Li – 1 water molecule

4

O 0.008684 0.091846 -0.120392
H -0.408756 -0.416625 -0.834340
H 0.946657 0.144857 -0.362340
Li -0.649396 0.218553 1.561495
4

O -0.018495 0.197587 -0.046841
H 0.586647 0.471913 0.662607
H 0.520759 0.218879 -0.853123
Li -1.294306 -1.065064 0.274987
4

O 0.006126 -0.080174 -0.071226
H 0.411206 0.185617 -0.913192
H 0.479778 -0.887663 0.186517
Li -1.069620 0.922747 0.959078
4

O 0.028197 0.115145 -0.034284
H 0.528863 0.103134 -0.865868
H -0.734636 0.689994 -0.199215
Li 0.218039 -1.079068 1.312845
4

O -0.006337 0.095098 -0.134557
H 0.939729 0.253726 -0.285142
H -0.282516 -0.495331 -0.852351
Li -0.754018 0.196665 1.516810
4

O 0.006638 0.062772 -0.114867
H -0.403323 -0.411922 -0.864819
H 0.946726 0.154604 -0.366219
Li -0.652851 0.233176 1.590329
4

O 0.058206 0.075076 -0.009535
H 0.593523 0.552286 0.654049
H 0.493159 0.261778 -0.864120
Li -1.350283 -1.065826 0.257237
4

O 0.162057 0.000996 -0.002596
H 0.355806 0.151959 -0.948793
H 0.428709 -0.925326 0.159670
Li -1.119082 0.912897 0.952895
4

O -0.064512 -0.003956 -0.119017
H 0.564426 0.158207 -0.849706
H -0.699148 0.737565 -0.170355
Li 0.239697 -1.062612 1.352555
4

O 0.015713 0.061090 -0.111298
H 0.950015 0.263012 -0.316142
H -0.288396 -0.480528 -0.866490
Li -0.780475 0.206584 1.538690

Li – 2 water molecules

7

O -1.372541 0.859183 0.771507
H -1.205509 0.719661 1.719084
H -1.270336 1.819182 0.657338
O 1.091372 -0.932795 -1.037013
H 1.903910 -0.407191 -0.952857
H 1.350396 -1.820287 -0.737095
Li -0.497293 -0.237754 -0.420963
7

O 0.927212 -0.052956 -1.563593
H 1.493146 0.597208 -2.009937
H 0.530649 -0.568941 -2.283969
O -0.685315 0.019930 1.802483
H -1.332962 0.735815 1.911223
H -1.193802 -0.787720 1.982955
Li 0.261818 0.056917 0.161267
7

O 0.325127 1.327093 -1.117153
H -0.442601 1.804858 -1.469595
H 0.872326 2.011754 -0.699536
O -0.171834 -1.603329 0.878281
H 0.293825 -1.495443 1.724859
H -1.107842 -1.663574 1.135031

Li 0.230998 -0.381356 -0.451889
7

O -0.164152 0.688628 1.614153
H -0.492616 1.602352 1.643293
H 0.350999 0.588164 2.430511
O -0.065428 -0.898140 -1.510788
H 0.508720 -1.523998 -1.979698
H -0.560201 -0.445214 -2.213453
Li 0.434876 0.018203 0.002567
7

O 0.288609 -1.129555 -1.441382
H 1.236671 -1.324988 -1.526094
H -0.112223 -1.997272 -1.262610
O -0.469098 1.379806 1.134430
H 0.323685 1.745802 1.560138
H -1.011611 1.062276 1.874656
Li -0.253954 0.273936 -0.347259
7

O -1.179107 0.903174 0.923035
H -0.965598 1.145983 1.845218
H -2.097271 1.212648 0.793413
O 1.099794 -1.031972 -0.877873
H 2.001756 -1.190512 -0.534307
H 1.103707 -1.451717 -1.760908
Li 0.036718 0.412396 -0.388582
7

O 0.804670 0.018105 -1.667823
H 1.339076 0.738520 -2.056414
H 1.008503 -0.761468 -2.221251
O -0.798864 -0.028525 1.673833
H -0.959401 0.750497 2.242148
H -1.402199 -0.713404 2.024129
Li 0.008960 -0.003472 0.005807
7

O 0.526355 1.468581 -1.049055
H 0.320251 2.374803 -0.743185
H 0.359503 1.503765 -2.012422
O -0.429959 -1.491554 0.996546
H -0.798268 -1.444389 1.900825
H -0.033500 -2.383774 0.943560
Li 0.055618 -0.027432 -0.036268
7

O 0.111038 0.942133 1.569610
H -0.675710 1.357783 1.975715
H 0.461689 0.361860 2.274485
O -0.157601 -0.821720 -1.556381
H 0.292059 -1.690707 -1.548205
H -0.161167 -0.567236 -2.500948
Li 0.141890 0.447883 -0.227687
7

O 0.343540 -1.130286 -1.274089
H -0.453878 -1.438952 -1.748205
H 1.074542 -1.646582 -1.667592
O -0.203044 1.173888 1.402127
H -1.108533 1.221975 1.768876
H 0.000099 2.097187 1.150726
Li 0.349356 -0.267227 0.360035

Li – 4 water molecules

13

O -1.328575 -0.337319 1.277913
H -2.113561 0.202554 1.454844
H -1.626265 -1.247947 1.431007
O -0.686366 0.468532 -1.835293
H -0.030687 0.750581 -2.491560
H -1.174758 -0.243186 -2.276861
O 1.377119 -1.217745 -0.305625
H 1.699508 -1.739072 0.446965
H 1.226578 -1.881126 -0.997171
O 0.714100 1.712344 0.757286
H 0.290788 1.785816 1.628399
H 1.658550 1.645859 0.971106
Li -0.006431 0.100708 -0.061011
13

O -0.812936 -0.100627 -1.927783
H -0.205210 -0.054014 -2.682993
H -1.330151 0.717666 -2.006341
O -0.159376 -1.797477 0.892646
H -0.705642 -1.441532 1.610881
H 0.596053 -2.206657 1.341409
O 1.802174 0.673258 -0.286513

H	2.197198	1.029643	0.524516
H	2.555545	0.333757	-0.792336
O	-1.066172	0.924437	0.896241
H	-0.919134	1.185598	1.817952
H	-2.031605	0.907325	0.804339
Li	0.079739	-0.172815	-0.190449

13

O	-1.115209	1.077389	0.974729
H	-0.659355	1.637404	1.622558
H	-1.736168	1.683267	0.539323
O	0.878747	0.699708	-1.683092
H	1.336505	1.550836	-1.589422
H	0.260473	0.851518	-2.415715
O	-0.721484	-1.678996	-0.739118
H	-1.049238	-1.646872	-1.651631
H	-0.058681	-2.387588	-0.752242
O	0.954682	-0.741869	1.540545
H	1.544835	-0.126937	2.005105
H	0.260921	-0.928238	2.193171
Li	0.057508	-0.044383	-0.068139

13

O	-1.454758	1.295526	0.255772
H	-2.087434	1.070037	0.956197
H	-2.023239	1.492685	-0.506641
O	1.028765	1.106060	-1.147733
H	0.921154	2.051062	-0.955991
H	1.988898	0.981449	-1.198688
O	-0.217348	-1.747366	-0.867876
H	0.470668	-2.316910	-0.489181
H	-0.079207	-1.819519	-1.825285
O	0.636261	-0.692475	1.573145
H	0.816227	-0.061849	2.288371
H	0.111822	-1.385457	2.005028
Li	-0.065197	-0.003434	-0.069352

13

O	-1.370690	-0.358869	-1.330588
H	-1.733798	0.375529	-1.850114
H	-1.039827	-0.978002	-1.999970
O	0.504869	1.835884	0.136555
H	0.666991	2.370478	-0.655954
H	-0.001371	2.426466	0.716876
O	1.346073	-1.333012	-0.416808
H	1.847550	-1.598951	0.371107
H	2.036439	-1.074462	-1.047514
O	-0.669526	-0.712652	1.653127
H	-1.524709	-0.371212	1.960018
H	-0.089621	-0.593309	2.422462
Li	-0.019279	-0.013840	-0.011130

13

O	-1.490567	-0.489313	1.180792
H	-2.329576	-0.776444	0.770529
H	-1.393785	-1.081955	1.950823
O	-0.786361	0.415022	-1.687585
H	-0.274681	0.072969	-2.447372
H	-0.945299	1.348927	-1.928739
O	1.125607	-1.511611	-0.333465
H	1.288813	-2.178802	0.362408
H	2.016649	-1.348492	-0.700603
O	0.900646	1.448121	0.931683
H	0.357546	2.104236	1.410883
H	1.549915	1.994756	0.448141
Li	-0.018909	0.002585	0.042505

13

O	-1.227059	1.271076	0.819385
H	-2.187840	1.097854	0.857051
H	-1.170596	2.172174	0.445816
O	1.013618	1.067290	-1.209592
H	0.452072	1.426935	-1.923820
H	1.759676	0.660523	-1.692177
O	-0.942523	-1.407027	-0.822787
H	-1.545470	-1.976175	-0.306101
H	-0.471380	-2.037250	-1.401987
O	1.263358	-0.490397	1.471515
H	2.045754	-1.054646	1.318409
H	0.935012	-0.781112	2.344539
Li	0.028911	-0.004004	0.075820

13

O	-0.598061	0.036862	-1.834454
H	-1.517006	-0.256131	-1.990990
H	-0.100064	-0.371497	-2.569082
O	-0.030998	-1.751933	0.756006
H	0.348435	-1.905103	1.643590
H	0.314387	-2.500070	0.230278
O	1.649258	1.005485	0.017175
H	2.162392	1.117350	0.841220
H	2.325696	0.750440	-0.640410

O	-1.435716	0.981169	0.919391
H	-1.553701	0.924570	1.887832
H	-1.548599	1.933057	0.729829
Li	-0.015541	0.034368	0.011186

13

O	-1.819030	0.805245	-0.006914
H	-2.071208	1.334403	0.775707
H	-2.125003	1.352193	-0.757036
O	1.279566	1.239195	-0.556909
H	1.092662	2.094964	-0.988705
H	2.156658	0.987456	-0.905019
O	-0.160671	-1.693299	-0.916925
H	0.669660	-2.201557	-1.003476
H	-0.555920	-1.752399	-1.809281
O	0.300918	-0.468065	1.870978
H	1.209436	-0.314734	2.197787
H	0.137449	-1.405370	2.095274
Li	-0.067904	-0.008222	0.022283

13

O	-1.348795	-0.638075	-1.220962
H	-2.284276	-0.391866	-1.079590
H	-1.213190	-0.474386	-2.175077
O	0.612824	1.793434	-0.051164
H	0.018076	2.508186	-0.353382
H	1.428475	1.944493	-0.568019
O	1.440630	-1.233646	-0.183036
H	2.333723	-1.016280	0.147258
H	1.597338	-1.537449	-1.097820
O	-0.916803	-0.166389	1.784499
H	-1.197570	-1.038496	2.124773
H	-0.474047	0.245049	2.552523
Li	-0.043282	-0.020529	0.068069

Li – 8 water molecules

25

O	2.184638	-1.954329	-0.674619
H	2.421932	-1.247382	-0.039055
H	3.003520	-2.187424	-1.130290
O	-2.869260	0.027390	2.523341
H	-2.520809	0.778960	3.020219
H	-2.757549	-0.732316	3.109145
O	-1.095573	1.734530	0.826510
H	-0.364607	1.932235	0.202181
H	-1.737307	2.444116	0.695230
O	0.457330	-0.452598	-2.135767
H	0.596314	-0.538290	-3.087907
H	1.115199	-1.054854	-1.709340
O	2.060608	0.148632	1.047048
H	1.883014	0.929874	0.483574
H	2.528678	0.469638	1.827697
O	1.085225	1.888500	-0.866767
H	0.914954	1.163338	-1.509621
H	1.445461	2.633295	-1.363470
O	-0.410787	-1.358624	1.006530
H	-0.174242	-2.019781	0.344382
H	0.419235	-0.873247	1.189881
O	-2.172824	-0.698568	-1.189943
H	-2.786234	-0.249618	-1.784087
H	-1.291697	-0.632815	-1.618843
Li	-1.861012	-0.084794	0.722588

