050	-1.2080	-3.5300
Cl	-6.8790	-1.6120	-4.2040
C	-4.5600	0.0560	-4.1770
Cl	-4.1970	-0.0450	-5.8810
C	-3.3630	0.5270	-3.2790
H	-3.3080	1.6260	-3.3490
C	-1.8940	0.0110	-3.3030

H	-1.4400	-0.0800	-4.2900
C	-1.1340	0.9780	-2.3680
H	-1.0630	2.0140	-2.6560
C	-1.5930	0.5800	-0.9890
H	-1.8630	1.3210	-0.2540
C	-2.5770	-0.5820	-1.2480
H	-2.7430	-1.2110	-0.3720
C	-1.8950	-1.2570	-2.4420
H	-0.8840	-1.6150	-2.2090
H	-2.3900	-2.1100	-2.8530
O	-0.2330	0.4270	-1.4030
C	-3.8440	0.1090	-1.8330
H	-4.0160	1.0110	-1.2240
C	-5.2430	-0.5380	-2.1230
Cl	-5.8800	-1.5090	-0.8200
C	-6.0690	0.6860	-2.5350
Cl	-7.2020	1.4580	-1.5440
C	-5.6600	1.0420	-3.7650
Cl	-6.1550	2.3690	-4.6920

41
CUP08031.xyz 0.0000000

C	-1.8050	-0.5680	0.2850
S	-1.1760	-2.2500	0.4940
H	-2.5900	-0.5700	-0.4740
H	-0.9930	0.0820	-0.0510
S	-2.4780	0.0750	1.8350
P	-3.0770	2.0540	1.3450
S	-4.3800	2.2210	-0.1070
O	-3.5740	2.7930	2.7140
C	-3.9680	4.1590	2.6850
H	-5.0200	4.2180	2.3910
H	-3.3650	4.7200	1.9640
C	-3.7850	4.7400	4.0720
H	-2.7380	4.6680	4.3850
H	-4.3750	4.1810	4.8060
H	-4.0900	5.7900	4.0990
O	-1.7440	2.9360	1.0140
C	-0.6670	2.9590	1.9390
H	-0.0200	2.0980	1.7470
H	-1.0360	2.8990	2.9680
C	0.1090	4.2450	1.7430
H	-0.5360	5.1130	1.9140
H	0.4780	4.3200	0.7150
H	0.9600	4.2970	2.4280
P	-0.2900	-2.7090	-1.3840
O	1.0860	-1.8580	-1.5880
C	1.9820	-1.5720	-0.5260
C	2.8060	-2.7760	-0.1200
H	3.2950	-3.2240	-0.9900
H	2.1800	-3.5450	0.3390
H	3.5730	-2.4890	0.6050
H	1.4470	-1.1540	0.3300
H	2.6560	-0.7870	-0.8860

O	0.3150	-4.2240	-1.3010
C	0.9750	-4.7950	-2.4230
H	1.6710	-4.0730	-2.8610
H	0.2320	-5.0750	-3.1750
C	1.7240	-6.0300	-1.9660
H	1.0360	-6.7550	-1.5180
H	2.4600	-5.7750	-1.1970
H	2.2410	-6.5060	-2.8040
S	-1.4570	-2.4650	-2.9400

24
CUP08032.xyz 0.0000000

C	0.6290	-0.2000	-0.0020
N	1.8680	0.3710	-0.3680
H	1.8860	1.3770	-0.4160
C	-0.4240	0.6830	0.2760
H	-0.2800	1.7590	0.2160
C	-1.6850	0.2010	0.6400
H	-2.4920	0.8970	0.8550
C	-1.9070	-1.1700	0.7280
H	-2.8860	-1.5480	1.0100
C	-0.8690	-2.0570	0.4500
H	-1.0380	-3.1290	0.5140
C	0.3930	-1.5750	0.0850
H	1.1690	-2.3010	-0.1300
C	3.0580	-0.2830	-0.6340
O	3.2530	-1.4800	-0.4270
N	4.0680	0.5450	-1.1430
C	3.8920	1.9160	-1.6070
H	4.6150	2.1350	-2.3990
H	4.0570	2.5900	-0.7630
H	2.8890	2.0700	-2.0130
C	5.4230	0.0190	-1.2320
H	6.1020	0.7080	-0.7210
H	5.7020	-0.0530	-2.2870
H	5.5180	-0.9690	-0.7730

22
CUP08033.xyz 0.0000000

Cl	0.2930	-1.7090	0.6080
C	0.8250	-0.1490	0.0110
C	2.3600	-0.0110	-0.2430
Cl	3.0130	-1.1120	-1.5040
Cl	3.3910	-0.2530	1.2190
C	2.1980	1.4830	-0.6880
C	1.2100	1.3510	-1.8960
H	1.7550	0.9910	-2.7790
C	0.2320	0.2270	-1.3910
H	0.2430	-0.6240	-2.0830
C	-1.1110	0.8850	-1.4320
H	-2.0280	0.3950	-1.1310

C	-1.0430	2.1410	-1.8890
H	-1.9030	2.7890	-1.9970
C	0.3450	2.5730	-2.2460
H	0.6400	3.4830	-1.7210
Cl	0.4060	2.9230	-3.9910
Cl	3.6850	2.3170	-1.0980
C	1.4440	2.0100	0.5190
C	0.6290	1.0350	0.9390
Cl	-0.4840	1.0830	2.2140
Cl	1.6090	3.5710	1.1520

24
CUP08034.xyz 0.0000000

C	1.2850	0.5310	-0.5780
C	1.2790	-0.1630	-1.9580
H	1.2610	0.5760	-2.7680
H	2.1780	-0.7760	-2.0920
H	0.4120	-0.8170	-2.0930
C	2.5340	1.4270	-0.5010
H	3.4510	0.8390	-0.6230
H	2.5210	2.1920	-1.2860
H	2.5960	1.9410	0.4640
C	0.0220	1.4070	-0.4080
H	0.1590	2.1120	0.4230
H	-0.1160	2.0140	-1.3130
C	-1.2360	0.6180	-0.1340
C	-2.5290	1.3270	-0.4210
H	-2.5920	1.5870	-1.4820
H	-2.5940	2.2480	0.1680
H	-3.4010	0.7120	-0.1750
C	-1.2180	-0.6330	0.3460
H	-2.1210	-1.2020	0.5370
C	0.0560	-1.3030	0.6780
O	0.0380	-2.4520	1.1090
C	1.3440	-0.5190	0.5450
H	2.1590	-1.2290	0.3550
H	1.5340	-0.0440	1.5150

