

SUPPLEMENTARY INFORMATION

Which Fullerenols are Water Soluble? Systematic Atomistic Investigation

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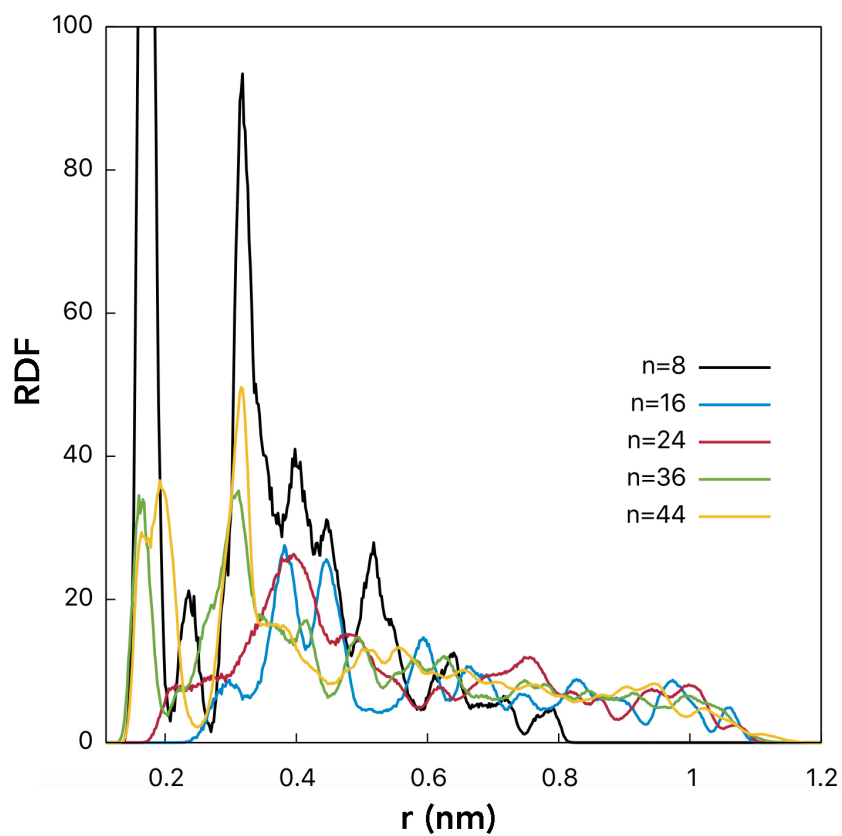


Figure S1: RDFs between the oxygen and hydrogen, both belonging to fullerenols.

Dipole Moments in Debye calculated at the B3LYP/6-31G(d,p) level of theory:

oh8	X=	0.9660	Y=	1.6946	Z=	-2.2726	Tot=	3.0
oh16	X=	5.2819	Y=	2.4310	Z=	-0.6962	Tot=	5.9
oh24	X=	0.0000	Y=	0.0000	Z=	0.0000	Tot=	0.0
oh36	X=	1.4096	Y=	-0.0726	Z=	5.6638	Tot=	5.8
oh44	X=	0.9929	Y=	-1.7108	Z=	-1.9816	Tot=	2.8

Reference geometries and CHELPG partial charges of the fullerenols determined by DFT calculations at the B3LYP/6-31G(d,p) level of theory.