25

O	1.965757	-1.772605	-1.613466
H	2.272382	-1.347148	-0.777745
H	2.696599	-1.622643	-2.233415
O	-2.985622	-0.425951	2.201271
H	-3.177380	0.441348	2.594685
H	-2.598777	-0.923135	2.939674
O	-1.301400	1.805180	0.982817
H	-0.430421	1.988602	0.551749
H	-1.917314	2.419625	0.557269
O	0.109113	0.046966	-2.132308
H	0.123577	0.324976	-3.061528
H	0.797934	-0.675421	-2.045295
O	2.419676	-0.276556	0.654435
H	2.143354	0.620106	0.334995
H	3.194567	-0.145712	1.222457
O	1.062008	1.813166	-0.339178
H	1.472637	2.605440	-0.720189
H	0.733210	1.279573	-1.111066
O	0.007878	-0.853115	1.609461
H	0.000569	-1.812384	1.742723
H	0.939888	-0.648660	1.345517
O	-2.184107	-0.660929	-0.957175
H	-2.301472	-1.614799	-1.075371
H	-1.396085	-0.430172	-1.512843
Li	-1.605703	-0.104850	0.844661

25

O	0.930146	-1.966981	-1.025504
H	1.346152	-2.694767	-1.512431
H	1.569408	-1.721151	-0.313293
O	-3.314984	0.443754	1.657757
H	-3.990955	0.714424	1.017148
H	-3.687217	-0.353304	2.066665
O	-0.277356	1.640736	1.288487
H	0.569302	1.672520	0.779191
H	-0.629592	2.541964	1.237563
O	0.516959	0.419845	-2.163376
H	0.688080	0.497073	-3.114703
H	0.713018	-0.523782	-1.916629
O	2.098260	-0.861432	1.174102
H	2.262007	0.025625	0.773596
H	2.926459	-1.116874	1.606504
O	1.974365	1.467193	-0.168056
H	1.540649	1.233642	-1.028678
H	2.463017	2.291692	-0.312626
O	-0.586926	-1.359231	1.222018
H	-0.404637	-1.798755	0.367386
H	0.325252	-1.154448	1.521544
O	-1.902078	0.327049	-1.024629
H	-2.412269	-0.383975	-1.439107
H	-1.092242	0.421961	-1.582622
Li	-1.552276	0.270491	0.847690

25

O	-1.165626	-1.887172	-1.174639
H	-0.993233	-1.321453	-1.962198
H	-1.443846	-2.748184	-1.523710
O	-0.698039	1.391572	0.977438
H	-1.493838	1.061365	0.495283
H	-0.809281	2.354092	0.983009
O	1.275326	1.374340	-1.509768
H	0.482360	1.087506	-2.028415
H	1.285903	2.339242	-1.597411
O	2.372347	1.032379	1.679653
H	2.222888	1.775258	2.283727
H	2.274196	0.231315	2.246361
O	1.076083	-1.186441	0.223968
H	0.278122	-1.613602	-0.158244
H	1.183870	-1.522764	1.135957
O	-0.934465	0.366618	-2.664828
H	-1.251076	0.550238	-3.563149
H	-1.689888	0.586362	-2.068569
O	1.847304	-1.380953	2.886791
H	2.582790	-1.939709	3.184709
H	1.216122	-1.396466	3.623926
O	-2.647670	0.293284	-0.588918
H	-3.617245	0.296473	-0.585846
H	-2.374662	-0.653787	-0.627633
Li	0.992860	0.743555	0.318091

25

O	1.503464	-2.224344	-0.140459
H	2.127685	-1.587910	0.276295
H	2.016068	-3.025144	-0.329481
O	-3.456137	0.120188	1.515063
H	-3.576392	0.775691	2.219665
H	-3.807499	-0.699211	1.897070
O	-1.089688	1.917753	0.420701
H	-0.207999	1.954410	-0.023886
H	-0.943920	2.356874	1.272343
O	0.542978	-0.586093	-2.015103
H	0.830317	-0.814488	-2.913020
H	0.923344	-1.291768	-1.424252
O	2.445837	0.041998	0.999549
H	2.255794	0.780190	0.370373
H	3.013748	0.411358	1.691867
O	1.342370	1.677943	-0.808567
H	1.115902	0.913310	-1.401679
H	1.733067	2.353544	-1.384037
O	-0.143689	-0.728475	1.433134
H	0.137654	-1.576191	1.037937
H	0.709667	-0.241155	1.457377
O	-2.050340	-0.432372	-1.320967
H	-2.465279	0.313943	-1.779909
H	-1.144094	-0.494872	-1.711974
Li	-1.722047	0.096613	0.572127

25

O	1.554437	-1.896904	-0.652987
H	2.115785	-1.221961	-0.154891
H	2.171162	-2.596003	-0.946708
O	-2.925027	-0.517300	2.123749
H	-3.785472	-0.055969	2.169881
H	-2.636850	-0.557201	3.057389
O	-1.001479	1.841007	0.869331
H	-0.229381	1.962450	0.238921
H	-1.673085	2.470519	0.542512

O	0.297636	-0.225263	-2.207321
H	0.440431	-0.329624	-3.169062
H	0.838843	-0.962760	-1.759998
O	2.380490	0.117268	0.837449
H	2.071383	0.879430	0.254999
H	3.278313	0.352602	1.141379
O	1.117953	1.808632	-0.759940
H	0.842748	1.137973	-1.469042
H	1.503521	2.569717	-1.236840
O	0.017986	-1.070741	1.471968
H	0.325624	-1.698107	0.770581
H	0.849963	-0.541925	1.592722
O	-2.003179	-0.679018	-0.894402
H	-2.734577	-0.186577	-1.315134
H	-1.222314	-0.505564	-1.498588
Li	-1.520706	-0.028813	0.882653

25

O	1.849269	-1.705582	-1.600844
H	2.117479	-1.242632	-0.747553
H	2.638494	-1.603825	-2.169853
O	-2.995587	-0.526696	2.206463
H	-3.801731	0.024116	2.251900
H	-2.778484	-0.689676	3.145654
O	-0.981507	1.802096	1.131355
H	-0.203885	1.971108	0.521024
H	-1.653983	2.450875	0.848100
O	0.145036	0.136794	-2.251462
H	0.058956	0.267530	-3.216753
H	0.811387	-0.636951	-2.119109
O	2.224974	-0.243304	0.601346
H	1.966238	0.660478	0.225384
H	3.094878	-0.125545	1.031422
O	1.109108	1.844932	-0.531060
H	1.577839	2.623748	-0.890600
H	0.754670	1.328311	-1.331080
O	-0.006454	-1.067106	1.820866
H	-0.045715	-2.005754	1.552373
H	0.889505	-0.770480	1.475906
O	-1.954120	-0.557423	-0.754217
H	-2.056607	-1.521575	-0.872940
H	-1.217811	-0.316456	-1.394679
Li	-1.501080	-0.066080	1.070491

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O	0.972871	-2.021511	-1.057601
H	1.380782	-2.790145	-1.502677
H	1.609104	-1.755070	-0.319655
O	-3.349137	0.140232	1.518722
H	-3.920020	0.930123	1.445414
H	-3.377052	-0.072723	2.472342
O	-0.518287	1.767870	1.342499
H	0.356454	1.799763	0.853758
H	-0.894788	2.659715	1.213227
O	0.647912	0.329740	-2.129725
H	0.961259	0.432665	-3.049871
H	0.821215	-0.640784	-1.874701
O	2.082624	-0.911528	1.054789
H	2.149063	0.032704	0.706001
H	2.941367	-1.109232	1.476037
O	1.754253	1.467915	-0.037894
H	1.426892	1.160613	-0.946798
H	2.449716	2.134171	-0.205911
O	-0.597642	-1.355609	1.101775
H	-0.370645	-1.828933	0.262159
H	0.316991	-1.167590	1.439556
O	-1.859523	0.437257	-1.217044
H	-2.336474	-0.325694	-1.596978
H	-0.979832	0.437986	-1.700046
Li	-1.594558	0.281337	0.710619

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O	-1.419242	-1.800910	-0.938534
H	-0.939024	-1.442999	-1.738585
H	-1.806070	-2.653001	-1.220335
O	-1.199413	1.952874	0.843217
H	-1.791758	1.493618	0.176955
H	-1.671066	1.847165	1.691778
O	1.295056	0.995431	-0.888895
H	0.743907	0.665271	-1.658210
H	1.563727	1.893849	-1.160723
O	1.795401	1.221877	2.168195
H	2.512639	1.724764	1.735079
H	2.187147	0.305563	2.266036
O	-0.067180	-0.984894	1.256982
H	-0.467679	-1.467723	0.485253
H	0.807814	-1.406759	1.443967
O	-0.420182	-0.025565	-2.665201
H	-0.412274	0.046235	-3.640341
H	-1.254816	0.435838	-2.359658
O	2.487154	-1.398001	2.151911
H	3.274201	-1.633594	1.620332

H	2.640017	-1.837970	3.012591
O	-2.484459	0.634874	-1.113903
H	-3.417892	0.765093	-1.374775
H	-2.389754	-0.348255	-0.934755
Li	0.405046	0.850284	0.827204

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O	1.414150	-2.011323	-0.226834
H	1.942890	-1.308580	0.270327
H	2.014873	-2.775257	-0.333456
O	-3.392464	0.311268	1.447248
H	-3.476219	0.596638	2.378457
H	-3.911551	-0.516463	1.418450
O	-0.931289	1.973638	0.452849
H	-0.060396	1.984014	-0.046255
H	-0.714858	2.391699	1.308216
O	0.559590	-0.486287	-2.163893
H	0.818339	-0.742273	-3.071283
H	0.961206	-1.189290	-1.546757
O	2.188857	0.115888	1.137586
H	2.048864	0.805947	0.416121
H	3.087802	0.268829	1.487913
O	1.375503	1.643397	-0.857865
H	1.133444	0.915808	-1.520632
H	1.868849	2.323069	-1.357936
O	-0.299749	-0.907149	1.618551
H	0.056161	-1.615593	1.025087
H	0.527840	-0.379468	1.762713
O	-1.879831	-0.667066	-1.073104
H	-2.571337	-0.292307	-1.652082
H	-1.041773	-0.592986	-1.618032
Li	-1.628089	0.165639	0.654777

Li – 12 water molecules

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O	-2.664938	0.621681	-1.159745
H	-2.590403	-0.278006	-0.737818
H	-3.599442	0.875403	-1.112513
O	2.223646	1.101829	2.664715
H	1.272579	1.348396	2.819287
H	2.715523	1.416316	3.438519
O	1.201647	1.133490	-2.668225
H	0.331704	0.825768	-3.022958
H	1.253518	2.061168	-2.943911
O	-1.008592	-1.151018	2.384572
H	-0.062627	-1.429987	2.378041
H	-1.319598	-1.337744	1.468655
O	-1.220638	0.106681	-3.312791
H	-1.882511	0.382283	-2.622426
H	-1.686511	0.147549	-4.162578
O	-2.004438	-1.723360	-0.139279
H	-1.431298	-2.047779	-0.885401
H	-2.697452	-2.395053	-0.038209
O	-0.416626	1.400364	2.672265
H	-1.010026	1.878495	3.271033
H	-0.750831	0.452255	2.635196
O	1.437828	-1.040957	-0.566536
H	0.829393	-1.612149	-1.079583
H	1.467228	-1.379120	0.355087
O	-0.440909	1.648191	-0.011570
H	-1.319837	1.373733	-0.355620
H	-0.521407	1.651182	0.970280
O	2.775787	1.671378	0.080197
H	2.822586	2.630987	-0.046443
H	2.678941	1.555768	1.057556
O	-0.407969	-2.197985	-2.217834
H	-0.458967	-2.995085	-2.767142
H	-0.715444	-1.443099	-2.785439
O	1.655305	-1.491062	2.133589
H	2.001902	-0.609567	2.426145
H	2.221894	-2.153693	2.556760
Li	1.169788	0.867208	-0.735323