18
CUP08035.xyz 0.0000000

C	1.1610	0.8790	-0.2460
H	1.1840	0.9330	-1.3410
Cl	2.6700	1.7190	0.2640
C	-0.1080	1.6070	0.2490
H	-0.1050	1.6930	1.3410
Cl	-0.1170	3.3000	-0.3850
C	-1.3720	0.8670	-0.2390
Cl	-2.8860	1.6930	0.2790
H	-1.4010	0.9200	-1.3340
C	-1.3960	-0.6230	0.1660
Cl	-1.7240	-0.8400	1.9220

H	-2.2470	-1.1110	-0.3250
C	-0.0950	-1.3520	-0.2300
H	-0.0890	-2.3690	0.1790
Cl	-0.0990	-1.5900	-2.0230
C	1.2020	-0.6100	0.1590
H	2.0540	-1.0900	-0.3370
Cl	1.5420	-0.8240	1.9130

38
CUP08036.xyz 0.0000000

P	0.4800	-2.0070	1.3280
S	0.7510	-2.7590	-0.4630
O	1.8540	-2.0730	2.2090
C	2.9450	-1.2350	1.8800
H	3.7870	-1.4910	2.5280
H	2.6830	-0.1880	2.0490
H	3.2500	-1.3810	0.8410
S	-0.3490	-0.0590	1.5290
C	-0.3980	0.6890	-0.1380
H	-0.7570	-0.0500	-0.8620
C	0.9890	1.1990	-0.5290
H	1.7380	0.4080	-0.4190
H	1.2890	2.0570	0.0840
O	-0.4000	-3.0200	2.2600
C	-1.7360	-3.3190	1.9010
H	-2.2700	-3.6520	2.7950
H	-1.7480	-4.1270	1.1650
H	-2.2450	-2.4420	1.4950
C	-1.4030	1.8330	-0.0960
O	-1.1160	3.0090	0.0890
O	-2.6670	1.3520	-0.2820
C	-3.6950	2.3510	-0.2580
H	-3.5180	3.0800	-1.0570
H	-3.6940	2.8590	0.7120
C	-5.0280	1.6630	-0.4760
H	-5.2080	0.9150	0.3030
H	-5.0360	1.1320	-1.4340
H	-5.8470	2.3870	-0.4660
C	1.0140	1.6250	-1.9770
O	0.0650	1.5540	-2.7440
O	2.2560	2.0870	-2.2930
C	2.4050	2.5180	-3.6520
H	1.7050	3.3360	-3.8580
H	2.2030	1.6800	-4.3280
C	3.8290	3.0010	-3.8430
H	4.5410	2.1990	-3.6200
H	4.0530	3.8250	-3.1580
H	3.9910	3.3410	-4.8700

20
CUP08037.xyz 0.0000000

N	0.0610	0.4920	0.1300
C	0.0540	1.9310	0.1400
H	-0.4870	2.2960	-0.7370
H	-0.4470	2.2810	1.0460
H	1.0850	2.2880	0.1200
H	0.9380	-0.0130	0.1360
C	-1.1010	-0.2410	0.1140
O	-0.7980	-1.5790	0.1080
N	-1.9760	-2.3450	0.0910
C	-1.7130	-3.6130	0.0860
C	-0.3270	-4.2040	0.0960
H	0.2200	-3.8600	-0.7870
H	-0.3410	-5.2970	0.0890
H	0.2020	-3.8710	0.9930
S	-3.0240	-4.7880	0.0650
C	-4.4660	-3.7000	0.0560
H	-4.4670	-3.0660	-0.8340
H	-4.4860	-3.0760	0.9540
H	-5.3730	-4.3110	0.0430
O	-2.2250	0.2500	0.1080

26
CUP08038.xyz 0.0000000

P	0.1240	-2.5330	1.1590
S	0.0300	-3.9120	-0.2110
O	1.4090	-1.5440	0.9970
C	1.4980	-0.7160	-0.1480
H	2.2730	0.0350	0.0260
H	0.5500	-0.2040	-0.3350
H	1.7780	-1.3120	-1.0200
O	-1.0640	-1.4470	1.2930
C	-2.4030	-1.6290	1.4850
O	0.3780	-3.0160	2.6860
C	-0.5380	-3.8540	3.3580
H	-0.0270	-4.3130	4.2080
H	-0.9030	-4.6500	2.7050
H	-1.3730	-3.2620	3.7370
C	-3.1110	-0.4750	1.8400
H	-2.5810	0.4700	1.9520
C	-4.4910	-0.5170	2.0580
H	-5.0100	0.3970	2.3360
C	-5.1680	-1.7320	1.9110
C	-4.4700	-2.8900	1.5490
H	-4.9800	-3.8440	1.4240
C	-3.0860	-2.8330	1.3340
H	-2.5850	-3.7490	1.0450
N	-6.6170	-1.7910	2.1350
O	-7.1960	-0.7420	2.4510
O	-7.1770	-2.8880	1.9950