OH8	x	y	z	q(e)
C	-3.63285	0.12947	2.03664	-0.220877
C	-2.92654	-1.01612	2.57889	0.130760
C	-1.77612	-0.5247	3.31927	-0.477645
C	-1.76988	0.9122	3.23614	-0.444045
C	-2.91563	1.32394	2.44189	0.136826
C	-4.21235	0.05842	0.76457	0.183531
C	-4.10814	-1.16324	-0.01189	0.103110
C	-4.0982	1.18184	-0.14729	0.094736
C	-3.91993	0.65497	-1.48800	0.019643
C	-3.9267	-0.79483	-1.40435	0.005324
C	-2.82739	-2.19108	1.83311	0.130833
C	-3.42632	-2.26673	0.51360	-0.051833
C	-1.57172	-2.92151	1.79513	-0.422906
C	-1.39526	-3.44804	0.46457	-0.177600
C	-2.54105	-3.04597	-0.33306	-0.070845
C	-0.55825	-1.21366	3.26141	0.127484
C	0.69026	-0.5104	3.19091	-0.151911
C	-0.45642	-2.43367	2.47872	0.250293
C	0.85933	-2.50379	1.90239	-0.179921
C	1.7341	-1.37754	2.46852	-0.070818
C	-0.54683	1.58078	3.10266	0.130118
C	-0.43729	2.70344	2.18586	0.255423
C	0.69634	0.86465	3.11278	-0.211310
C	1.74732	1.63658	2.29601	-0.017175
C	0.87698	2.6949	1.60571	-0.240752
C	-2.81024	2.40582	1.56708	0.129400
C	-3.40913	2.33393	0.24742	-0.006868
C	-1.54802	3.11426	1.44538	-0.347482
C	-1.36937	3.48384	0.06325	-0.146765
C	-2.51868	3.00346	-0.68323	-0.082375
C	-0.11417	-3.46057	-0.09764	-0.118645
C	1.0414	-3.01704	0.64123	0.087020
C	0.05658	-3.07689	-1.48138	0.070375
C	1.31465	-2.37904	-1.60256	0.076130
C	2.14669	-2.57931	-0.35259	-0.326753
C	2.23592	-0.59996	1.27475	0.421471
C	2.24639	0.72552	1.20040	0.438971
C	2.93087	-1.28604	0.13544	-0.038127
C	3.20443	-0.07036	-0.92824	0.482489
C	2.93862	1.2638	-0.01677	0.020155
C	1.06104	3.05865	0.29259	0.069488
C	-0.08958	3.42031	-0.49777	-0.184958
C	2.16424	2.50426	-0.63903	-0.396286
C	1.33869	2.16626	-1.86738	0.066876
C	0.08428	2.88072	-1.82916	0.070305
C	-2.34884	2.49693	-1.97263	-0.085829
C	-3.06142	1.30098	-2.38424	0.060751
C	-1.02121	2.44855	-2.55834	-0.053958
C	-0.91149	1.23195	-3.32551	-0.116641
C	-2.17184	0.52022	-3.22580	0.001483
C	-3.07315	-1.54567	-2.21931	0.032164
C	-2.37085	-2.69324	-1.67286	-0.027232
C	-2.17876	-0.87367	-3.14521	-0.071678
C	-0.92453	-1.60098	-3.15958	-0.086767

C	-1.04362	-2.72222	-2.25880	-0.038840
C	0.2948	0.53039	-3.30761	-0.054857
C	0.28618	-0.9099	-3.22403	-0.080408
C	1.42869	-1.31462	-2.44489	0.180534
C	2.42066	-0.15104	-2.32334	-0.709778
C	1.44665	1.01331	-2.58349	0.132787
O	2.79924	-1.7859	3.31090	0.001567
O	3.1063	-3.6456	-0.54215	-0.112292
O	4.17038	-1.72145	0.68657	-0.087373
O	4.56301	-0.08411	-1.28320	-0.144442
O	3.33854	-0.26256	-3.39988	-0.033447
O	4.21654	1.74066	0.44301	-0.126152
O	3.17172	3.49574	-0.96343	-0.099286
O	2.81065	2.14906	3.08714	-0.010633
H	3.5473	-1.98386	2.72168	0.318008
H	3.25368	-3.73655	-1.49443	0.267435
H	4.36663	-2.56666	0.23595	0.292945
H	5.02809	0.38174	-0.56320	0.318358
H	4.20434	-0.01424	-3.02828	0.308923
H	4.34768	2.58841	-0.03570	0.308780
H	2.84507	4.36224	-0.68677	0.282144
H	3.59616	2.16692	2.51703	0.318868