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O	-2.487991	0.872906	-1.040741
H	-2.073348	1.303781	-1.833348
H	-3.416840	1.153054	-1.038247
O	2.202529	1.885170	1.641701
H	1.950417	2.653062	2.177304
H	2.069284	1.113969	2.247840
O	0.533305	2.905521	-1.050147
H	1.329426	3.314231	-1.421831
H	0.026880	2.596856	-1.840849
O	2.021371	-2.195624	1.056782
H	2.893193	-2.610978	0.974605
H	2.059818	-1.613387	1.858769
O	0.181238	-0.607284	-2.885882
H	0.512424	-1.161815	-3.608974
H	-0.527709	-1.135063	-2.431449

O	-0.951937	-0.744098	2.669064
H	-0.915346	-1.533939	2.046314
H	-1.560432	-0.986925	3.383095
O	1.670749	-0.377405	3.020239
H	1.997213	-0.533090	3.919801
H	0.683015	-0.500717	3.060005
O	-0.923476	1.797076	-3.013986
H	-0.490671	0.919052	-3.184848
H	-1.223322	2.141175	-3.868980
O	-0.900925	1.471322	1.101292
H	-1.548930	1.291226	0.381481
H	-1.023181	0.722178	1.729638
O	1.570332	-0.075466	-0.559287
H	1.183775	-0.354158	-1.418221
H	1.771470	-0.897778	-0.057367
O	-1.735056	-1.665338	-1.344278
H	-2.167839	-0.782595	-1.190729
H	-2.403741	-2.211550	-1.786589
O	-0.636377	-2.710846	0.941637
H	-0.984557	-2.356208	0.090321
H	0.342616	-2.675039	0.868393
Li	0.844932	1.502271	0.261816

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O	-1.893614	0.772115	-1.733501
H	-1.527727	1.593971	-1.310335
H	-2.585446	1.090675	-2.334579
O	0.862466	0.964866	2.546615
H	1.374495	1.355660	3.271677
H	1.042684	-0.013915	2.578799
O	3.069332	0.248150	-3.035836
H	2.173115	0.144008	-3.412755
H	3.352647	1.129345	-3.323839
O	-2.864340	-0.241983	0.705906
H	-2.621519	0.037667	-0.207561
H	-2.547529	0.510009	1.258539
O	0.472682	-0.221500	-2.639338
H	0.189092	-1.118893	-2.349243
H	-0.356833	0.289582	-2.476585
O	-0.305837	-2.498210	-1.287542
H	-0.446033	-3.413832	-1.573173
H	-0.703413	-2.438576	-0.379726
O	-1.597203	1.849418	1.950953
H	-0.733090	1.519009	2.315750
H	-1.983926	2.407099	2.643568
O	2.143941	-1.646695	-0.477845
H	1.352163	-2.130885	-0.813443
H	2.007294	-1.651252	0.497126
O	-0.694299	2.736216	-0.389067
H	-0.835943	3.676137	-0.580800
H	-1.090598	2.577368	0.509823
O	1.700919	1.462099	0.000175
H	0.933394	2.037996	-0.225959
H	1.539006	1.258522	0.951260
O	-1.171526	-2.176172	1.249656
H	-1.679543	-2.928906	1.592239
H	-1.846225	-1.439358	1.105127
O	1.271844	-1.627713	2.159787
H	1.570499	-2.244310	2.845955
H	0.344229	-1.903937	1.928964
Li	1.967243	0.088460	-1.307542

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O	-2.348548	1.134926	-0.276849
H	-2.392343	0.489277	-1.032131
H	-3.199673	1.600215	-0.291869
O	0.202862	-0.054101	2.689502
H	0.220790	-0.228336	3.644131
H	0.991085	-0.539938	2.322046
O	-0.135006	2.642387	-0.752257
H	0.080296	2.806271	0.191843
H	-0.983997	2.141605	-0.671472
O	2.233419	-1.227623	1.433508
H	1.747780	-1.849091	0.827627
H	2.882776	-1.762674	1.915251
O	0.571296	-0.346088	-1.905029
H	-0.377174	-0.435452	-2.144976
H	0.746279	-1.162704	-1.380961
O	-1.861747	-2.636545	-0.194101
H	-2.027883	-2.020221	0.590999
H	-2.378886	-3.440509	-0.031657
O	0.584708	2.514362	1.907120
H	0.929800	3.065903	2.624847
H	0.384717	1.633106	2.314795
O	0.783339	-2.566916	-0.331949
H	-0.194337	-2.735357	-0.231090
H	1.142845	-3.343174	-0.788690
O	-2.169960	-0.832547	1.649435
H	-2.321404	-0.071250	1.041204
H	-1.296437	-0.620917	2.060399
O	1.987136	2.057569	-2.957404
H	2.576712	2.825403	-2.899313

H	2.522413	1.388088	-3.412133
O	-2.144489	-0.780394	-2.093385
H	-2.180451	-1.583033	-1.509520
H	-2.736063	-0.955561	-2.840824
O	2.424458	1.224840	0.286925
H	2.487345	0.324401	0.679757
H	1.921215	1.746904	0.951705
Li	1.239319	1.351247	-1.305835

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O	-1.117883	-0.890764	-3.871817
H	-0.609062	-1.718004	-3.834251
H	-0.911322	-0.531925	-4.748254
O	-2.441199	-1.705286	0.801327
H	-3.072028	-2.438428	0.865400
H	-1.532369	-2.113381	0.799795
O	0.140290	-2.319812	0.789565
H	0.396115	-3.227187	1.020047
H	0.394328	-1.771494	1.592355
O	2.384360	0.588722	1.167936
H	1.845236	1.365644	0.849287
H	3.124676	0.986311	1.653887
O	0.813836	1.550068	-2.376445
H	0.755566	2.028085	-1.513670
H	1.684873	1.110644	-2.302941
O	0.857302	2.494046	0.157999
H	-0.062789	2.441795	0.536875
H	1.159314	3.401992	0.316294
O	0.669277	-0.751703	2.850005
H	-0.205945	-0.306673	2.901420
H	1.267968	-0.154692	2.344617
O	-1.796746	0.249146	-1.005900
H	-1.783086	0.995575	-0.364465
H	-2.146705	-0.506581	-0.483319
O	3.036585	-0.011444	-1.385874
H	2.921781	0.126629	-0.411254
H	3.867056	-0.500950	-1.485824
O	-1.954737	0.119688	2.700869
H	-2.569737	0.184281	3.447689
H	-2.304122	-0.596090	2.107140
O	-1.606382	2.099275	0.955644
H	-2.288967	2.786894	0.992655
H	-1.794437	1.470498	1.705427
O	0.840955	-1.463397	-1.762334
H	0.625468	-1.803650	-0.862292
H	1.723841	-1.034045	-1.651185
Li	-0.388013	-0.038764	-2.249446

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O	-2.511485	0.667799	-1.271685
H	-2.546515	-0.186984	-0.724114
H	-3.423970	1.018454	-1.288679
O	2.160562	0.938661	2.583707
H	1.172852	1.160871	2.704571
H	2.599539	1.184889	3.421516
O	1.160610	1.326850	-2.751213
H	0.337822	0.859127	-3.083147
H	1.006786	2.261986	-2.986622
O	-0.989642	-1.271033	2.469747
H	-0.038911	-1.550853	2.326312
H	-1.427178	-1.424427	1.581763
O	-1.045954	-0.118729	-3.293130
H	-1.736420	0.254511	-2.650278
H	-1.481038	-0.153905	-4.168253
O	-2.191433	-1.577093	0.052992
H	-1.574008	-1.982118	-0.647084
H	-2.957007	-2.185267	0.097175
O	-0.423637	1.229949	2.538439
H	-0.941724	1.701941	3.219716
H	-0.742723	0.240408	2.557576
O	1.550538	-0.861089	-0.665215
H	0.873734	-1.452997	-1.093692
H	1.616876	-1.207474	0.270556
O	-0.393910	1.859846	-0.074829
H	-1.248986	1.521789	-0.460610
H	-0.483709	1.698815	0.908785
O	2.734120	1.828969	0.115811
H	2.768481	2.804571	0.110994
H	2.622355	1.591742	1.083698
O	-0.493246	-2.223203	-1.822639
H	-0.441565	-3.091119	-2.269642
H	-0.721202	-1.543300	-2.538947
O	1.630793	-1.565409	1.940341
H	1.972961	-0.683439	2.299680
H	2.262233	-2.241913	2.255361
Li	1.192810	1.033633	-0.808404

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O	-2.640256	0.710591	-1.099475
H	-2.150628	1.208611	-1.834492
H	-3.588111	0.926016	-1.203661
O	1.851406	1.986517	1.853943

H	2.793756	2.173058	1.679528
H	1.868733	1.151065	2.408963
O	0.621136	3.029309	-1.012977
H	1.454233	3.288957	-1.452199
H	0.059736	2.673124	-1.763157
O	1.924061	-2.000751	0.973971
H	2.701968	-2.592792	0.979102
H	1.964672	-1.484505	1.843758
O	0.233628	-0.549601	-2.826918
H	0.493070	-1.041415	-3.630866
H	-0.464730	-1.118135	-2.358330
O	-0.918540	-0.718201	2.681990
H	-0.921024	-1.541359	2.047701
H	-1.557848	-0.914471	3.394844
O	1.640528	-0.411989	3.060576
H	1.959846	-0.657368	3.951331
H	0.627953	-0.536816	3.084465
O	-0.954317	1.783855	-2.806806
H	-0.477084	0.908811	-2.999639
H	-1.226193	2.142515	-3.674798
O	-0.973342	1.336447	0.955498
H	-1.683843	1.134587	0.287903
H	-1.064547	0.614240	1.641299
O	1.736188	0.121776	-0.676887
H	1.287119	-0.193647	-1.507775
H	1.879326	-0.704801	-0.133564
O	-1.612568	-1.682492	-1.344323
H	-2.146729	-0.823219	-1.238037
H	-2.222332	-2.308909	-1.783949
O	-0.694080	-2.660901	1.019861
H	-1.043827	-2.307400	0.150406
H	0.300069	-2.570246	0.935559
Li	0.814879	1.543091	0.251499

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O	-2.128191	0.851262	-1.552062
H	-1.725653	1.714297	-1.200321
H	-2.825913	1.127834	-2.179386
O	1.018945	1.075973	2.376963
H	1.517339	1.368510	3.165320
H	1.046446	0.057160	2.384224
O	3.082804	0.512467	-2.772291
H	2.828407	0.089922	-3.616968
H	3.980311	0.159602	-2.610460
O	-2.776233	-0.237961	0.827744
H	-2.649072	0.116970	-0.103478
H	-2.359571	0.483417	1.383864
O	0.154167	-0.296606	-2.438978
H	0.000593	-1.252681	-2.199858
H	-0.712519	0.135786	-2.192357
O	-0.039955	-2.752975	-1.358484
H	-0.216576	-3.654470	-1.689629
H	-0.570113	-2.653572	-0.503138
O	-1.449775	1.814979	1.988437
H	-0.509889	1.559033	2.284333
H	-1.825322	2.352970	2.713308
O	2.185001	-1.518323	-0.438137
H	1.500763	-2.142151	-0.813206
H	1.925067	-1.498418	0.526281
O	-0.872229	2.809891	-0.366326
H	-1.067916	3.759439	-0.492320
H	-1.156868	2.587510	0.582426
O	1.599610	1.678980	-0.213051
H	0.753202	2.179508	-0.383139
H	1.531625	1.492821	0.765571
O	-1.185482	-2.219907	0.963928
H	-1.666696	-2.945899	1.408961
H	-1.861374	-1.416500	0.918931
O	1.077810	-1.491466	2.032527
H	1.373076	-2.120822	2.720247
H	0.163836	-1.823148	1.719469
Li	1.742748	0.148808	-1.385695

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O	-2.440105	1.182638	-0.465315
H	-2.397517	0.477478	-1.192965
H	-3.263775	1.683031	-0.631777
O	0.155842	0.122049	2.680669
H	0.154427	0.012750	3.652931
H	0.879079	-0.506949	2.335282
O	-0.032500	2.290706	-0.770735
H	0.262750	2.502558	0.161397
H	-0.981523	1.973909	-0.679014
O	1.996117	-1.325178	1.515146
H	1.576754	-1.979275	0.857476
H	2.641046	-1.839163	2.040073
O	0.724174	-0.684552	-2.148304
H	-0.263685	-0.698745	-2.294780
H	0.868076	-1.494108	-1.580520
O	-1.762664	-2.429205	-0.035199
H	-1.976456	-1.722293	0.708771
H	-2.365417	-3.183994	0.117160