CUP08039.xyz	0.0000000		
C	0.6940	0.8660	0.1950
O	1.9230	1.1890	-0.3430
C	1.8360	1.9760	-1.5260
H	1.3740	2.9480	-1.3220
H	1.2980	1.4440	-2.3190
H	2.8550	2.1590	-1.8800
N	-0.4170	1.3400	-0.3640
C	-1.5440	0.9790	0.2390
N	-1.6110	0.1980	1.3190
C	-0.4360	-0.2310	1.7910
C	-0.4510	-1.0830	3.0200
H	-1.3630	-1.6870	3.0590
H	-0.4120	-0.4470	3.9100
H	0.4080	-1.7600	3.0320
N	0.7500	0.0840	1.2720
N	-2.7790	1.4260	-0.2140
H	-3.5570	1.1000	0.3370
C	-2.9930	2.2370	-1.2900
N	-4.3590	2.5620	-1.4090
H	-4.9200	2.4170	-0.5520
S	-4.8860	3.8870	-2.3050
C	-6.6620	3.7940	-2.1660
O	-2.1540	2.6690	-2.0640
C	-7.3140	3.8820	-0.9290
C	-8.7150	3.9120	-0.8800
H	-9.2350	3.9610	0.0740
C	-9.4580	3.8620	-2.0600
H	-10.5440	3.8850	-2.0200
C	-8.8090	3.7740	-3.2900
H	-9.3920	3.7370	-4.2090
C	-7.4150	3.7420	-3.3480
H	-6.9320	3.6950	-4.3220
O	-4.5580	3.6720	-3.6990
O	-4.5060	5.0990	-1.6100
C	-6.5880	3.8330	0.3370
O	-5.7640	2.9580	0.5730
O	-6.9580	4.8640	1.1290
C	-6.2590	4.9250	2.3740
H	-5.1840	5.0370	2.2040
H	-6.4660	4.0320	2.9720
H	-6.6180	5.8010	2.9220

42			
CUP08040.xyz	0.0000000		
C	1.0250	0.8690	0.5270
N	2.1810	1.5620	0.2030
C	3.3400	0.8180	-0.3060
C	4.6250	1.1340	0.4600
H	4.4800	0.9890	1.5350
H	4.9040	2.1840	0.3200
C	5.7780	0.2580	-0.0070
H	5.9740	0.4050	-1.0740
H	5.5590	-0.8010	0.1610

H	6.6900	0.5070	0.5430
H	3.4750	1.0680	-1.3660
H	3.1500	-0.2630	-0.2710
C	2.2070	3.0290	0.2640
H	1.3000	3.4530	-0.1800
H	3.0360	3.4080	-0.3460
C	2.3490	3.5360	1.6980
H	3.2290	3.0910	2.1760
H	1.4760	3.2390	2.2900
C	2.4760	5.0510	1.7410
H	1.5960	5.5310	1.3020
H	3.3610	5.3870	1.1920
H	2.5680	5.3940	2.7770
C	-0.1100	0.8640	-0.3110
C	-1.3060	0.1940	-0.0020
H	-2.1560	0.2350	-0.6820
C	-1.3780	-0.5320	1.1840
S	-2.8850	-1.3610	1.6180
C	-2.6750	-2.9850	0.9360
H	-1.8040	-3.4550	1.3950
H	-2.5490	-2.9040	-0.1460
H	-3.5720	-3.5660	1.1620
C	-0.2910	-0.5800	2.0530
H	-0.3490	-1.1380	2.9870
C	0.8840	0.1090	1.7040
N	-0.0590	1.5230	-1.5990
O	-0.7560	2.5380	-1.7350
O	0.6370	0.9970	-2.4780
N	1.9810	0.0020	2.6370
O	2.0160	0.8200	3.5650
O	2.7620	-0.9440	2.4700
O	-3.9590	-0.7020	0.9010
O	-2.9110	-1.4740	3.0630

13			
CUP08041.xyz			
	0.000000		
C	-0.0320	0.4230	0.3050
C	0.3050	-0.9490	-0.2190
O	1.3240	-1.1480	-0.8810
C	-0.6400	-2.0790	0.1340
O	-1.9320	-1.7240	-0.3280
H	-0.6200	-2.2060	1.2230
H	-0.2860	-2.9890	-0.3650
H	0.7810	1.1150	0.0700
H	-0.1530	0.3810	1.3910
H	-0.9500	0.7850	-0.1640
N	-2.9030	-2.7140	-0.0430
O	-4.0250	-2.4130	-0.4480
O	-2.5240	-3.7180	0.5610

CUP08042.xyz	0.0000000		
N	0.0420	1.2980	0.4520
C	-0.0480	2.7180	0.2380
H	-0.0430	2.9220	-0.8360
H	-0.9800	3.0900	0.6730
H	0.8070	3.2010	0.7160
H	0.8170	0.9100	0.9730
C	-0.9030	0.4270	-0.0340
O	-0.5640	-0.8560	0.3140
N	-1.5140	-1.7670	-0.1840
C	-1.2210	-2.9760	0.1620
S	0.0960	-3.6200	1.0840
C	1.3660	-3.5930	-0.2000
H	1.5370	-2.5720	-0.5520
H	1.0720	-4.2200	-1.0460
H	2.3020	-3.9810	0.2100
O	-1.8900	0.7680	-0.6770
C	-2.0670	-4.1590	-0.2130
O	-1.7170	-4.8050	-1.1970
N	-3.1990	-4.4180	0.5630
C	-3.6190	-3.6230	1.7100
H	-3.6720	-4.2760	2.5860
H	-4.6110	-3.2120	1.5040
H	-2.9370	-2.8010	1.9290
C	-4.0430	-5.5520	0.2230
H	-4.0840	-6.2300	1.0810
H	-3.6630	-6.1010	-0.6420
H	-5.0490	-5.1870	-0.0020

32			
CUP08043.xyz	0.0000000		
P	0.4570	-2.4500	-0.6850
S	-0.8440	-3.8930	-0.6790
O	0.5710	-1.6100	-2.0690
C	-0.5750	-0.9360	-2.5650
H	-1.1370	-0.4840	-1.7410
H	-1.2180	-1.6570	-3.0780
C	-0.1220	0.1380	-3.5330
H	0.4520	-0.3010	-4.3560
H	0.5380	0.8550	-3.0320
H	-0.9780	0.6770	-3.9470
O	0.2270	-1.3020	0.4310
C	0.9800	-0.1820	0.6530
O	2.0010	-2.8930	-0.4560
C	2.3570	-3.5650	0.7430
H	1.8210	-3.1340	1.5940
C	3.8510	-3.4270	0.9480
H	4.1340	-2.3720	1.0230
H	4.3980	-3.8440	0.0960
H	4.1690	-3.9420	1.8590
H	2.0860	-4.6210	0.6520
C	2.1170	0.1700	-0.0730
H	2.4880	-0.4440	-0.8890
C	2.8140	1.3430	0.2380