OH16	x	y	z	q(e)
C	1.781946	-2.939092	0.811086	0.056291
C	0.617242	-3.095635	1.640156	-0.008831
C	0.818960	-2.319221	2.943467	0.129696
C	2.634489	-1.986053	1.347595	0.058171
C	2.044452	-1.451770	2.548349	0.046597
C	1.772950	-3.310228	-0.659455	0.119565
C	2.352792	-2.145620	-1.458276	0.074580
C	1.497456	-1.839953	-2.559199	-0.021462
C	0.343325	-3.345050	-1.203764	0.028335
C	0.277354	-2.753824	-2.612219	0.150603
C	-0.606742	-3.260692	1.057578	0.017623
C	-0.732135	-3.408293	-0.402515	0.041377
C	-2.159474	-3.013262	-0.813844	0.145036
C	-1.795216	-2.567908	1.529831	0.031534
C	-2.595755	-2.257361	0.453916	-0.010588
C	-0.390228	-1.463481	3.245188	0.029119
C	-1.825030	-1.827915	2.858934	0.163130
C	-2.408018	-0.428394	2.633421	-0.027676
C	-0.266306	-0.118953	3.461220	0.027242
C	-1.521701	0.536156	3.056515	0.059531
C	3.627863	-1.194725	0.514900	0.160343
C	3.403545	0.303041	0.775365	0.013742
C	3.279598	1.012000	-0.381298	0.070312
C	3.244251	-1.245125	-0.961913	0.007957
C	3.466414	0.114252	-1.613361	0.136613
C	2.140260	-0.124141	2.876851	0.031287
C	0.955866	0.566285	3.293576	0.020626
C	0.969189	1.899000	2.727908	0.070755
C	3.044073	0.865002	2.129719	0.143239
C	2.088795	2.060529	1.972901	-0.007816
C	-1.781037	2.940394	-0.809133	0.057047
C	-2.629085	1.984763	-1.341359	0.050243
C	-2.042693	1.458564	-2.544751	0.070283
C	-0.618964	3.100959	-1.639451	-0.000423
C	-0.823931	2.323183	-2.941702	0.131018
C	-1.790934	3.322675	0.657614	0.133616
C	-0.355144	3.361523	1.210689	-0.011708
C	-0.292369	2.748991	2.612938	0.143470
C	-2.368316	2.157060	1.454397	0.102877
C	-1.504029	1.838692	2.543621	0.014067
C	-3.640852	1.197312	-0.518757	0.160573
C	-3.261123	1.251777	0.961726	-0.004141
C	-3.474498	-0.120446	1.615710	0.164980
C	-3.419285	-0.298160	-0.772225	0.069317
C	-3.288899	-1.005759	0.380920	0.096627
C	-2.139855	0.130494	-2.867455	0.010320
C	-3.054104	-0.863457	-2.124152	0.152007

C	-2.095864	-2.058795	-1.970291	0.018763
C	-0.957983	-0.563458	-3.280901	0.020604
C	-0.981806	-1.905105	-2.733408	0.093640
C	0.604072	3.272906	-1.057488	0.028126
C	1.788939	2.574558	-1.526196	0.064611
C	2.586163	2.260774	-0.453124	0.034331
C	0.724709	3.418016	0.406559	0.030074
C	2.149114	3.006319	0.812135	0.109770
C	0.385613	1.463998	-3.238909	0.003093
C	0.264867	0.118700	-3.461655	0.016474
C	1.525420	-0.537767	-3.069339	0.050921
C	1.817527	1.825537	-2.843355	0.138655
C	2.416190	0.428204	-2.645822	-0.039576
O	-2.553650	-2.542580	3.863209	-0.537168
H	-1.986358	-3.267546	4.166834	0.307811
O	2.505834	2.662616	-3.796427	-0.548107
H	2.559412	2.148571	-4.616852	0.299497
O	-4.986486	1.545476	-0.834848	-0.528164
H	-5.123758	2.456703	-0.536318	0.310783
O	4.951693	-1.651041	0.804231	-0.546334
H	5.537285	-1.190748	0.182684	0.313669
O	-0.443230	3.658522	3.708713	-0.531960
H	0.297617	4.280367	3.684115	0.297553
O	0.290662	-3.704674	-3.678558	-0.539775
H	1.027362	-4.308322	-3.500074	0.313689
O	4.202660	1.164081	2.916753	-0.532861
H	4.706027	1.832701	2.428865	0.309118
O	-4.262893	-1.187346	-2.802506	-0.517593
H	-4.027201	-1.680066	-3.602444	0.313356
O	-2.559076	4.504544	0.908925	-0.540061
H	-2.121972	5.238570	0.453064	0.307722
O	2.401477	-4.570105	-0.941042	-0.547482
H	3.344200	-4.471056	-0.738444	0.313117
O	-1.179342	3.150633	-4.057458	-0.533255
H	-0.381651	3.647083	-4.295618	0.314150
O	1.043620	-3.158470	4.084987	-0.538057
H	1.773891	-3.757656	3.868316	0.314670
O	4.820022	0.181548	-2.117517	-0.554263
H	4.896390	1.009873	-2.616067	0.306232
O	-4.798055	-0.341835	2.123282	-0.533956
H	-4.793559	-0.079842	3.055238	0.308834
O	3.073352	4.094482	0.999131	-0.543265
H	2.844094	4.522870	1.836303	0.298088
O	-3.024034	-4.101248	-1.135170	-0.531428
H	-3.224569	-4.570451	-0.312061	0.308854