O	1.052954	2.388476	1.656212
H	1.307499	3.068170	2.309850
H	0.682699	1.608758	2.182141
O	0.808515	-2.704397	-0.338316
H	-0.196203	-2.737313	-0.169954
H	1.075283	-3.617254	-0.565350
O	-2.236409	-0.543044	1.614840
H	-2.399971	0.177443	0.937484
H	-1.358011	-0.285458	2.026649
O	1.718424	2.422316	-2.753490
H	1.009219	2.820109	-2.181437
H	2.514263	2.945385	-2.534605
O	-1.981560	-0.823026	-2.094335
H	-2.010883	-1.554067	-1.389339
H	-2.589555	-1.109404	-2.804664
O	2.624331	0.860323	0.056341
H	2.537476	-0.005970	0.546700
H	2.236104	1.506735	0.711646
Li	1.343392	0.954630	-1.401023

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O	-0.755499	-0.139681	-4.057737
H	-0.270955	-0.782680	-4.611969
H	-0.076398	0.551683	-3.850815
O	-2.399808	-1.685589	1.003170
H	-3.098042	-2.320936	1.257057
H	-1.523741	-2.207429	1.008005
O	0.024564	-2.630997	0.954752
H	0.231399	-3.526293	1.288852
H	0.451420	-1.965822	1.632741
O	2.269911	0.884305	1.061022
H	1.704671	1.648492	0.693767
H	3.009712	1.318308	1.531730
O	0.803017	1.165886	-2.302116
H	0.708482	1.870573	-1.598542
H	1.676758	0.735923	-2.062953
O	0.700693	2.655553	-0.064727
H	-0.233801	2.529896	0.314343
H	0.909690	3.605497	0.035408
O	0.892481	-0.858712	2.598669
H	0.015187	-0.404516	2.751478
H	1.418410	-0.193355	2.062369
O	-2.071910	0.013465	-1.070442
H	-1.984745	0.822515	-0.489351
H	-2.337655	-0.692886	-0.418558
O	2.800304	-0.277116	-1.253909
H	2.749928	0.133350	-0.331269
H	3.748680	-0.315539	-1.485586
O	-1.608540	0.219015	2.620158
H	-2.120380	0.305036	3.449168
H	-2.045797	-0.541510	2.103631
O	-1.691907	2.011860	0.725165
H	-2.393858	2.680420	0.853432
H	-1.701148	1.430472	1.560154
O	0.634146	-1.857554	-1.537227
H	0.441956	-2.237916	-0.629439
H	1.535186	-1.442332	-1.428899
Li	-0.489114	-0.386361	-2.064578

Li – 16 water molecules

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O	3.377019	1.253820	-0.968564
H	3.509326	1.854219	-1.717762
H	3.263172	1.853398	-0.190189
O	-2.089830	-2.185850	0.827756
H	-1.172737	-2.577484	0.853302
H	-2.697092	-2.876934	1.131999
O	-0.517661	1.753003	3.316198
H	-1.063749	2.104963	4.035212
H	-1.118171	1.190720	2.758996
O	0.079631	3.289969	1.023207
H	-0.225286	2.817629	1.828856
H	1.053814	3.150772	1.028339
O	-2.108084	-1.096383	-1.691711
H	-2.592655	-0.254114	-1.533422
H	-2.136351	-1.548536	-0.814298
O	-0.980271	2.788810	-1.317585
H	-0.578957	2.974179	-0.411280
H	-1.098341	3.653161	-1.740534
O	-0.276131	-2.495442	-3.017937
H	-0.363241	-2.543308	-3.982303
H	-1.051295	-1.967559	-2.701001
O	-1.766000	0.392576	1.433603
H	-2.322718	0.799957	0.723472
H	-1.975545	-0.572026	1.386306
O	2.810287	2.739568	1.238030
H	2.701508	2.088043	1.971571
H	3.349265	3.454274	1.611401
O	0.385994	-3.112024	0.557111

H	0.835641	-3.549750	1.296685
H	0.239604	-3.830166	-0.124289
O	0.255870	0.597670	-2.386926
H	-0.142273	1.462149	-2.119950
H	-0.462292	-0.038300	-2.192130
O	1.993194	0.879434	3.059048
H	1.100942	1.154510	3.389512
H	2.281957	0.143439	3.619016
O	1.827823	-1.731707	-1.375402
H	1.205167	-1.988170	-2.091037
H	1.399276	-2.104278	-0.570670
O	-0.085444	-4.730991	-1.480461
H	0.738917	-5.143078	-1.782885
H	-0.237566	-4.006703	-2.137565
O	-3.045311	1.266203	-0.748958
H	-3.902837	1.715649	-0.690184
H	-2.383133	1.958615	-1.024200
O	0.881290	0.212386	0.649408
H	1.323524	0.333596	1.515564
H	-0.078564	0.313270	0.839470
Li	1.666646	0.189288	-1.068309

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O	3.478801	0.629694	-0.888767
H	3.778456	0.855334	-1.781778
H	3.352804	1.503820	-0.445323
O	-1.730869	-3.589100	-0.271816
H	-1.064071	-3.696690	-1.003421
H	-2.091343	-4.477953	-0.123903
O	-0.317670	2.339211	2.922182
H	-0.930284	2.713176	3.573654
H	-0.646102	1.426350	2.724297
O	0.134122	3.609448	0.492133
H	-0.084029	3.210351	1.365832
H	1.097854	3.445860	0.378345
O	-3.318787	-1.761991	-1.551041
H	-3.184016	-0.962887	-0.986586
H	-2.881928	-2.483703	-1.041477
O	-1.357274	2.283863	-1.214715
H	-0.800977	2.840475	-0.585832
H	-1.750809	2.899223	-1.851997
O	-1.264468	-1.410971	-3.159209
H	-1.526228	-1.265300	-4.081287
H	-2.117099	-1.517665	-2.633662
O	-1.001340	-0.073513	1.937606
H	-1.660260	0.046950	1.207230
H	-0.791284	-1.039906	1.969594
O	2.887616	3.022015	0.409278
H	2.867987	2.832672	1.377845
H	3.438547	3.814958	0.318284
O	-0.115198	-2.586864	1.597760
H	0.094654	-3.230513	2.291592
H	-0.760282	-3.043202	0.995748
O	0.419870	0.331368	-1.951483
H	-0.197662	1.073617	-1.756656
H	-0.152603	-0.316015	-2.425187
O	2.354205	2.304915	2.944486
H	1.387632	2.361127	3.152839
H	2.772818	1.863640	3.698480
O	1.753946	-2.136489	-0.505667
H	1.270955	-2.646996	-1.194467
H	1.225339	-2.290096	0.309444
O	0.098516	-3.450835	-2.225738
H	0.307633	-4.173023	-2.837705
H	-0.365592	-2.751283	-2.762352
O	-2.795218	0.427958	-0.011342
H	-3.591684	0.819423	0.380717
H	-2.339119	1.175052	-0.492025
O	1.604934	0.210712	1.217759
H	1.977788	0.891088	1.813743
H	0.658447	0.142573	1.483940
Li	1.738749	-0.190108	-0.654153

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O	3.402355	1.266580	-0.365114
H	3.194187	1.739067	-1.187457
H	3.255312	1.941580	0.343034
O	-2.210206	-2.575227	1.277779
H	-1.348605	-2.924920	0.928982
H	-2.539723	-3.236133	1.905518
O	-0.775028	1.906247	3.101312
H	-1.430975	2.322434	3.680289
H	-1.233239	1.149182	2.646750
O	0.075324	3.145886	0.737905
H	-0.319289	2.754476	1.549232
H	1.040786	3.151868	0.928974
O	-3.149050	-1.837780	-1.225130
H	-2.990981	-2.166894	-0.312067
H	-3.019811	-0.862693	-1.160549
O	-0.821153	2.405480	-1.601212
H	-0.468883	2.725429	-0.713183
H	-1.014426	3.200012	-2.122104

O	0.959134	-1.640621	-3.473696
H	1.166282	-1.935986	-4.372925
H	0.125108	-2.111660	-3.215727
O	-1.606019	-0.003792	1.511862
H	-2.066666	0.326486	0.699630
H	-1.894405	-0.945066	1.614632
O	2.720233	2.991540	1.564160
H	2.523451	2.431705	2.358666
H	3.194555	3.771541	1.889902
O	0.068622	-3.270152	-0.021042
H	0.322114	-4.197356	0.115989
H	-0.339519	-3.257829	-0.929938
O	1.236306	0.743604	-2.213169
H	0.455886	1.338809	-2.130862
H	0.991197	0.017043	-2.827264
O	1.778937	1.281764	3.353871
H	0.827540	1.520725	3.502813
H	2.099255	0.858699	4.164440
O	2.295907	-1.954627	-1.084258
H	1.969159	-1.974311	-2.012885
H	1.590424	-2.424056	-0.583528
O	-1.106223	-2.950889	-2.409987
H	-1.411291	-3.762476	-2.845154
H	-1.936505	-2.500862	-2.052170
O	-2.763437	0.822076	-0.803095
H	-3.550525	1.362342	-0.631033
H	-2.088056	1.441024	-1.201364
O	1.099430	-0.197110	1.140668
H	1.428268	0.263367	1.943166
H	0.116538	-0.157052	1.213836
Li	1.940590	-0.032945	-0.551951

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O	3.353399	0.792016	0.125320
H	3.705780	1.098461	-0.723635
H	3.279951	1.612909	0.671956
O	-2.878694	-2.179575	0.545430
H	-2.045205	-2.700527	0.376681
H	-3.483137	-2.776311	1.012661
O	-0.578081	1.895483	2.771355
H	-1.188355	2.409358	3.322002
H	-1.123874	1.190686	2.330762
O	0.472456	3.268114	0.635375
H	0.029027	2.823871	1.395297
H	1.422430	3.264565	0.886215
O	-3.173177	-1.147190	-1.967670
H	-3.114696	-0.198880	-1.703471
H	-3.185110	-1.612724	-1.098372
O	-0.336875	2.424659	-1.675411
H	0.006448	2.801646	-0.804023
H	-0.229172	3.127714	-2.334602
O	-0.817452	-1.299167	-3.074749
H	-0.928120	-1.005920	-3.992234
H	-1.737563	-1.275976	-2.660619
O	-1.666132	0.089509	1.207610
H	-1.981832	0.578317	0.405609
H	-2.190191	-0.748330	1.190768
O	2.985596	2.934954	1.686259
H	2.743268	2.382893	2.473639
H	3.751953	3.468717	1.945858
O	-0.558144	-3.376508	0.063255
H	-0.562045	-4.269753	0.441658
H	-0.283866	-3.509147	-0.880287
O	1.119152	0.156945	-1.788498
H	0.694214	1.047216	-1.789864
H	0.438850	-0.397233	-2.236993
O	1.916014	1.199247	3.392218
H	0.973008	1.505039	3.380352
H	2.112551	0.957504	4.310337
O	2.125021	-2.410046	-0.363863
H	1.851352	-2.793295	-1.223917
H	1.358427	-2.635307	0.199565
O	0.565624	-3.420691	-2.428680
H	0.394238	-4.199278	-2.979616
H	0.022834	-2.683971	-2.821321
O	-2.626910	1.348366	-1.009790
H	-3.269237	2.036298	-0.775994
H	-1.827760	1.831665	-1.365048
O	1.002731	-0.646657	1.538734
H	1.353447	-0.075512	2.255049
H	0.052172	-0.412767	1.430352
Li	1.889827	-0.434865	-0.158572

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O	2.921614	1.227598	-1.528900
H	2.609552	1.833631	-2.218198
H	3.140360	1.817443	-0.767577
O	-2.103607	-2.410301	1.491512
H	-1.188501	-2.753771	1.249563
H	-2.388969	-2.921176	2.264196
O	0.140088	1.644087	3.179372
H	-0.298232	2.161572	3.871303