H	3.6980	1.5970	-0.3420
C	2.3640	2.1590	1.2830
C	1.2240	1.8110	2.0160
H	0.8570	2.4310	2.8310
C	0.5370	0.6380	1.6940
H	-0.3500	0.3630	2.2610
N	3.0920	3.3870	1.6120
O	2.6610	4.0820	2.5430
O	4.0970	3.6610	0.9410

34			
CUP08044.xyz		0.0000000	
C	-0.4050	-0.5120	-0.4220
S	-1.4740	-1.8620	-0.0400
C	-0.6090	-3.2050	-0.9050
H	0.4060	-3.2960	-0.5050
H	-0.5420	-2.9620	-1.9710
C	-1.3650	-4.5190	-0.7160
H	-2.3850	-4.4330	-1.1090
H	-1.4420	-4.7650	0.3500
C	-0.6620	-5.6630	-1.4320
H	0.3520	-5.8050	-1.0440
H	-0.5950	-5.4710	-2.5080
H	-1.2150	-6.5970	-1.2870
N	-0.7660	0.7380	0.0900
C	-1.9180	1.0140	0.9600
H	-1.6530	1.8340	1.6370
H	-2.1330	0.1510	1.5950
C	-3.1560	1.3880	0.1590
H	-3.4490	0.5850	-0.5240
H	-2.9800	2.2860	-0.4430
H	-3.9960	1.5890	0.8310
C	0.0760	1.8830	-0.2640
H	-0.5550	2.7770	-0.3360
H	0.5090	1.7200	-1.2580
C	1.1990	2.0920	0.7540
H	1.8150	1.1860	0.8150
H	0.7720	2.2480	1.7520
C	2.0750	3.2860	0.3770
H	1.4630	4.1940	0.3230
H	2.5120	3.1290	-0.6160
C	3.1930	3.4980	1.3860
H	3.8430	2.6190	1.4410
H	2.7890	3.6900	2.3850
H	3.8070	4.3570	1.0970
O	0.5950	-0.6950	-1.1110

30			
CUP08045.xyz		0.0000000	
P	-0.1950	-3.2630	0.5110
S	-0.9760	-4.6020	-0.6860

O	1.4360	-3.2690	0.4430
C	2.0870	-2.9720	-0.7840
H	1.5270	-2.2190	-1.3450
H	2.1470	-3.8860	-1.3830
C	3.4800	-2.4600	-0.4790
H	4.0480	-3.2030	0.0900
H	3.4310	-1.5560	0.1380
H	4.0220	-2.2300	-1.4000
S	-0.8510	-1.2570	0.3260
C	0.1140	-0.4100	1.5970
H	1.1770	-0.5410	1.3820
H	-0.1130	-0.8530	2.5700
S	-0.2830	1.3570	1.6300
C	0.8310	1.8580	2.9760
H	1.8630	1.6170	2.7000
H	0.5730	1.3050	3.8840
C	0.7040	3.3490	3.2310
H	-0.3140	3.6220	3.5290
H	0.9760	3.9340	2.3450
H	1.3770	3.6470	4.0420
O	-0.3370	-3.6980	2.0790
C	-1.6290	-3.8690	2.6440
H	-1.9820	-4.8810	2.4210
H	-2.3340	-3.1480	2.2200
C	-1.5280	-3.6740	4.1430
H	-1.1560	-2.6710	4.3770
H	-0.8180	-4.3860	4.5780
H	-2.5020	-3.8100	4.6210

40			
CUP08046.xyz			
	0.0000000		
C	0.6340	0.8570	-0.4910
N	1.9190	1.3570	-0.3570
C	2.1770	2.7650	-0.6850
H	2.5770	3.2750	0.2000
H	1.2510	3.2840	-0.9620
C	3.1170	2.8830	-1.8500
H	2.7880	2.2990	-2.7010
C	3.0450	0.5150	0.0770
H	3.8880	1.1570	0.3590
H	3.3980	-0.0970	-0.7600
C	2.7090	-0.3670	1.2810
H	1.8850	-1.0500	1.0460
H	2.3830	0.2560	2.1200
C	3.9120	-1.1910	1.7150
H	4.7480	-0.5450	2.0010
H	4.2460	-1.8510	0.9090
H	3.6530	-1.8120	2.5780
C	-0.4290	1.2630	0.3400
C	-1.7410	0.7610	0.2400
H	-2.5150	1.1080	0.9260
C	-2.0490	-0.1950	-0.7330
C	-3.4400	-0.7680	-0.8400
F	-3.6020	-1.8710	-0.0610

F	-3.7630	-1.1480	-2.1060
F	-4.4070	0.1100	-0.4560
C	-1.0260	-0.6370	-1.5780
H	-1.2390	-1.3870	-2.3420
C	0.2740	-0.1100	-1.4470
N	-0.1900	2.2020	1.4140
O	-0.3540	3.4020	1.1570
O	0.1070	1.7290	2.5180
N	1.2510	-0.5950	-2.3950
O	1.7570	-1.7000	-2.1570
O	1.4640	0.1040	-3.3930
C	4.5990	3.0790	-1.6510
H	4.9930	3.1610	-0.6440
H	5.2720	2.5930	-2.3490
C	3.7570	4.2130	-2.1600
H	3.8660	4.4940	-3.2020
H	3.5820	5.0500	-1.4940