OH24	x	y	z	q(e)
C	-0.327629	3.362866	1.726688	0.152948
C	2.336658	-2.982410	-0.288998	0.153100
C	0.000000	3.471171	0.240436	0.088716
C	1.700750	-2.690403	-1.651252	0.050198
C	-1.074479	3.260270	-0.531860	0.021868
C	0.327629	-3.362866	-1.726688	0.152948
C	-2.336658	2.982410	0.288998	0.153100
C	0.000000	-3.471171	-0.240436	0.088716
C	-1.700750	2.690403	1.651252	0.050198
C	1.074479	-3.260270	0.531860	0.021868
C	0.657970	2.427998	2.389055	0.044532
C	3.006123	-1.735586	0.240436	0.088716
C	1.414514	3.514810	-0.288998	0.153100
C	2.061375	-1.666364	-2.422557	0.051557
C	-1.001453	3.046966	-2.026323	0.154984
C	-0.657970	-2.427998	-2.389055	0.044532
C	-3.006123	1.735586	-0.240436	0.088716
C	-1.414514	-3.514810	0.288998	0.153100
C	-2.061375	1.666364	2.422557	0.051557
C	1.001453	-3.046966	2.026323	0.154984
C	0.298892	1.396540	3.165123	0.052401
C	3.076142	-1.397698	1.726688	0.152948
C	2.286237	2.560661	0.531860	0.021868
C	3.139476	-0.656199	-2.026323	0.154984

C	0.412426	2.618386	-2.422557	0.051557
C	-0.298892	-1.396540	-3.165123	0.052401
C	-3.076142	1.397698	-1.726688	0.152948
C	-2.286237	-2.560661	-0.531860	0.021868
C	-3.139476	0.656199	2.026323	0.154984
C	-0.412426	-2.618386	2.422557	0.051557
C	-2.138023	-2.390767	-2.026323	0.154984
C	-3.360716	0.699609	0.531860	0.021868
C	-1.479582	-2.818094	1.651252	0.050198
C	-1.135984	1.041927	3.473311	0.154832
C	1.773723	-1.783818	2.389055	0.044532
C	2.138023	2.390767	2.026323	0.154984
C	3.360716	-0.699609	-0.531860	0.021868
C	1.479582	2.818094	-1.651252	0.050198
C	1.135984	-1.041927	-3.473311	0.154832
C	-1.773723	1.783818	-2.389055	0.044532
C	1.470328	0.462828	3.473311	0.154832
C	3.180332	0.127691	1.651252	0.050198
C	3.006123	1.735586	-0.240436	0.088716
C	2.431693	0.644181	-2.389055	0.044532
C	0.334343	1.504755	-3.473311	0.154832
C	-1.470328	-0.462828	-3.473311	0.154832
C	-3.180332	-0.127691	-1.651252	0.050198
C	-3.006123	-1.735586	0.240436	0.088716
C	-2.431693	-0.644181	2.389055	0.044532
C	-0.334343	-1.504755	3.473311	0.154832
C	-2.473802	-0.952021	-2.422557	0.051557
C	-3.751172	-0.532400	-0.288998	0.153100
C	-2.748513	-1.965168	1.726688	0.152948
C	-1.358885	-0.439422	3.165123	0.052401
C	1.059993	-0.957118	3.165123	0.052401
C	2.473802	0.952021	2.422557	0.051557
C	3.751172	0.532400	0.288998	0.153100
C	2.748513	1.965168	-1.726688	0.152948
C	1.358885	0.439422	-3.165123	0.052401
C	-1.059993	0.957118	-3.165123	0.052401
O	-5.151093	-0.810385	-0.287394	-0.541561
H	-5.586872	-0.027055	-0.656390	0.313311
O	-2.820790	-3.390113	-2.792595	-0.552802
H	-3.737797	-3.413298	-2.481645	0.314363
O	-4.224398	2.037192	-2.292149	-0.545015
H	-4.147534	1.971798	-3.255249	0.315400
O	-1.925572	-0.516625	-4.823857	-0.544414
H	-2.082733	-1.449862	-5.031122	0.315584
O	2.820790	3.390113	2.792595	-0.552802
H	3.737797	3.413298	2.481645	0.314363
O	5.151093	0.810385	0.287394	-0.541561
H	5.586872	0.027055	0.656390	0.313311
O	1.925572	0.516625	4.823857	-0.544414
H	2.082733	1.449862	5.031122	0.315584
O	4.224398	-2.037192	2.292149	-0.545015
H	4.147534	-1.971798	3.255249	0.315400
O	0.347939	-4.677032	-2.292149	-0.545015
H	0.366140	-4.577769	-3.255249	0.315400
O	1.410197	-1.409281	-4.823857	-0.544414
H	2.296984	-1.078768	-5.031122	0.315584
O	3.277360	-4.055785	-0.287394	-0.541561
H	2.816866	-4.824845	-0.656390	0.313311
O	4.346319	-0.747819	-2.792595	-0.552802
H	4.824902	-1.530378	-2.481645	0.314363
O	-3.277360	4.055785	0.287394	-0.541561
H	-2.816866	4.824845	0.656390	0.313311
O	-4.346319	0.747819	2.792595	-0.552802
H	-4.824902	1.530378	2.481645	0.314363
O	-0.347939	4.677032	2.292149	-0.545015
H	-0.366140	4.577769	3.255249	0.315400
O	-1.410197	1.409281	4.823857	-0.544414
H	-2.296984	1.078768	5.031122	0.315584
O	1.873732	4.866170	-0.287394	-0.541561
H	2.770005	4.851900	-0.656390	0.313311
O	3.876459	2.639840	-2.292149	-0.545015