H	-0.553206	1.051155	2.783747
O	0.477746	3.004715	0.757275
H	0.307898	2.587733	1.631682
H	1.456179	2.969711	0.656691
O	-3.555763	-1.499240	-0.646354
H	-3.538743	-0.534103	-0.455269
H	-3.139228	-1.915167	0.144321
O	-1.050813	2.333107	-1.255749
H	-0.452369	2.593517	-0.487768
H	-1.211164	3.152130	-1.750406
O	-1.716320	-1.634676	-2.495125
H	-2.185003	-1.772303	-3.333404
H	-2.438433	-1.591371	-1.790804
O	-1.398388	0.160723	1.678193
H	-2.084518	0.599952	1.113428
H	-1.711695	-0.776120	1.779364
O	3.220975	2.677110	0.729189
H	3.762564	3.426411	1.019732
H	3.182970	2.044465	1.489238
O	0.349473	-3.056079	0.811849
H	0.287908	-3.269066	-0.149835
H	0.728817	-2.145494	0.817438
O	0.212497	0.308002	-2.522623
H	-0.250281	1.103760	-2.163546
H	-0.501349	-0.370284	-2.572789
O	2.562084	0.808865	2.537789
H	1.750350	1.119028	3.014247
H	3.061534	0.266611	3.167121
O	2.398505	-1.770493	-1.856973
H	2.764725	-1.624821	-2.741829
H	1.658789	-2.417006	-1.987447
O	0.234011	-3.300516	-1.904597
H	0.165837	-4.153519	-2.359575
H	-0.551625	-2.757508	-2.194612
O	-3.149615	1.160523	-0.094316
H	-3.786748	1.811531	0.237716
H	-2.466090	1.674567	-0.606188
O	1.020876	-0.394381	0.619120
H	1.641463	-0.054474	1.309516
H	0.119710	-0.101204	0.914677
Li	1.581874	-0.128667	-1.237468

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O	3.242884	0.906154	-0.618629
H	3.536120	1.259746	-1.480178
H	3.084498	1.725084	-0.058575
O	-1.702526	-2.208757	0.768794
H	-0.838630	-2.746617	0.686856
H	-2.405009	-2.863379	0.952828
O	-0.617888	2.174721	3.028298
H	-1.115751	2.411542	3.835421
H	-1.124797	1.411521	2.594531
O	0.042719	3.874767	1.014909
H	-0.297558	3.342184	1.791214
H	1.009670	3.610240	0.971005
O	-1.916104	-1.075438	-1.652876
H	-2.457312	-0.255500	-1.456816
H	-1.856215	-1.538000	-0.759086
O	-0.997039	2.851158	-1.090110
H	-0.581864	3.283411	-0.238705
H	-1.099756	3.575411	-1.738766
O	-0.231240	-2.469591	-3.120955
H	-0.312341	-2.388613	-4.091874
H	-0.960982	-1.894088	-2.736459
O	-1.720051	0.311553	1.581982
H	-2.229055	0.674299	0.791033
H	-1.782577	-0.685014	1.484043
O	2.588997	2.924750	1.028330
H	2.448065	2.363919	1.861810
H	3.252939	3.595156	1.287560
O	0.431548	-3.589552	0.210798
H	0.827902	-4.191950	0.871174
H	0.083242	-4.188897	-0.545993
O	0.273104	0.608509	-1.882677
H	-0.130580	1.491757	-1.640416
H	-0.492440	-0.024397	-1.800457
O	1.866145	1.344690	2.987462
H	0.934692	1.677479	3.207471
H	2.314847	1.181710	3.840168
O	1.874407	-1.953650	-1.431084
H	1.228175	-2.061339	-2.180383
H	1.473974	-2.546365	-0.733400
O	-0.490879	-4.828291	-1.885956
H	0.219545	-5.410776	-2.222657
H	-0.419168	-4.010266	-2.470438
O	-2.915296	1.172025	-0.644643
H	-3.808578	1.560420	-0.564195
H	-2.280245	1.941511	-0.857747
O	0.915994	-0.310637	1.065330
H	1.360057	0.143610	1.830641
H	-0.028133	-0.003243	1.137268
Li	1.610820	-0.140498	-0.711343

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O	3.419318	0.770509	-0.938001
H	3.698422	1.009596	-1.842688
H	3.235251	1.657240	-0.504275
O	-1.718925	-3.568739	-0.226032
H	-1.017861	-3.717918	-0.949307
H	-2.099312	-4.450741	-0.041828
O	-0.203390	2.272088	3.032180
H	-0.681356	2.663836	3.789374
H	-0.639450	1.377269	2.855864
O	0.074365	3.583011	0.633146
H	-0.093600	3.150981	1.518400
H	1.051103	3.429264	0.483319
O	-3.095406	-1.663293	-1.584285
H	-2.991699	-0.872749	-0.971368
H	-2.737506	-2.421828	-1.039820
O	-1.133033	2.117869	-1.087298
H	-0.621968	2.695665	-0.384124
H	-1.588742	2.761153	-1.666059
O	-1.102506	-1.531426	-3.193517
H	-1.417057	-1.576429	-4.118190
H	-1.959028	-1.544130	-2.599645
O	-1.242579	-0.028691	2.237870
H	-1.870358	0.116742	1.460143
H	-0.875998	-0.958328	2.105351
O	2.766895	3.037218	0.392479
H	2.807781	2.695913	1.335715
H	3.372351	3.805766	0.380727
O	-0.183500	-2.368860	1.540928
H	0.084253	-2.995302	2.242714
H	-0.830481	-2.892089	0.959262
O	0.547903	0.420543	-2.340757
H	-0.080017	1.075244	-1.915037
H	-0.059127	-0.272200	-2.728403
O	2.387461	1.927377	2.768150
H	1.446410	2.089625	3.093220
H	2.829394	1.370630	3.437358
O	1.716682	-2.031199	-0.449196
H	1.283206	-2.640084	-1.108660
H	1.110457	-2.096546	0.340694
O	0.135551	-3.519424	-2.070649
H	0.337981	-4.280237	-2.649959
H	-0.307797	-2.815658	-2.661593
O	-2.708958	0.422642	0.068168
H	-3.554182	0.870030	0.275753
H	-2.138242	1.135410	-0.403562
O	1.026611	0.606616	0.772178
H	1.627296	0.928275	1.491630
H	0.194408	0.359166	1.250619
Li	1.664450	-0.124035	-0.865791

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O	3.739154	0.797293	0.036318
H	4.172743	1.073633	-0.793871
H	3.375362	1.653702	0.413460
O	-2.087539	-2.608279	1.144618
H	-1.218623	-2.970643	0.766403
H	-2.442615	-3.315520	1.718652
O	-0.863952	2.068120	2.851100
H	-1.502204	2.350611	3.535403
H	-1.220607	1.197225	2.467739
O	-0.091096	3.611359	0.753889
H	-0.473047	3.122075	1.540232
H	0.893163	3.437392	0.834959
O	-3.204381	-1.916716	-1.237990
H	-2.949437	-2.247139	-0.327708
H	-3.036109	-0.932554	-1.164716
O	-0.856960	2.373894	-1.350234
H	-0.555077	2.903717	-0.502812
H	-1.076720	3.050634	-2.021501
O	0.775585	-1.403134	-3.355230
H	1.046107	-1.647203	-4.261187
H	-0.032407	-1.969098	-3.140767
O	-1.475491	-0.074195	1.525759
H	-1.958815	0.229061	0.689908
H	-1.765786	-1.030119	1.631427
O	2.520908	2.924454	1.161498
H	2.299725	2.453627	2.033386
H	3.072156	3.688599	1.425260
O	0.081177	-3.383346	-0.164291
H	0.292910	-4.332864	-0.056208
H	-0.382757	-3.329398	-1.068876
O	1.257146	0.815683	-1.899338
H	0.461036	1.403940	-1.753224
H	0.956732	0.118185	-2.541807
O	1.668751	1.489899	3.173766
H	0.692990	1.747146	3.257896
H	2.030573	1.460644	4.081075
O	2.250719	-1.967059	-1.139774
H	1.835244	-1.853238	-2.041371
H	1.550291	-2.480358	-0.649763

O	-1.169942	-2.912314	-2.429217
H	-1.461066	-3.695518	-2.937646
H	-2.037660	-2.491786	-2.032502
O	-2.691949	0.685762	-0.701710
H	-3.505398	1.184436	-0.485284
H	-2.023269	1.387459	-1.037418
O	1.191834	-0.409589	1.273296
H	1.461053	0.166259	2.036831
H	0.192580	-0.338204	1.280780
Li	2.057853	-0.128006	-0.412666

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O	3.567599	0.441183	0.008935
H	4.025770	0.740696	-0.799356
H	3.374234	1.290160	0.508840
O	-2.505725	-2.145374	0.529938
H	-1.660456	-2.715035	0.461010
H	-3.182937	-2.723206	0.933834
O	-0.795813	2.155051	2.808815
H	-1.393170	2.509008	3.496905
H	-1.287690	1.383606	2.371786
O	0.403894	3.639616	0.860883
H	-0.118635	3.188781	1.585385
H	1.344101	3.334352	1.034607
O	-3.015574	-1.044080	-1.889409
H	-2.929546	-0.084374	-1.617919
H	-2.904348	-1.527387	-1.016180
O	-0.235267	2.522628	-1.354368
H	0.041508	2.987987	-0.464325
H	-0.183485	3.215074	-2.043088
O	-0.767581	-1.369406	-3.072442
H	-0.920002	-1.227575	-4.027813
H	-1.697736	-1.250975	-2.618874
O	-1.741069	0.249897	1.319465
H	-2.069217	0.718455	0.486773
H	-2.123211	-0.677628	1.235351
O	2.827567	2.584837	1.451686
H	2.485394	2.077652	2.259528
H	3.497905	3.204596	1.803165
O	-0.315464	-3.535811	0.223593
H	-0.342896	-4.436207	0.604851
H	-0.156747	-3.682060	-0.767260
O	1.097942	0.257032	-1.988109
H	0.606859	1.100031	-1.772516
H	0.410267	-0.328479	-2.418340
O	1.582946	1.147155	3.236235
H	0.658752	1.559646	3.278245
H	1.809916	0.870011	4.145260
O	2.157607	-2.434913	-0.548294
H	1.788175	-2.864282	-1.365040
H	1.444666	-2.671355	0.098131
O	0.423563	-3.545569	-2.301519
H	0.303340	-4.304882	-2.904392
H	-0.090188	-2.767367	-2.711576
O	-2.529215	1.423857	-0.925906
H	-3.230290	2.092441	-0.794246
H	-1.678355	1.940094	-1.170035
O	0.859380	-0.515961	1.204451
H	1.204633	-0.018023	1.993574
H	-0.104216	-0.246076	1.172672
Li	1.896962	-0.481301	-0.405823

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O	2.901128	1.193971	-1.569080
H	2.225449	1.547677	-2.183134
H	2.923858	1.866449	-0.821309
O	-2.058122	-2.384272	1.355449
H	-1.150552	-2.838750	1.144635
H	-2.467251	-2.905432	2.074291
O	0.119660	1.794083	3.011627
H	-0.193195	1.954960	3.923380
H	-0.482660	1.072683	2.619404
O	0.271415	3.561179	0.956516
H	0.108959	3.015204	1.779005
H	1.243920	3.388926	0.781551
O	-3.418949	-1.406686	-0.764419
H	-3.360078	-0.434044	-0.542529
H	-2.996985	-1.850925	0.030424
O	-0.999769	2.553682	-1.030903
H	-0.480566	2.970931	-0.228539
H	-1.204955	3.299066	-1.629966
O	-1.551614	-1.582655	-2.510031
H	-1.971110	-1.660290	-3.390201
H	-2.341079	-1.525362	-1.832482
O	-1.179258	0.071875	1.594963
H	-1.871209	0.530422	1.013969
H	-1.551200	-0.862283	1.715026
O	2.828784	2.768764	0.580493
H	3.553073	3.393395	0.785417
H	2.855248	2.070835	1.314927
O	0.292604	-3.279760	0.785164
H	0.227635	-3.465919	-0.199610