35

cup0847a.xyz	0.000000		
C	0.00000	0.00000	0.00000
N	1.36429	0.00000	0.00000
H	1.80311	0.85231	0.00000
C	2.19029	-1.20549	0.00000
C	3.05853	-1.22422	1.26644
N	-0.55730	1.14410	0.00000
C	-1.82999	1.16503	0.00000
S	-2.63802	2.72374	0.00000
C	-4.41124	2.43067	0.00000
N	-2.54432	0.11122	0.00000
C	-1.92812	-1.00228	0.00000
N	-2.71274	-2.11837	0.00000
H	-3.66231	-1.98770	0.00000
C	-2.20110	-3.48723	0.00000
C	-2.68502	-4.20831	1.26645
C	-2.68502	-4.20831	-1.26645
N	-0.65838	-1.08943	0.00000
C	3.05853	-1.22422	-1.26644
H	1.55564	-2.12450	0.00000
H	2.42460	-1.22108	2.18324
H	3.72553	-0.33275	1.31026
H	3.70060	-2.13438	1.30228
H	-4.94642	3.40634	0.00000
H	-4.70535	1.85872	0.90859
H	-4.70535	1.85872	-0.90859
H	-1.08429	-3.49624	0.00000
H	-3.79790	-4.24148	1.31021
H	-2.32317	-3.68774	2.18323
H	-2.30947	-5.25692	1.30237
H	-3.79790	-4.24148	-1.31021
H	-2.30947	-5.25692	-1.30237
H	-2.32317	-3.68774	-2.18323
H	3.70060	-2.13438	-1.30228
H	2.42460	-1.22108	-2.18324

H	3.72553	-0.33275	-1.31026
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22

CUP08048.xyz	0.0000000		
C	0.3940	1.2020	-0.1540
H	1.1660	1.9640	-0.1900
C	-0.9070	1.5790	-0.5060
H	-1.0990	2.6090	-0.7990
C	-1.9440	0.6450	-0.4800
Cl	-3.5250	1.1760	-0.9260
C	-1.6730	-0.6720	-0.1000
Cl	-2.9010	-1.8870	-0.0420
C	-0.3700	-1.0460	0.2520
H	-0.1770	-2.0750	0.5460
C	0.6750	-0.1110	0.2280
N	1.9590	-0.5690	0.5960
H	2.0260	-1.5480	0.8530
C	3.1350	0.1690	0.6460
C	4.3050	-0.6940	1.0930
H	4.4080	-1.5300	0.3920
H	4.0750	-1.1060	2.0820
C	5.6110	0.0770	1.1570
H	5.5410	0.9110	1.8640
H	5.8740	0.4890	0.1770
H	6.4260	-0.5780	1.4820
O	3.2650	1.3580	0.3760

23

CUP08049.xyz	0.0000000		
C	1.0680	0.9410	0.2520
H	1.9490	1.6050	0.2350
N	-0.0290	1.3950	-0.2540
N	-1.1420	0.5820	-0.2430
C	-2.3050	1.1990	-0.8360
C	-1.1110	-0.7160	0.3000
O	-2.0580	-1.4970	0.3460
C	0.1950	-1.1570	0.8600
Cl	0.2610	-2.7550	1.5360
C	1.2810	-0.3820	0.8570
N	2.5260	-0.6760	1.3390
H	3.2870	-0.0100	1.2860
H	2.6900	-1.5850	1.7610
C	-2.2230	2.5100	-1.3490
H	-1.2900	3.0670	-1.3050
C	-3.3250	3.1460	-1.9310
H	-3.2260	4.1570	-2.3170
C	-4.5430	2.4840	-2.0160
H	-5.4020	2.9720	-2.4670
C	-4.6540	1.1910	-1.5190
H	-5.6040	0.6650	-1.5810
C	-3.5490	0.5570	-0.9360
H	-3.7130	-0.4510	-0.5710