H	3.781394	2.605971	-3.255249	0.315400
O	0.515375	1.925907	-4.823857	-0.544414
H	-0.214251	2.528631	-5.031122	0.315584
O	-1.525529	4.137932	-2.792595	-0.552802
H	-1.087104	4.943677	-2.481645	0.314363
O	1.525529	-4.137932	2.792595	-0.552802
H	1.087104	-4.943677	2.481645	0.314363
O	-0.515375	-1.925907	4.823857	-0.544414
H	0.214251	-2.528631	5.031122	0.315584
O	-3.876459	-2.639840	2.292149	-0.545015
H	-3.781394	-2.605971	3.255249	0.315400
O	-1.873732	-4.866170	0.287394	-0.541561
H	-2.770005	-4.851900	0.656390	0.313311

OH36	x	y	z	q(e)
C	-0.835253	-3.142030	1.785020	0.145255
C	0.876023	3.709699	0.840710	0.269906
C	-1.906752	-2.384189	1.055260	0.038357
C	-0.023517	3.742600	-0.485730	0.185988
C	-2.206323	-3.025418	-0.265620	0.205648
C	0.880603	3.227769	-1.651440	0.212235
C	-0.805923	-3.646470	-0.678830	0.262262
C	1.925782	2.359718	-0.983950	-0.032863
C	0.048057	-3.785810	0.662410	0.227886
C	2.230442	3.016148	0.358670	0.163892
C	-0.100082	-2.216740	2.696710	0.107605
C	0.163402	2.939290	1.913420	0.081186
C	-2.876841	-1.543648	1.753230	0.232719
C	-1.360477	3.025911	-0.381920	0.003173
C	-2.983852	-2.049858	-1.271660	0.268130
C	0.127262	2.358940	-2.598990	0.058866
C	-0.085852	-2.685530	-1.515030	-0.047505
C	3.035361	1.722617	-1.697390	0.296856
C	1.389587	-3.067881	0.540190	0.116810
C	3.009282	2.144307	1.397660	0.225745
C	1.208938	-1.951171	2.694600	0.059125
C	0.911572	2.214329	3.014360	0.137462
C	-1.942121	-0.695329	2.486600	0.020844
C	-2.135577	3.106571	0.859690	0.213846
C	-3.043591	-0.674108	-0.689360	0.026380
C	-1.182058	2.068221	-2.573590	0.157831
C	-0.823672	-1.948850	-2.548300	0.130342
C	2.032761	0.862698	-2.347190	0.076930
C	2.241397	-2.960722	-0.680180	0.225272
C	3.582691	0.851287	0.751770	0.204136
C	0.953041	1.315559	-3.312300	0.145260
C	1.321518	-2.869871	-1.923050	0.187419
C	3.580261	0.669077	-0.688050	0.176943
C	2.174508	-2.661582	1.791610	0.195048
C	2.082201	1.498298	2.401000	0.061629
C	-0.912541	-1.185670	3.433300	0.140801
C	-1.157238	2.720641	1.964210	0.064129
C	-3.541600	-0.535517	0.750360	0.167623
C	-2.139058	2.782082	-1.663510	0.174396
C	-2.034331	-1.238979	-2.030640	0.062147
C	1.522249	-0.687892	3.473650	0.128520
C	-0.147169	1.206980	3.448530	0.064269
C	-2.522149	0.662732	2.676630	0.165408
C	-2.655318	1.826722	0.341220	0.058116
C	-3.512040	0.405703	-1.660210	0.200813
C	-1.491719	0.840231	-3.426080	0.175453
C	0.209709	-1.033630	-3.081250	0.139883
C	2.620810	-0.545582	-2.513260	0.149810
C	2.784399	-1.660523	-0.242300	-0.017682
C	3.507020	-0.303803	1.782040	0.211700
C	-0.084040	0.216170	-3.425660	0.000483
C	1.587319	-1.651812	-2.928260	0.217712
C	3.453809	-0.769133	-1.218310	0.254160
C	3.298569	-1.731463	1.148340	0.191865
C	2.344150	0.201958	2.595450	0.086310