H	0.751847	-2.388129	0.808033
O	0.202249	0.437992	-2.210128
H	-0.258607	1.226192	-1.803601
H	-0.515728	-0.240844	-2.374351
O	2.465876	0.854967	2.339145
H	1.626228	1.210168	2.787245
H	3.063238	0.568993	3.058372
O	2.265253	-1.885479	-2.199763
H	3.024539	-2.349018	-1.795173
H	1.525124	-2.568304	-2.166503
O	0.143469	-3.454653	-1.887861
H	-0.000091	-4.283513	-2.385260
H	-0.587792	-2.808896	-2.189142
O	-2.933660	1.164447	-0.037672
H	-3.602432	1.731820	0.394195
H	-2.276073	1.797041	-0.501113
O	1.171766	-0.718984	0.611900
H	1.765029	-0.285693	1.296655
H	0.259573	-0.359907	0.857102
Li	1.674750	-0.319714	-1.219191

Li – 20 water molecules

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O	3.030852	2.516043	1.000321
H	3.755158	3.158109	1.050387
H	3.401522	1.697183	0.574361
O	-0.088127	-0.186219	-0.122204
H	0.606963	-0.005505	-0.806282
H	0.358447	-0.476241	0.720221
O	-1.656324	-1.347845	-3.181861
H	-2.094798	-1.399341	-2.298833
H	-1.657280	-0.383477	-3.381954
O	3.699031	0.262232	-0.232480
H	4.597052	0.212590	-0.596398
H	3.562540	-0.586640	0.275094
O	-2.967167	-0.001181	2.865699
H	-3.452226	0.057313	3.702890
H	-2.376871	-0.818368	2.936500
O	0.844542	-2.041343	-2.668901
H	1.160519	-2.547956	-3.432920
H	-0.110907	-1.802456	-2.884660
O	0.618615	2.992343	-0.102949
H	0.656542	3.034616	-1.083847
H	1.549160	2.908178	0.205913
O	-2.405172	-1.351044	-0.592630
H	-1.540638	-0.876564	-0.457079
H	-3.092701	-0.734559	-0.230066
O	-2.094405	2.067198	-0.903426
H	-2.885576	1.620824	-0.532408
H	-2.039632	1.775724	-1.843304
O	1.711480	0.384710	-2.044165
H	1.558456	-0.515510	-2.433764
H	2.530618	0.333074	-1.489587
O	-1.289058	-1.995027	3.010583
H	-1.366240	-2.602572	2.236305
H	-0.426796	-1.543043	2.849661
O	-1.114540	1.866728	2.199949
H	-1.729610	1.210474	2.602708
H	-0.279593	1.856497	2.712512
O	3.042130	-1.932481	1.103333
H	2.406412	-2.512459	0.571703
H	3.688752	-2.527904	1.512192
O	-3.974939	0.542402	0.476036
H	-4.933522	0.408335	0.422981
H	-3.723965	0.346818	1.419404
O	-1.308378	-3.366478	0.678432
H	-1.855667	-2.695354	0.185296
H	-1.761475	-4.215219	0.555970
O	0.617080	2.637724	-2.855173
H	1.135889	1.808087	-2.672939
H	1.155335	3.156756	-3.472498
O	1.278147	-3.288082	-0.262008
H	1.114596	-2.856609	-1.134929
H	0.380383	-3.333301	0.143747
O	1.497789	1.816805	3.072351
H	1.964300	1.879254	3.920100
H	2.136435	2.151715	2.389496
O	-1.667259	1.395424	-3.484458
H	-2.254049	1.901889	-4.067419
H	-0.826250	1.921021	-3.425012
O	0.983641	-0.717930	2.245756
H	1.241443	0.168420	2.607464
H	1.826411	-1.191777	2.033028
Li	-0.682018	1.664861	0.326585

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O	2.769518	2.750534	0.538524
H	2.543763	2.508269	1.466738
H	3.120831	1.907581	0.175594

O	-0.149706	0.209773	-0.153081
H	0.452541	0.303670	-0.941571
H	0.435707	-0.125625	0.580129
O	-1.712990	-0.915118	-3.051175
H	-2.091350	-1.152349	-2.173094
H	-1.790357	0.068160	-3.069496
O	3.640462	0.347627	-0.552653
H	4.515899	0.368277	-0.970664
H	3.549487	-0.569538	-0.182121
O	-2.308724	0.058160	3.076994
H	-2.715061	0.180898	3.949176
H	-1.730784	-0.748702	3.163305
O	0.649682	-2.078118	-2.773011
H	0.874036	-2.535617	-3.598334
H	-0.253347	-1.665922	-2.930780
O	0.322683	3.117895	-0.607146
H	0.435759	3.003200	-1.577256
H	1.236124	3.009891	-0.230862
O	-2.243417	-1.367265	-0.420718
H	-1.439132	-0.780829	-0.343302
H	-2.960661	-0.845183	0.021830
O	-2.663344	2.413202	-0.244821
H	-3.253290	1.707644	0.105565
H	-2.549225	2.225669	-1.204755
O	1.573996	0.338017	-2.193168
H	1.411283	-0.583013	-2.523101
H	2.428126	0.330298	-1.684092
O	-0.579882	-1.972317	3.116853
H	-0.842304	-2.606397	2.390264
H	-0.449055	-2.514946	3.910595
O	-0.705291	2.096249	2.304037
H	-1.226916	1.363819	2.707593
H	0.207685	2.017673	2.661327
O	3.093101	-2.088219	0.424789
H	2.359402	-2.676397	0.049019
H	3.707598	-2.680277	0.885310
O	-3.873411	0.296172	0.922726
H	-4.808224	0.103255	1.090432
H	-3.406128	0.200253	1.794448
O	-1.170112	-3.337292	0.962155
H	-1.696297	-2.663267	0.439114
H	-1.722286	-4.134795	0.993762
O	0.581432	2.510980	-3.235896
H	1.074907	1.679089	-2.997929
H	1.150959	3.018629	-3.832813
O	1.131665	-3.513677	-0.495471
H	0.902889	-3.068635	-1.346545
H	0.296770	-3.494126	0.028554
O	1.940127	1.731409	2.910853
H	1.872320	0.786027	2.606163
H	2.410721	1.707391	3.758215
O	-2.005127	1.837355	-2.900677
H	-2.599758	2.184762	-3.583169
H	-1.107796	2.175218	-3.148390
O	1.401040	-0.639403	1.869815
H	0.791419	-1.198016	2.415812
H	2.084010	-1.244604	1.477486
Li	-0.839472	1.977349	0.370280
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O	3.301476	2.174031	0.809524
H	4.120755	2.683245	0.905679
H	3.547615	1.327522	0.350542
O	-0.124589	-0.022993	-0.025939
H	0.554414	0.029583	-0.749501
H	0.279075	-0.506355	0.748428
O	-1.793425	-0.673672	-3.323449
H	-2.249649	-0.827967	-2.452285
H	-2.423655	-0.959390	-4.003251
O	3.703294	-0.161151	-0.448631
H	4.573899	-0.297326	-0.854481
H	3.472520	-1.026482	-0.007581
O	-2.611335	0.131498	2.965158
H	-2.166480	-0.770119	3.035886
H	-3.068645	0.262153	3.810288
O	0.523638	-1.986842	-2.952010
H	0.809685	-2.474100	-3.740320
H	-0.355540	-1.583805	-3.189668
O	0.895175	3.193831	0.064704
H	0.913361	3.202377	-0.921292
H	1.806483	2.918302	0.315239
O	-2.514293	-0.932704	-0.791885
H	-1.629356	-0.557150	-0.525884
H	-3.173630	-0.358516	-0.320068
O	-2.094967	2.526163	-0.192265
H	-2.859577	1.991162	0.116634
H	-2.065578	2.384080	-1.175437
O	1.610224	0.279942	-2.071308
H	1.358921	-0.546940	-2.555738
H	2.468443	0.097290	-1.611523
O	-1.313992	-2.169996	3.053445
H	-1.581485	-2.592705	2.201991

H	-0.413012	-1.825573	2.845687
O	-0.620965	1.957382	2.468019
H	-1.266016	1.280219	2.778216
H	0.256209	1.726544	2.843334
O	2.818255	-2.397039	0.670428
H	2.036774	-2.807870	0.176957
H	3.375658	-3.129927	0.973098
O	-3.934039	0.736444	0.729872
H	-4.898334	0.764635	0.820913
H	-3.565432	0.489010	1.621220
O	-1.803462	-3.080020	0.547878
H	-2.215228	-2.338141	0.026059
H	-2.346037	-3.861175	0.356891
O	0.858184	2.772466	-2.629513
H	1.231441	1.855404	-2.542072
H	1.401462	3.217397	-3.297740
O	0.724305	-3.294603	-0.566360
H	0.630881	-2.858489	-1.445478
H	-0.174836	-3.242145	-0.164550
O	1.982256	1.299201	2.964086
H	2.519017	1.318471	3.771289
H	2.557110	1.675189	2.245145
O	-1.793811	2.100254	-2.846490
H	-0.852951	2.384665	-2.910418
H	-1.779062	1.143263	-3.068415
O	1.022118	-1.087111	2.139374
H	1.435759	-0.271525	2.521790
H	1.764537	-1.630044	1.775023
Li	-0.455869	1.885793	0.553383

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O	3.118856	2.538936	0.906900
H	2.773839	2.239839	1.780088
H	3.394560	1.696965	0.476464
O	0.143733	-0.143803	0.117207
H	0.662675	0.032099	-0.710334
H	-0.721947	-0.561801	-0.133197
O	-1.791814	-0.620862	-3.116532
H	-2.406122	-0.912685	-3.807614
H	-1.774273	0.376099	-3.165253
O	3.691200	0.185569	-0.378199
H	4.590578	0.097800	-0.730455
H	3.476016	-0.700372	0.030537
O	-2.526937	-0.029494	3.035218
H	-2.973169	0.073379	3.890107
H	-2.043889	-0.911853	3.088032
O	0.588651	-1.911996	-2.846120
H	0.829069	-2.387283	-3.656497
H	-0.290279	-1.492720	-3.037580
O	0.724960	2.905889	-0.306470
H	0.814567	2.975803	-1.280553
H	1.645439	2.821747	0.054292
O	-2.257436	-1.091420	-0.556210
H	-2.972351	-0.540435	-0.145011
H	-2.260812	-0.942216	-1.537325
O	-2.115455	2.312685	-0.188741
H	-2.888950	1.772767	0.086729
H	-2.076331	2.252163	-1.169609
O	1.650204	0.397828	-2.067422
H	1.471644	-0.468369	-2.507792
H	2.503844	0.311060	-1.565800
O	-1.123356	-2.269039	3.121198
H	-1.322740	-2.722277	2.265448
H	-0.222688	-1.896015	2.976273
O	-0.641364	1.878768	2.473829
H	0.221054	1.753654	2.928329
H	-1.255813	1.186222	2.811439
O	2.937857	-2.116440	0.692740
H	2.179560	-2.591480	0.219746
H	3.610271	-2.794555	0.860109
O	-3.882753	0.522513	0.801145
H	-4.843669	0.418298	0.868285
H	-3.505413	0.316001	1.699184
O	-1.516637	-3.256496	0.643058
H	-1.933458	-2.511796	0.127268
H	-2.048293	-4.044504	0.451297
O	0.851312	2.716581	-2.997192
H	1.269385	1.832724	-2.803180
H	1.448320	3.189231	-3.596104
O	0.968032	-3.315567	-0.500712
H	0.800054	-2.850037	-1.352290
H	0.095200	-3.318306	-0.040332
O	1.947207	1.496934	3.176815
H	1.808412	0.527249	2.996080
H	2.328198	1.541171	4.067677
O	-1.725262	2.024521	-2.937180
H	-2.302741	2.535311	-3.525591
H	-0.809239	2.375070	-3.097060
O	1.235923	-0.968861	2.421014
H	0.784998	-0.652261	1.592995
H	1.977260	-1.492775	2.028493
Li	-0.454938	1.718905	0.560220