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25
CUP08050.xyz      0.0000000
C      1.1220      0.4910      0.0000
N      2.2850      1.2210      0.0000
C      3.5820      0.5910      0.0000
H      3.6980     -0.0420     -0.8880
H      3.6980     -0.0420      0.8870
C      4.6720      1.6500     -0.0010
H      4.5970      2.2910      0.8840
H      4.5960      2.2910     -0.8860
H      5.6600      1.1800     -0.0010
H      2.1730      2.2240      0.0000
N     -0.0100      1.1960      0.0000
C     -1.1540      0.5090      0.0000
N     -2.3050      1.2570      0.0000
C     -3.6120      0.6480     -0.0010
H     -3.7390      0.0160      0.8860
H     -3.7380      0.0180     -0.8890
C     -4.6850      1.7240      0.0000
H     -4.5990      2.3650     -0.8840
H     -4.6000      2.3630      0.8860
H     -5.6810      1.2710     -0.0010
H     -2.1770      2.2590      0.0010
N     -1.2180     -0.8160     -0.0010
C     -0.0310     -1.4070     -0.0010
Cl     -0.0450     -3.1170     -0.0020
N      1.1650     -0.8350     -0.0010
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41
CUP08051.xyz      0.0000000
C      1.4580      0.1460      0.8640
S      2.7260      0.9710      1.8130
N      2.8210      2.4830      1.0770
H      2.8760      2.4070      0.0460
C      0.3260     -0.3240      1.5440
H      0.1900     -0.1380      2.6080
C     -0.6430     -1.0630      0.8630
H     -1.5190     -1.4310      1.3940
C     -0.4870     -1.3390     -0.4940
H     -1.2440     -1.9130     -1.0220
C      0.6380     -0.8720     -1.1760
H      0.7360     -1.0800     -2.2400
C      1.6170     -0.1310     -0.5000
C      3.5050      3.5730      1.6540
O      3.8500      3.5720      2.8240
N      3.7100      4.5610      0.7370
H      3.3610      4.4650     -0.2020
C      4.3840      5.7570      0.9570
N      4.9230      6.0510      2.1480
C      5.5640      7.2320      2.2630
```

C	6.1660	7.5610	3.5950
H	5.9860	6.7550	4.3140
H	5.7230	8.4780	3.9950
H	7.2480	7.6950	3.4990
C	5.6740	8.1170	1.2090
H	6.1910	9.0630	1.3120
C	5.0880	7.7340	0.0190
C	5.1560	8.6330	-1.1780
H	4.6450	8.1810	-2.0350
H	6.1980	8.8120	-1.4590
H	4.6720	9.5900	-0.9600
N	4.4410	6.5580	-0.1220
O	2.2110	1.1200	3.1580
O	3.9510	0.2480	1.5450
C	2.7300	0.4110	-1.2800
O	3.0540	1.5910	-1.2170
O	3.2960	-0.5670	-2.0220
C	4.4240	-0.1440	-2.7910
H	5.2120	0.2380	-2.1350
H	4.1240	0.6160	-3.5200
H	4.8110	-1.0120	-3.3320

27
CUP08052.xyz 0.0000000

C	1.1350	0.9150	0.3810
N	0.0440	1.7340	0.2560
H	0.2390	2.7170	0.4150
C	-1.2280	1.3400	-0.0550
C	-2.2230	2.4600	-0.1830
H	-3.2330	2.1230	-0.4320
H	-1.9090	3.1540	-0.9700
H	-2.2880	3.0170	0.7580
C	-1.4860	0.0380	-0.2040
Cl	-3.0490	-0.5880	-0.5800
C	-0.3870	-0.9470	-0.0110
N	0.9230	-0.4420	0.1360
C	2.0760	-1.4240	0.1210
C	1.9560	-2.4170	-1.0660
H	1.1390	-3.1330	-0.9500
H	2.8630	-3.0230	-1.1740
H	1.8000	-1.8780	-2.0070
C	2.1030	-2.2050	1.4500
H	2.1960	-1.5220	2.3020
H	2.9470	-2.9040	1.4840
H	1.1910	-2.7910	1.6040
C	3.4740	-0.7740	-0.0550
H	3.7860	-0.2160	0.8340
H	3.4970	-0.1060	-0.9230
H	4.2500	-1.5340	-0.2090
O	2.1930	1.4430	0.7150
O	-0.6690	-2.1420	0.0420

35

CUP08053.xyz	0.0000000		
C	1.0120	0.5410	0.0050
N	2.1950	1.2350	-0.0010
H	2.0600	2.2370	-0.0060
C	3.5460	0.6880	0.0000
C	3.8040	-0.1490	-1.2600
H	3.2040	-1.0640	-1.2800
H	4.8550	-0.4540	-1.3210
H	3.5660	0.4190	-2.1670
C	3.8080	-0.1340	1.2700
H	4.8590	-0.4390	1.3320
H	3.2070	-1.0480	1.3030
H	3.5730	0.4440	2.1710
C	4.5190	1.8840	-0.0080
H	5.5630	1.5520	-0.0070
H	4.3700	2.5230	0.8710
H	4.3670	2.5120	-0.8940
N	-0.0850	1.2900	0.0020
C	-1.2350	0.6190	0.0070
S	-2.7670	1.5330	0.0050
C	-2.1450	3.2340	0.0000
H	-1.5480	3.4260	-0.8960
H	-1.5460	3.4310	0.8930
H	-2.9950	3.9220	-0.0020
N	-1.3500	-0.7070	0.0150
C	-0.2030	-1.3730	0.0160
N	-0.3010	-2.7430	0.0240
H	-1.2380	-3.1160	0.0270
C	0.8680	-3.5860	0.0270
H	1.4820	-3.3850	0.9120
H	1.4800	-3.3940	-0.8630
C	0.4520	-5.0480	0.0350
H	-0.1490	-5.2900	-0.8480
H	-0.1470	-5.2810	0.9220
H	1.3340	-5.6960	0.0370
N	0.9920	-0.7880	0.0120

38

CUP08054.xyz	0.0000000		
N	1.1300	1.0140	-0.1060
C	0.0040	1.4580	0.4600
C	-0.0640	2.9050	0.8330
H	-0.7100	3.0490	1.7050
H	-0.4680	3.4830	-0.0040
H	0.9310	3.2880	1.0780
N	-1.0780	0.7120	0.6810
C	-0.9650	-0.5580	0.2980
O	-2.0830	-1.3320	0.5380
C	-1.9710	-2.6600	0.0390
H	-1.1680	-3.2070	0.5440
H	-1.8280	-2.6660	-1.0480