C	0.122170	-0.087060	3.639180	0.066729
C	-1.522649	1.781581	3.102620	0.183557
C	-3.293299	0.897412	1.351180	0.261797
C	-3.259978	1.872862	-1.049770	0.212422
C	-2.622740	-0.110248	-2.862260	0.239576
O	2.041168	-2.171032	-4.178940	-0.624329
H	1.929887	-3.143962	-4.088290	0.354703
O	1.482472	1.824628	-4.538800	-0.581347
H	2.073381	1.137128	-4.883720	0.340133
O	-1.341322	-2.851489	-3.577130	-0.589145
H	-1.909422	-2.321729	-4.164650	0.318761
O	-1.898889	1.246581	-4.729490	-0.570193
H	-1.180619	1.795901	-5.078300	0.335894
O	-1.469462	-1.770319	4.633050	-0.590089
H	-2.147691	-1.144958	4.938150	0.341835
O	-2.145538	2.506342	4.173620	-0.599234
H	-1.586167	3.276411	4.353880	0.357151
O	2.268259	-0.896882	4.675390	-0.581504
H	1.849409	-1.631642	5.147660	0.356486
O	1.291343	3.153029	4.025410	-0.573132
H	1.835662	2.678918	4.671510	0.351310
O	1.557114	4.349868	-2.246650	-0.592007
H	0.952854	5.102579	-2.085200	0.345491
O	-2.635787	3.971162	-2.276120	-0.590506
H	-3.528937	4.085923	-1.897170	0.348600
O	1.135764	4.984289	1.362840	-0.577012
H	1.942894	5.299438	0.922500	0.339110
O	-2.966186	4.224562	1.124330	-0.592980
H	-3.722357	3.878843	1.622920	0.330869
O	-0.950434	-4.891099	-1.353870	-0.605471
H	-1.716435	-5.350239	-0.972060	0.321479
O	3.256557	-3.970193	-0.834230	-0.605829
H	2.880886	-4.614393	-1.462220	0.328803
O	-1.453624	-4.245559	2.515130	-0.588974
H	-1.878083	-3.856779	3.298920	0.350063
O	2.726307	-3.758983	2.495300	-0.578579
H	3.430657	-4.099923	1.916690	0.338604
O	-3.920582	-2.260507	2.501060	-0.618209
H	-4.146151	-1.670887	3.241830	0.337261
O	-4.494829	1.594453	1.704170	-0.576088
H	-4.975509	1.782444	0.879370	0.337445
O	-4.903640	0.306614	-2.000340	-0.612488
H	-5.307470	-0.257496	-1.314790	0.360442
O	-4.081032	-2.651687	-1.916190	-0.610107
H	-4.394693	-3.354047	-1.323970	0.344103
O	4.004362	2.872556	2.076110	-0.575758
H	2.983184	4.343577	-0.911200	0.363068
O	4.716100	-0.338734	2.542830	-0.578631
H	4.708950	0.405516	3.162940	0.363404
O	4.824429	-1.195524	-1.449360	-0.592899
H	4.870928	-2.116254	-1.133700	0.355218
O	4.026892	2.457406	-2.363840	-0.582667
H	4.291132	1.935286	-3.137510	0.347099
O	3.153453	4.081077	0.019770	-0.602674
H	4.304493	3.560156	1.454250	0.362727
O	4.919861	0.971616	-0.037700	-0.424415
H	5.374600	0.079865	-0.118160	0.405260
O	4.568258	-2.416924	1.186910	-0.604908
H	4.989248	-2.181114	2.031460	0.346648
O	0.362426	-5.135611	0.953020	-0.581229
H	0.065846	-5.312040	1.861740	0.344332
O	-3.148263	-4.105148	-0.003040	-0.606634
H	-3.006914	-4.405598	0.911900	0.346205
O	-4.940171	-0.787706	0.621830	-0.602755
H	-5.123971	-1.501836	1.266070	0.342200
O	-0.398436	5.099930	-0.761280	-0.584656
H	-1.232906	5.080811	-1.272390	0.348648
O	-3.455190	0.412353	3.759420	-0.578989
H	-3.745929	1.281363	4.086850	0.358012
O	1.516307	-4.110992	-2.698690	-0.635184
H	0.651946	-4.564021	-2.690560	0.354998