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O	2.878478	2.435559	0.641409
H	3.466841	3.201160	0.736007
H	2.527811	2.267154	1.556788
O	-0.060863	0.075171	-0.078681
H	0.666283	0.152179	-0.756779
H	0.383062	-0.244240	0.753165
O	-1.592698	-1.009369	-3.279942
H	-2.021179	-1.170733	-2.407123
H	-1.665215	-0.027901	-3.350483
O	4.032033	0.158841	-0.331059
H	3.709721	0.967318	0.133659
H	3.754142	-0.602111	0.229652
O	-2.565031	-0.076196	2.948669
H	-3.017087	-0.010548	3.804375
H	-2.067419	-0.936160	2.976312
O	0.855922	-1.953263	-2.904768
H	1.156788	-2.336328	-3.742879
H	-0.067913	-1.594716	-3.080547
O	0.458230	3.039936	-0.581472
H	0.545866	2.879761	-1.549325
H	1.362822	2.879400	-0.223821
O	-2.347449	-1.119909	-0.686801
H	-1.502035	-0.628316	-0.501148
H	-3.057892	-0.602298	-0.229855
O	-2.424788	2.375920	-0.392582
H	-3.138237	1.793060	-0.048722
H	-2.357495	2.173929	-1.354265
O	1.888902	0.252400	-1.908948
H	1.701598	-0.610572	-2.360716
H	2.755101	0.179526	-1.414139
O	-0.984713	-2.252785	2.860704
H	-1.108178	-2.728951	1.991674
H	-0.979488	-2.940365	3.544814
O	-0.904839	2.000268	2.269770
H	-1.435763	1.258560	2.641608
H	-0.028969	1.972605	2.711680
O	3.019040	-1.994222	1.050726
H	2.432294	-2.520369	0.420625
H	3.586898	-2.638513	1.500556
O	-3.996666	0.478372	0.744118
H	-4.937540	0.252883	0.800949
H	-3.597129	0.244735	1.622518
O	-1.203643	-3.194151	0.402110
H	-1.763224	-2.486662	-0.030677
H	-1.659270	-4.032905	0.227365
O	0.750203	2.250423	-3.134349
H	1.310767	1.502782	-2.781847
H	1.317633	2.783136	-3.711303
O	1.361189	-3.236062	-0.540098
H	1.226181	-2.813158	-1.420456
H	0.453328	-3.235466	-0.155296
O	1.717228	1.777650	2.961253
H	1.558905	0.800576	2.837775
H	2.137641	1.873601	3.829933
O	-1.875651	1.717817	-3.083411
H	-2.379904	2.174447	-3.774125
H	-0.935723	2.002632	-3.214730
O	1.084925	-0.673878	2.245559
H	0.406411	-1.288531	2.624169
H	1.849603	-1.235476	1.942384
Li	-0.735687	1.882777	0.353402

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O	2.812038	2.392352	0.964915
H	3.547133	3.028711	1.070312
H	3.228795	1.564602	0.556630
O	-0.182150	0.203659	0.015938
H	0.537352	0.208997	-0.702366
H	0.238906	-0.176130	0.861598
O	-1.534293	-1.267451	-3.255039
H	-1.891239	-1.397189	-2.322252
H	-1.527235	-0.265431	-3.323429
O	3.679593	0.170634	-0.182761
H	4.604285	0.092832	-0.489884
H	3.455681	-0.709135	0.289299
O	-2.692194	0.115064	2.710385
H	-3.247703	0.214936	3.508919
H	-2.155203	-0.767170	2.863609
O	0.856279	-2.045978	-2.759249
H	1.250498	-2.431342	-3.566587
H	-0.111499	-1.753859	-3.021955
O	0.552443	3.285782	-0.298410
H	0.688243	3.137000	-1.276417
H	1.423158	3.009174	0.104649
O	-2.117722	-1.406830	-0.672127
H	-1.352947	-0.769191	-0.435961
H	-2.924845	-0.910169	-0.317010
O	-2.483808	2.250170	-0.684989
H	-3.110037	1.552424	-0.345397
H	-2.265347	1.951920	-1.615848

O	1.664609	0.248357	-1.862278
H	1.488716	-0.651806	-2.301890
H	2.534291	0.193826	-1.353097
O	-1.262932	-1.977244	3.083274
H	-1.340314	-2.586022	2.289726
H	-0.379553	-1.534595	2.892972
O	-1.086012	2.240786	2.239269
H	-1.641701	1.455494	2.518461
H	-0.204305	2.110893	2.682885
O	2.811230	-1.982156	0.963434
H	2.190087	-2.578727	0.358391
H	3.427982	-2.593449	1.412551
O	-3.902800	0.193216	0.405868
H	-4.859895	0.003048	0.457899
H	-3.546138	0.141526	1.360944
O	-1.183938	-3.351502	0.764128
H	-1.651671	-2.649950	0.181980
H	-1.703068	-4.171255	0.639356
O	0.758438	2.449655	-2.864295
H	1.241406	1.595212	-2.590441
H	1.260126	2.820782	-3.616870
O	1.240049	-3.389339	-0.454379
H	1.060228	-2.934844	-1.331695
H	0.345772	-3.426362	0.001416
O	1.449562	1.702751	3.100559
H	1.903943	1.878052	3.947717
H	2.069227	2.033145	2.368831
O	-1.646485	1.424385	-3.143599
H	-2.134849	1.838915	-3.882896
H	-0.731070	1.862196	-3.160115
O	0.901202	-0.707757	2.228969
H	1.213180	0.147720	2.667576
H	1.711634	-1.218676	1.910100
Li	-0.820073	2.036207	0.321499

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O	2.913042	2.536661	0.544235
H	2.618270	2.297748	1.469137
H	3.187848	1.665248	0.146874
O	-0.090486	0.311263	-0.042888
H	0.531640	0.339868	-0.848358
H	0.468324	-0.034320	0.730852
O	-1.892712	-1.201195	-3.061085
H	-2.111006	-1.336365	-2.088676
H	-1.899557	-0.198040	-3.124800
O	3.625950	0.174023	-0.680665
H	4.515135	0.113969	-1.081728
H	3.470005	-0.714031	-0.212298
O	-2.261248	0.162532	3.117014
H	-2.723629	0.231134	3.975665
H	-1.721070	-0.692973	3.169643
O	0.556921	-1.947052	-2.899691
H	0.839039	-2.329561	-3.754118
H	-0.440257	-1.666865	-3.029775
O	0.556953	3.396613	-0.370988
H	0.559024	3.277819	-1.359592
H	1.472614	3.069135	-0.086137
O	-2.072613	-1.338813	-0.411064
H	-1.283861	-0.693246	-0.306514
H	-2.818314	-0.847340	0.065822
O	-2.501727	2.323299	-0.393454
H	-3.055161	1.621750	0.047559
H	-2.402982	2.012317	-1.339733
O	1.482010	0.367777	-2.151111
H	1.236850	-0.534948	-2.547618
H	2.394172	0.280969	-1.718243
O	-0.690503	-1.954221	3.053269
H	-0.867220	-2.594168	2.276935
H	-0.558211	-2.513304	3.844861
O	-0.791087	2.315682	2.315299
H	-1.288701	1.542999	2.704502
H	0.141846	2.205673	2.656478
O	2.909916	-2.025357	0.541850
H	2.236593	-2.625323	0.002834
H	3.575459	-2.631877	0.922570
O	-3.696892	0.247378	0.916739
H	-4.644551	0.057753	1.062665
H	-3.256550	0.205479	1.830485
O	-1.007187	-3.306431	0.852472
H	-1.539662	-2.589522	0.337207
H	-1.574169	-4.104023	0.857193
O	0.409944	2.576094	-2.969469
H	0.938220	1.729618	-2.769026
H	0.786750	2.941732	-3.793877
O	1.203581	-3.418283	-0.731088
H	0.935946	-2.916825	-1.559459
H	0.379244	-3.439490	-0.162172
O	1.802543	1.805991	2.903480
H	1.702967	0.820893	2.682056
H	2.223552	1.841884	3.784555
O	-1.984746	1.487227	-2.933770
H	-2.571014	1.898148	-3.600547

H	-1.087835	1.947851	-3.059388
O	1.310653	-0.584746	2.011182
H	0.644962	-1.163793	2.501828
H	1.991216	-1.203381	1.583291
Li	-0.715746	2.133715	0.380146

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O	3.158178	1.959815	0.954670
H	3.966565	2.501204	1.053121
H	3.446316	1.136133	0.439712
O	-0.108770	0.226075	0.084339
H	0.566129	0.181300	-0.675055
H	0.306276	-0.264487	0.876122
O	-1.838286	-0.604772	-3.169499
H	-2.146980	-0.798292	-2.212681
H	-2.540837	-0.968318	-3.745013
O	3.677258	-0.206564	-0.465175
H	4.574049	-0.363462	-0.821050
H	3.384610	-1.081139	-0.025387
O	-2.480874	0.208414	2.903465
H	-2.053912	-0.742338	2.935746
H	-2.973013	0.293687	3.744080
O	0.439916	-1.893380	-3.040999
H	0.724590	-2.255756	-3.903239
H	-0.466268	-1.457834	-3.206377
O	0.949520	3.222185	-0.058293
H	0.987018	3.141321	-1.054986
H	1.806470	2.813311	0.248584
O	-2.282571	-0.984429	-0.652958
H	-1.422093	-0.507046	-0.361799
H	-3.003530	-0.435542	-0.194449
O	-2.201961	2.622568	-0.298563
H	-2.912180	2.004351	0.021613
H	-2.102771	2.404584	-1.283809
O	1.559739	0.205402	-1.955512
H	1.267774	-0.613171	-2.474827
H	2.463163	0.017921	-1.547343
O	-1.318790	-2.078240	2.972028
H	-1.513493	-2.565210	2.117523
H	-0.391448	-1.736343	2.788939
O	-0.657012	2.165995	2.474416
H	-1.283770	1.428384	2.731299
H	0.225096	1.896012	2.847258
O	2.622880	-2.326190	0.596813
H	1.896955	-2.781006	-0.007882
H	3.187017	-3.049988	0.934143
O	-3.812808	0.648868	0.705723
H	-4.776441	0.516235	0.800567
H	-3.406817	0.466200	1.623708
O	-1.553428	-3.185152	0.521661
H	-1.962658	-2.385922	0.036613
H	-2.175095	-3.924447	0.366486
O	0.860615	2.611208	-2.678349
H	1.217692	1.675456	-2.517816
H	1.420323	2.989922	-3.384760
O	0.794402	-3.400435	-0.818023
H	0.623818	-2.889810	-1.661652
H	-0.075730	-3.367666	-0.318208
O	1.848164	1.261141	3.122172
H	2.372605	1.321286	3.944603
H	2.453829	1.577039	2.372322
O	-1.797745	2.121078	-2.881861
H	-0.823404	2.340377	-2.923254
H	-1.825189	1.138113	-3.053973
O	0.960301	-1.004248	2.143035
H	1.399034	-0.227499	2.618341
H	1.682986	-1.557178	1.706167
Li	-0.527721	2.095920	0.530152

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O	3.097699	2.298175	0.937296
H	2.733006	2.028355	1.828702
H	3.316867	1.432641	0.494176
O	-0.022567	0.275494	0.164596
H	0.593388	0.272821	-0.643963
H	-0.818881	-0.294616	-0.099655
O	-1.793274	-0.756588	-3.095296
H	-2.444125	-1.037119	-3.769337
H	-1.777351	0.266564	-3.119104
O	3.656730	-0.038051	-0.396495
H	4.551398	-0.137218	-0.777092
H	3.427914	-0.936707	0.024321
O	-2.375923	0.106407	2.959973
H	-2.885375	0.153605	3.793239
H	-1.880979	-0.811103	2.995729
O	0.581615	-1.887164	-2.943047
H	0.899924	-2.209661	-3.809647
H	-0.344074	-1.512329	-3.115817
O	0.840473	3.323517	-0.047936
H	0.874044	3.236485	-1.038866
H	1.726973	2.943156	0.264849
O	-2.114308	-1.187895	-0.526359