H	-2.9110	-3.1770	0.2530

N	0.1080	-1.1060	-0.2670
C	1.1270	-0.2760	-0.4460
N	2.3330	-0.7240	-0.9720
H	3.0430	-0.0120	-1.0210
C	2.5930	-1.9940	-1.3950
N	3.9660	-2.1630	-1.6580
H	4.5950	-1.5080	-1.1880
O	1.7930	-2.9050	-1.5270
S	4.6430	-3.6970	-1.8020
C	6.3540	-3.4670	-1.9890
O	4.5540	-4.3780	-0.5290
O	4.2280	-4.3010	-3.0480
C	7.0650	-3.9050	-3.1460
H	6.6150	-4.3720	-4.0150
C	8.4190	-3.6900	-3.0270
H	9.1940	-3.9330	-3.7430
S	8.8260	-2.9780	-1.5290
C	7.1800	-2.9060	-1.0300
C	6.8950	-2.3170	0.2630
O	7.5930	-2.4050	1.2650
O	5.7460	-1.5740	0.1930
C	5.3920	-0.9470	1.4330
H	6.1730	-0.2460	1.7430
H	5.2140	-1.7030	2.2040
H	4.4670	-0.3870	1.2760

20			
CUP08055.xyz		0.0000000	
P	0.1670	-0.6350	-1.5770
O	0.3470	-0.1370	-3.1080
C	-0.7560	-0.2690	-3.9840
H	-0.4320	-0.0100	-4.9950
H	-1.5550	0.4140	-3.6840
H	-1.1240	-1.2980	-3.9830
C	1.7680	-0.2780	-0.8350
C	1.9540	-0.8050	0.5940
Cl	0.7170	-0.1960	1.7280
Cl	3.5650	-0.2460	1.2040
Cl	1.9770	-2.5920	0.6440
H	2.5220	-0.7350	-1.4880
O	1.9740	1.1480	-0.9270
H	2.8710	1.3480	-0.6000
O	-0.8620	0.4530	-0.9680
C	-2.1630	0.0180	-0.6190
H	-2.6640	-0.4110	-1.4900
H	-2.7370	0.8790	-0.2680
H	-2.1090	-0.7230	0.1830
O	-0.2950	-2.0580	-1.4710

39		
CUP08056.xyz		0.0000000

C	1.2960	0.5040	-0.3180
N	2.4480	1.2650	-0.2050
C	2.4060	2.7130	0.0550
H	2.0650	3.2500	-0.8360
H	3.4240	3.0770	0.2470
C	1.5410	3.0740	1.2630
H	1.9250	2.5710	2.1580
H	0.5090	2.7340	1.1180
C	1.5300	4.5750	1.5080
H	1.1220	5.1100	0.6440
H	2.5410	4.9500	1.6990
H	0.9100	4.8120	2.3790
C	3.7590	0.6220	-0.3750
H	3.6710	-0.4700	-0.3950
H	4.3930	0.8730	0.4840
C	4.4310	1.0700	-1.6750
H	4.5250	2.1610	-1.7080
H	3.8150	0.7780	-2.5320
C	5.8120	0.4510	-1.8270
H	5.7540	-0.6420	-1.8410
H	6.4690	0.7500	-1.0030
H	6.2730	0.7780	-2.7640
C	0.3420	0.6810	-1.3370
C	-0.8340	-0.0870	-1.4530
H	-1.5330	0.1000	-2.2700
C	-1.1050	-1.1000	-0.5280
C	-2.3690	-1.9170	-0.6240
F	-2.2300	-3.1710	-0.1150
F	-2.7990	-2.0780	-1.9050
F	-3.4010	-1.3460	0.0540
C	-0.1940	-1.3090	0.5130
H	-0.3910	-2.0770	1.2610
C	0.9690	-0.5180	0.5970
N	0.5510	1.6660	-2.3730
O	-0.0920	2.7200	-2.2760
O	1.3080	1.3590	-3.3030
N	1.8160	-0.7650	1.7450
O	2.6050	-1.7160	1.6620
O	1.6440	-0.0480	2.7380

34			
CUP08057.xyz			
		0.0000000	
N	0.3300	-0.4700	0.0000
C	0.2670	1.0050	0.0000
H	0.8160	1.3400	0.8880
H	0.8160	1.3400	-0.8870
C	-1.0910	1.7120	0.0000
H	-1.6670	1.4290	0.8890
H	-1.6670	1.4290	-0.8880
C	-0.9230	3.2260	0.0000
H	-0.3770	3.5610	-0.8870
H	-0.3770	3.5610	0.8880
H	-1.9030	3.7150	0.0000
C	1.6760	-1.0900	0.0000

H	1.7340	-1.7340	0.8860
H	1.7340	-1.7340	-0.8860
C	2.8940	-0.1600	0.0000
H	2.8810	0.4870	0.8840
H	2.8810	0.4870	-0.8840
C	4.1930	-0.9550	0.0000
H	4.2630	-1.5920	-0.8870
H	4.2630	-1.5920	0.8870
H	5.0520	-0.2760	0.0000
C	-0.8380	-1.2580	0.0000
S	-0.6000	-3.0170	0.0000
C	-2.3310	-3.5730	0.0000
H	-2.8350	-3.1800	-0.8890
H	-2.8350	-3.1800	0.8890
C	-2.3870	-5.0990	0.0000
H	-1.8780	-5.5010	0.8840
H	-1.8770	-5.5000	-0.8840
C	-3.8260	-5.5940	0.0000
H	-4.3620	-5.2430	-0.8880
H	-4.3620	-5.2430	0.8870
H	-3.8500	-6.6880	0.0000
O	-1.9840	-0.8240	0.0010

28
CUP08058.xyz 0.0000000

C	0.00000	0.00000	0.00000
C	1.41174	0.00000	0.00000
C	2.08882	1.23615	0.00000
C	1.37146	2.43375	0.00000
C	-0.04075	2.44329	0.00000
C	-0.71136	1.19837	0.00000
N	2.20715	-1.34446	0.00000
O	1.60501	-2.44457	-0.00665
O	3.40441	-1.34572	0.00738
N	-0.73120	3.74355	0.00000
N	-2.08037	3.92341	0.00038
C	-2.77127	5.22544	0.00038
C	-4.18564	5.23244	0.00081
C	-2.09928	6.46883	-0.00043
C	-2.80854	7.66938	-0.00039
C	-4.22095	7.66197	0.00048
C	-4.90458	6.42606	0.00130
N	-4.93387	8.86349	0.00052
H	-0.54329	-0.95922	0.00047
H	3.19085	1.25835	0.00000
H	1.93649	3.38090	0.00000
H	-1.80968	1.13129	0.00000
H	-4.74759	4.28316	0.00114
H	-1.00058	6.53299	-0.00112
H	-2.26262	8.62778	-0.00103
H	-6.00719	6.40259	0.00198
H	-4.46440	9.70038	-0.00003
H	-5.89338	8.85243	0.00111

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CUP08059.xyz	0.000000		
C	0.00000	0.00000	0.00000
C	1.34677	0.00000	0.00000
C	2.09903	1.28717	0.01401
C	1.41177	2.45371	-0.00765
C	-0.04361	2.46586	-0.00708
C	-0.73921	1.29046	-0.00137
N	-2.13612	1.34098	0.00000
C	-0.75723	-1.28002	0.00745
C	2.08613	-1.29187	-0.00389
N	3.47111	1.27642	0.01193
C	-0.05443	-2.57201	0.06655
C	1.36750	-2.57742	0.06403
C	4.32907	2.19733	0.55425
C	4.02981	3.01872	1.57380
C	5.69706	2.25247	-0.02284