O	3.496110	-0.288523	-3.616200	-0.579610
H	3.377159	-1.082483	-4.189000	0.361282
O	-3.354051	-0.588567	-3.967920	-0.579081
H	-4.135191	-1.033597	-3.600080	0.342209
O	-4.511978	2.568673	-1.037620	-0.609476
H	-5.099598	2.016014	-1.601000	0.356325

OH44	x	y	z	q(e)
C	1.574924	-1.762308	2.398856	0.203933
C	1.041148	-0.801338	3.129918	0.178266
C	0.531458	-3.059737	0.724149	0.097949
C	-0.573948	-3.238083	0.025785	0.203699
C	2.212132	0.087471	-2.114346	0.066150
C	1.226759	-0.009584	-2.996570	0.195689
C	-1.049422	-2.375863	-2.054563	0.102276
C	-0.571173	-1.536565	-2.944825	0.176228
C	-1.012971	0.815943	-3.064957	0.123579
C	-1.563502	1.793926	-2.375712	0.187684
C	0.537697	3.129299	-0.032799	0.104297
C	-0.567631	3.114919	-0.753009	0.186334
C	-1.212346	0.006230	2.934952	0.126929
C	-2.291146	-0.077184	2.174739	0.198005
C	0.620397	1.557540	2.981777	0.169061
C	1.099553	2.431777	2.121926	0.213110
C	-0.713122	-2.522864	2.904430	0.203775
C	-2.082422	-2.662137	2.026082	0.204872
O	-0.794315	-3.421188	4.022664	-0.612411
H	-0.861277	-2.850371	4.838996	0.426986
O	-2.908952	-3.625882	2.694421	-0.617687
H	-3.485775	-3.112168	3.319410	0.405601
C	-1.298324	3.396153	1.565230	0.167325
C	-1.868779	2.316794	2.565333	0.149612
O	-2.535433	3.077157	3.616159	-0.661744
H	-3.401680	2.553429	3.757288	0.429228
O	-1.678297	4.693571	2.101159	-0.641100
H	-2.162584	4.507411	2.956319	0.427503
C	-3.623904	0.312786	-1.774426	0.174405
C	-2.927566	-0.898514	-2.610541	0.201103
O	-4.883663	0.530373	-2.449745	-0.620901
H	-4.781442	1.418981	-2.926023	0.426667
O	-3.856464	-1.316418	-3.620011	-0.597058
H	-3.481639	-1.022571	-4.497241	0.425772
C	2.977357	0.902705	2.603041	0.188264
C	3.647717	-0.312032	1.736289	0.145360
C	2.103355	2.661331	-1.996209	0.216304
C	0.742799	2.525187	-2.893238	0.173160
O	3.927456	1.248181	3.620375	-0.598538
H	4.713597	0.653896	3.502146	0.412369
O	4.931276	-0.548028	2.420916	-0.676939
H	4.796600	-1.476246	2.851522	0.432844
O	2.911058	3.652403	-2.682709	-0.615197
H	2.913656	4.455704	-2.076651	0.433745
O	0.938525	3.396027	-4.031597	-0.653729
H	1.862966	3.788971	-3.892184	0.431037
C	1.314328	-3.407667	-1.550654	0.222543
C	1.911019	-2.319124	-2.544948	0.171470
O	2.662906	-3.053973	-3.549121	-0.652391
H	2.555414	-4.025641	-3.287115	0.442424
O	1.776394	-4.649666	-2.097312	-0.633397
H	1.845095	-5.286162	-1.335211	0.441553
C	-2.985548	-1.348135	1.901582	0.055023
C	-1.953546	-3.268539	0.570632	0.079318
C	0.631421	-2.907943	2.172565	0.039113
C	-0.400482	-1.092381	3.494082	0.045438
O	-0.626033	-1.172307	4.927517	-0.624064
H	-0.664878	-0.255982	5.308150	0.441165
O	1.152706	-4.171482	2.686695	-0.615739
H	0.636328	-4.338804	3.522546	0.417369
O	-3.976072	-1.458533	2.975138	-0.576935
H	-4.830366	-1.655886	2.479574	0.413110
O	-2.312436	-4.686268	0.618616	-0.580956