C	5.03446	3.97546	2.09914
C	6.60953	3.11465	0.44688
C	6.26136	4.02550	1.56327
C	2.05874	-3.81153	0.11910
C	-0.75328	-3.78958	0.12327
C	-0.05556	-5.00368	0.17836
C	1.34381	-5.01519	0.17648
H	-1.85586	-3.80478	0.12560
H	-0.61231	-5.95462	0.22324
H	1.88619	-5.97444	0.22003
H	3.16103	-3.83986	0.11748
H	-0.57421	3.43245	-0.01374
H	1.93192	3.42457	-0.04188
H	-2.64655	0.52717	0.00000
H	-2.58686	2.18757	-0.00172
O	-1.96920	-1.28136	-0.02851
O	3.29433	-1.32170	-0.07791
H	3.88580	0.50819	-0.38926
H	3.03716	2.99727	2.05165
H	5.96250	1.57554	-0.85252
H	7.62100	3.15147	0.00862
H	4.76472	4.64184	2.93561
H	7.01392	4.73376	1.94823

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CUP08060.xyz	0.000000		
C	0.00000	0.00000	0.00000
C	1.34503	0.00000	0.00000
C	2.08392	1.29332	0.00000
C	1.40579	2.46213	0.00000
C	-0.04895	2.47092	0.00000
C	-0.73964	1.29172	0.00000
N	-2.13659	1.34387	0.00000
C	-0.74869	-1.28470	0.00000
C	2.08704	-1.28943	0.00000
N	3.44901	1.33696	0.00000

C	-0.04831	-2.58591	0.00000
C	1.37723	-2.58787	0.00000
C	2.07442	-3.82896	0.00000
C	-0.74644	-3.81348	0.00000
C	-0.04093	-5.02141	0.00000
N	-2.11099	-3.86683	0.00000
C	1.35798	-5.02990	0.00000
N	3.43848	-3.89100	0.00000
H	-0.58614	-5.97998	0.00000
H	1.89341	-5.99396	0.00000
H	-0.58185	3.43621	0.00000
H	1.94613	3.42351	0.00000
H	-2.64805	0.53103	0.00000
H	-2.58624	2.19101	0.00000
O	-1.96024	-1.25782	0.00000
O	3.29723	-1.28173	0.00000
H	3.96554	0.52667	0.00000
H	3.91734	2.17451	0.00000
H	-2.57392	-4.70736	0.00000
H	-2.63399	-3.06046	0.00000
H	3.89669	-4.73405	0.00000
H	3.96600	-3.08732	0.00000

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CUP08061.xyz	0.000000		
C	0.00000	0.00000	0.00000
C	1.50187	0.00000	0.00000
C	2.21057	1.31254	0.00000
C	2.22756	-1.31481	0.00000
C	1.49770	2.46758	0.00000
C	0.03181	2.47505	0.00000
C	-0.70013	1.32014	0.00000
N	-2.09551	1.38825	0.00000
C	-0.71853	-1.32015	0.00000
C	0.04019	-2.58839	0.00000
C	1.47222	-2.58557	0.00000
C	2.16380	-3.82054	0.00000
C	-0.64150	-3.81639	0.00000
C	0.06170	-5.02921	0.00000
C	1.45922	-5.03201	0.00000
H	-1.74398	-3.84427	0.00000
H	-0.48989	-5.98426	0.00000
H	2.00861	-5.98830	0.00000
H	3.26633	-3.84540	0.00000
H	3.31275	1.34253	0.00000
H	-0.48616	3.44860	0.00000
H	2.03363	3.43173	0.00000
H	-2.61338	0.57792	0.00000
H	-2.53594	2.24034	0.00000
O	-1.93525	-1.33562	0.00000
O	3.44245	-1.32615	0.00000

CUP08062.xyz		0.0000000	
C	0.00000	0.00000	0.00000
C	1.39932	0.00000	0.00000
C	2.08873	1.21777	0.00000
C	1.38141	2.42355	0.00000
C	-0.02945	2.44341	0.00000
C	-0.70729	1.20708	0.00000
N	-0.71247	3.75291	0.00000
N	-2.05807	3.94184	0.00000
C	-2.73977	5.25072	0.00000
C	-4.15064	5.27693	0.00000
C	-2.06609	6.48935	0.00000
C	-2.76927	7.69467	0.00000
C	-4.18645	7.72803	0.00000
C	-4.85700	6.47898	0.00000
N	-4.89907	8.95119	0.00000
C	-4.18459	10.23094	0.00000
C	-6.36472	8.96036	0.00000
H	-0.54637	-0.95846	0.00000
H	1.95503	-0.95290	0.00000
H	3.19186	1.22481	0.00000
H	1.95297	3.36694	0.00000
H	-1.80625	1.14841	0.00000
H	-4.72108	4.33255	0.00000
H	-0.96673	6.54493	0.00000
H	-2.17454	8.62153	0.00000
H	-5.95635	6.41551	0.00000
H	-3.55653	10.32126	0.91546
H	-3.55653	10.32125	-0.91546
H	-4.88219	11.09791	0.00000
H	-6.75286	8.45833	-0.91543
H	-6.77523	9.99466	0.00000
H	-6.75286	8.45833	0.91543

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CUP08063.xyz		0.0000000	
C	0.00000	0.00000	0.00000
C	1.41851	0.00000	0.00000
C	2.09415	1.23284	0.00000
N	1.32017	2.38954	-0.01050
C	-0.06074	2.49330	-0.01056
N	-0.63715	1.21899	-0.00629
C	-0.80969	-1.26622	0.01621
C	2.18767	-1.29583	-0.01023
O	3.45315	1.31074	0.00174
N	-0.76736	3.69643	-0.02267
C	4.09874	2.52054	0.23418
O	4.60518	2.69730	1.34342
N	4.19190	3.49785	-0.72525
C	4.72364	4.81123	-0.36002
C	-2.21752	3.66845	-0.19371
C	-0.03460	4.94761	-0.20242
C	3.54168	3.33303	-2.02505
H	-0.43242	-1.97954	0.78333
H	-0.78051	-1.75601	-0.98336

H	-1.87497	-1.05143	0.25986
H	3.26114	-1.15551	-0.26862
H	2.14115	-1.77508	0.99385
H	1.77172	-2.00201	-0.76383
H	5.67688	4.71209	0.20773
H	3.97512	5.35830	0.25776
H	4.94183	5.42010	-1.26621
H	-2.67378	2.85685	0.41755
H	-2.67309	4.62875	0.13766
H	-2.46399	3.50553	-1.26764
H	0.90663	4.94830	0.39341
H	-0.64345	5.81472	0.13938
H	0.21261	5.08420	-1.27985
H	3.49851	2.26309	-2.33033
H	2.51170	3.75449	-1.99046
H	4.11498	3.86883	-2.81484