H	-2.680117	-4.820410	1.538996	0.421214
C	0.852503	-1.427763	-3.357040	0.065383
C	2.933315	-1.223869	-1.977286	0.121738
C	1.792887	-3.358438	-0.029104	0.128519
C	-0.295175	-3.472321	-1.427633	0.066712
O	3.965880	-1.092632	-3.018140	-0.608694
H	4.083807	-1.989935	-3.417781	0.422383
O	0.946967	-1.690886	-4.765860	-0.576433
H	1.730233	-2.288788	-4.876801	0.398815
O	-0.753368	-4.751522	-1.890740	-0.570023
H	-1.606674	-4.618812	-2.376168	0.405718
O	2.050859	-4.768717	0.267568	-0.603492
H	1.840158	-4.931311	1.226878	0.426831
C	-0.814515	1.394841	3.322227	0.043506
C	-2.976178	1.247050	2.018864	0.094048
C	-1.818466	3.396244	0.037260	0.122552
C	0.295842	3.436156	1.400756	0.033241
O	-0.997761	1.482757	4.769871	-0.590594
H	-1.509156	2.308247	4.948475	0.401893
O	-4.018064	1.319999	3.056530	-0.592531
H	-4.857528	1.553485	2.563514	0.419485
O	-2.092421	4.760116	-0.309319	-0.513072
H	-2.513498	5.187333	0.471117	0.381597
O	0.778315	4.793066	1.651611	-0.591171
H	-0.018971	5.311381	1.937394	0.410446
C	-0.635855	2.971482	-2.214330	0.050389
C	1.927725	3.217774	-0.538588	0.117439
C	2.952119	1.349913	-1.881241	0.089602
C	0.400131	1.105501	-3.506628	0.042490
O	0.444385	1.129056	-4.958853	-0.584362
H	0.648732	2.073699	-5.191924	0.404919
O	-1.133774	4.166377	-2.826624	-0.556220
H	-0.583565	4.297001	-3.640054	0.392146
O	2.168511	4.652330	-0.653324	-0.615327
H	1.888948	5.083643	0.198749	0.432325
O	3.950256	1.413057	-2.963307	-0.590865
H	4.100618	0.473461	-3.291136	0.430523
C	-1.577594	-0.508332	-3.375911	0.038662
C	-2.538466	-2.269785	-1.840642	0.127223
C	-4.067386	0.036264	-0.219195	0.182178
C	-2.931701	1.788864	-1.817084	0.067690
O	-3.716854	2.569297	-2.782029	-0.588551
H	-4.027315	3.377226	-2.278820	0.435919
O	-5.516372	0.081463	-0.280278	-0.611291
H	-5.727301	0.204784	-1.276515	0.444632
O	-3.004179	-3.384464	-2.658417	-0.590563
H	-3.681894	-2.992842	-3.276037	0.414436
O	-1.875066	-0.572683	-4.803597	-0.619795
H	-1.112730	-0.193803	-5.308217	0.431483
C	2.585914	2.306122	1.889524	0.106438
C	1.632511	0.526230	3.427963	0.040668
C	4.088210	-0.060014	0.187998	0.183698
C	2.935083	-1.767052	1.825431	0.052441
O	1.888676	0.580185	4.841432	-0.578808
H	2.759908	1.056229	4.919090	0.403947
O	3.740697	-2.546182	2.789650	-0.590458
H	4.092672	-3.316224	2.236576	0.429810
O	5.529767	-0.113197	0.175017	-0.601865
H	5.817107	-0.236860	1.126192	0.427653
O	3.090344	3.366034	2.709686	-0.541996
H	3.873311	3.739826	2.229194	0.401017
C	-3.758853	-1.393405	0.504112	0.193002
C	-3.071686	-2.555808	-0.371547	0.172957
O	-5.046352	-1.904496	0.896360	-0.609054
H	-5.175564	-2.748991	0.366009	0.430208
O	-4.132367	-3.521487	-0.518764	-0.612667
H	-3.705458	-4.412466	-0.377828	0.418114
C	3.750648	1.389393	-0.504331	0.188341
C	3.074809	2.565171	0.391980	0.197002
O	5.019239	1.962186	-0.882323	-0.608681
H	5.063930	1.878223	-1.886131	0.423518

O	4.101204	3.556565	0.561359	-0.623627
H	4.842985	3.283956	-0.058163	0.424717
C	-3.707955	1.432844	0.633137	0.124168
O	-5.039736	1.938688	1.001309	-0.673946
H	-5.666620	1.230196	0.538306	0.444461
C	-3.106031	2.511210	-0.382655	0.172015
O	-4.152995	3.487988	-0.586284	-0.612425
H	-4.897789	3.238972	0.029298	0.412910
C	3.689478	-1.457784	-0.638961	0.166041
C	3.077733	-2.512521	0.404745	0.169383
O	4.115275	-3.487729	0.642835	-0.618304
H	4.822322	-3.292582	-0.047455	0.422070
O	4.949412	-2.064861	-1.026454	-0.621280
H	5.640701	-1.363572	-0.803264	0.426517