H	-2.866004	-0.648333	-0.109478
H	-2.156276	-1.071525	-1.528876
O	-2.262243	2.476584	-0.260126
H	-2.914982	1.798617	0.068846
H	-2.155250	2.266384	-1.229967
O	1.586527	0.312570	-1.929496
H	1.335410	-0.539532	-2.412843
H	2.478632	0.161848	-1.468707
O	-1.039019	-2.082333	3.030010
H	-1.202133	-2.618882	2.198849
H	-0.138798	-1.674251	2.832174
O	-0.721564	2.221683	2.542444
H	0.180853	2.008248	2.913528
H	-1.292042	1.439344	2.795446
O	2.774571	-2.243950	0.676580
H	2.099488	-2.758327	0.063381
H	3.397006	-2.915704	1.018903
O	-3.716029	0.415767	0.752935
H	-4.675400	0.262841	0.859729
H	-3.297638	0.285801	1.676977
O	-1.236394	-3.323566	0.633945
H	-1.684790	-2.559887	0.131274
H	-1.838547	-4.087670	0.531234
O	0.739486	2.633043	-2.690299
H	1.177481	1.730504	-2.510547
H	1.213362	3.016308	-3.454981
O	1.063022	-3.462211	-0.774005
H	0.854666	-2.929897	-1.594049
H	0.204370	-3.471576	-0.252247
O	1.817716	1.497755	3.187817
H	1.667757	0.525605	2.925233
H	2.194293	1.472279	4.089203
O	-1.734235	1.835985	-2.872169
H	-2.242861	2.343248	-3.536507
H	-0.783113	2.205066	-2.919833
O	1.169069	-0.834629	2.223085
H	0.701953	-0.402069	1.426490
H	1.851520	-1.429486	1.773013
Li	-0.538288	2.123641	0.604626

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O	2.875100	2.326608	0.817268
H	3.588105	2.977226	0.977988
H	2.489849	2.139886	1.737168
O	-0.038446	0.311349	-0.028357
H	0.650168	0.299251	-0.782903
H	0.418655	-0.069759	0.792470
O	-1.610962	-1.152791	-3.247352
H	-1.897358	-1.289432	-2.292807
H	-1.614763	-0.149827	-3.307717
O	3.781233	0.141046	-0.505425
H	3.502941	0.913751	0.070197
H	3.496195	-0.673685	0.004395
O	-2.515257	0.112372	2.870728
H	-3.045837	0.164986	3.690379
H	-2.004207	-0.760235	2.939372
O	0.802880	-1.952487	-2.899347
H	1.149729	-2.315802	-3.738083
H	-0.174215	-1.650612	-3.104098
O	0.616721	3.392191	-0.299994
H	0.697209	3.235553	-1.283488
H	1.489298	3.059628	0.060790
O	-1.995343	-1.313774	-0.621454
H	-1.221090	-0.672267	-0.423642
H	-2.787290	-0.833687	-0.212561
O	-2.433893	2.313230	-0.589103
H	-3.037114	1.610251	-0.222304
H	-2.259770	2.026828	-1.533215
O	1.689972	0.329295	-1.993232
H	1.472115	-0.557166	-2.434895
H	2.588832	0.235558	-1.493767
O	-0.996859	-2.042531	2.926097
H	-1.100169	-2.672517	2.129189
H	-0.971059	-2.607555	3.724015
O	-0.958526	2.269321	2.270393
H	-1.498631	1.492930	2.589915
H	-0.061441	2.139325	2.686986
O	2.805201	-2.042712	0.747128
H	2.197735	-2.637150	0.138427
H	3.431718	-2.655339	1.180668
O	-3.768821	0.228683	0.563816
H	-4.719381	0.005678	0.607391
H	-3.418060	0.163843	1.513825
O	-1.105294	-3.349125	0.677718
H	-1.561963	-2.598730	0.138189
H	-1.696578	-4.124899	0.598560
O	0.707056	2.540369	-2.869862
H	1.204929	1.677740	-2.637277
H	1.177294	2.931527	-3.632391
O	1.244076	-3.452840	-0.704656
H	1.046379	-2.941008	-1.546263
H	0.372007	-3.486512	-0.214698

O 1.588662 1.705820 3.027724
H 1.474380 0.713848 2.825946
H 1.988832 1.758840 3.917748
O -1.708364 1.534775 -3.094273
H -2.219655 1.976284 -3.801782
H -0.792916 1.974251 -3.121477
O 1.117012 -0.669559 2.140599
H 0.400304 -1.255709 2.540174
H 1.820977 -1.278377 1.724089
Li -0.728139 2.114278 0.340453

Na – 1 water molecule

4

O 0.161018 -0.000760 -0.028458
H 0.456151 -0.010091 -0.952739
H 0.933492 -0.288488 0.480450
Na -1.870180 0.362037 0.607888
4

O 0.138446 0.148965 0.060974
H 0.749758 0.347160 -0.665455
H 0.709692 -0.154110 0.783483
Na -1.932677 -0.427306 -0.227076
4

O 0.163035 0.003637 0.080164
H 0.477941 -0.913312 0.124490
H 0.487107 0.416005 0.894222
Na -1.360034 0.619146 -1.330832
4

O 0.027830 -0.036636 0.232976
H 0.495807 -0.886749 0.246906
H 0.665709 0.594536 0.599751
Na -1.450440 0.417425 -1.296239
4

O 0.038499 0.134503 0.085962
H -0.196390 1.073882 0.080286
H 0.890425 0.091201 0.547914
Na -0.901153 -1.568126 -0.870057
4

O 0.215029 0.141569 -0.032949
H 0.447856 -0.067021 -0.959615
H 0.891643 -0.339724 0.483492
Na -1.874048 0.327873 0.616214
4

O 0.139718 0.206090 0.080365
H 0.750730 0.324909 -0.673983
H 0.710296 -0.175311 0.777184
Na -1.935525 -0.440978 -0.231641
4

O 0.242066 0.000685 0.021641
H 0.478946 -0.936397 0.169474
H 0.427413 0.420252 0.885261
Na -1.380375 0.640936 -1.308332
4

O 0.133249 -0.021043 0.084452
H 0.473861 -0.904955 0.324112
H 0.633741 0.587310 0.662423
Na -1.501946 0.427265 -1.287593
4

O 0.066002 0.123903 0.070105
H -0.210675 1.061148 0.080253
H 0.903182 0.118479 0.574058
Na -0.927129 -1.572071 -0.880311

Na – 2 water molecules

7

O 1.261643 -1.738650 -0.437656
H 1.057831 -2.377214 -1.138891
H 2.229693 -1.676904 -0.449496
O -1.191775 1.789526 0.511184
H -1.267199 2.047053 1.443590
H -2.085901 1.924325 0.158507
Na -0.004292 0.031865 -0.087239
7

O 0.654821 0.590262 1.955827
H 0.716857 1.483811 2.328296

H 1.541854 0.218504 2.085428
O -0.939392 -0.569835 -1.877017
H -1.352548 -1.448747 -1.870538
H -0.315519 -0.620668 -2.620024
Na -0.307387 0.348144 -0.002022
7

O -0.056700 -0.002158 2.218949
H -0.848785 -0.333085 2.671826
H 0.152912 0.819920 2.690174
O 0.054468 -0.013222 -2.193795
H 0.810703 0.338329 -2.689551
H -0.243948 -0.768533 -2.724346
Na 0.033402 -0.054657 0.009480
7

O 0.053969 0.094426 2.188281
H -0.679520 0.303939 2.786647
H 0.645745 -0.461243 2.719080
O 0.016605 0.016479 -2.171768
H 0.527670 0.572813 -2.779209
H -0.532919 -0.535712 -2.748884
Na -0.018784 0.085265 0.006271
7

O 1.800508 -0.947068 -0.837898
H 1.747039 -1.406830 -1.690819
H 2.442984 -1.467115 -0.330422
O -1.677331 1.139203 0.789066
H -2.558744 1.201508 0.389679
H -1.780494 1.525863 1.672143
Na 0.006686 -0.055260 0.069422
7

O 1.429444 -1.611453 -0.501405
H 1.744839 -1.741655 -1.417509
H 1.344301 -2.522895 -0.158109
O -1.363578 1.680981 0.428339
H -1.047479 2.589845 0.600968
H -2.136807 1.592085 1.019684
Na 0.029281 0.013092 0.028033
7

O 0.893385 0.540601 1.945523
H 1.734517 1.038085 1.978146
H 0.368355 0.938062 2.668704
O -0.883594 -0.536178 -1.962230
H -0.347962 -1.011561 -2.628392
H -1.746062 -0.995536 -1.998839
Na -0.019956 0.028000 -0.002961
7

O -0.058425 0.036269 2.222504
H -0.809274 -0.369855 2.699794
H 0.037948 0.907812 2.655342
O 0.290545 -0.322709 -2.178593
H 0.858634 0.296896 -2.678413
H -0.492139 -0.425707 -2.755664
Na 0.074763 -0.136113 0.017768
7

O 0.182846 -0.086351 2.204854
H 0.241104 0.727378 2.744132
H -0.432770 -0.650517 2.713847
O -0.127519 -0.143200 -2.202551
H -0.552096 0.571839 -2.717323
H 0.654768 -0.374046 -2.742285
Na 0.046430 0.030865 -0.000257
7

O 1.798613 -1.016229 -0.751160
H 2.048440 -1.947258 -0.590244
H 2.073288 -0.861160 -1.676208
O -1.711841 1.000532 1.016050
H -1.650032 1.934875 1.297106
H -2.600585 0.945263 0.612106
Na 0.022766 -0.065723 0.153522

Na – 4 water molecules

13

O -0.753349 1.849181 -0.821450
H -0.442353 1.983979 -1.730613
H -1.718823 1.851867 -0.911554
O -0.768800 -1.780943 -0.741404
H -1.732650 -1.886309 -0.724144
H -0.440365 -2.656512 -0.483248
O -0.347084 0.612778 2.304590
H -1.199069 1.052608 2.449195

H	-0.308159	-0.053347	3.008131
O	2.138206	-0.212333	-0.909947
H	2.915896	0.309490	-0.658945
H	2.482492	-1.118035	-0.962202
Na	0.174056	0.047576	0.181589

13

O	0.486100	1.382947	0.014961
H	0.628485	0.889136	0.855081
H	0.387983	2.307072	0.287698
O	0.310384	-0.136334	-3.169338
H	0.932079	-0.880068	-3.207291
H	0.849816	0.624946	-3.435853
O	0.495778	-0.345828	2.136551
H	1.222009	-0.990461	2.155754
H	0.477198	0.028859	3.032253
O	-1.740549	-0.734309	0.584282
H	-1.033855	-0.706131	1.269282
H	-2.182673	-1.584054	0.723388
Na	-0.832755	0.144225	-1.253296

13

O	-1.700968	-1.037602	0.274263
H	-0.907994	-1.499078	0.632792
H	-2.188508	-1.728657	-0.198087
O	0.779817	-1.826490	1.206595
H	0.858398	-2.232616	2.085575
H	1.354853	-2.363694	0.638418
O	0.659673	0.874889	0.903236
H	0.907222	-0.053788	1.116314
H	1.497291	1.359396	0.880237
O	-0.407607	2.292740	-2.243419
H	-0.409084	3.229868	-1.992034
H	0.461017	2.169030	-2.658633
Na	-0.905638	0.821973	-0.650464

13

O	-0.580649	1.561076	-0.919343
H	-0.152278	2.409642	-0.725190
H	-1.518987	1.739317	-0.752350
O	-1.520649	-1.631311	-0.215511
H	-2.266249	-1.392332	0.356311
H	-1.917385	-1.655326	-1.100737
O	0.298843	-0.337593	2.247075
H	-0.493863	-0.682538	2.686240
H	0.539468	0.436369	2.778729
O	2.288028	-0.063038	-1.089526
H	2.353997	0.718276	-1.660339
H	2.653676	-0.775683	-1.635895
Na	0.304627	-0.282984	0.002073

13

O	-2.025256	-0.110057	-1.422183
H	-2.480791	0.710612	-1.673227
H	-2.536842	-0.812232	-1.854692
O	2.775051	0.478239	1.815457
H	3.272449	-0.166843	2.341785
H	3.460416	0.990075	1.359081
O	0.722890	-0.018996	-1.367574
H	-0.235969	-0.083151	-1.581576
H	1.139145	-0.722964	-1.885705
O	-1.302241	-0.302384	1.232693
H	-1.855545	0.244178	1.810631
H	-1.742594	-0.258896	0.352494
Na	0.848961	0.054374	0.847888

13

O	-0.865729	1.624575	-1.446132
H	-0.660992	2.557530	-1.236037
H	-1.830457	1.645079	-1.604505
O	-1.068155	-1.926295	-0.392769
H	-0.611162	-2.718936	-0.048047
H	-1.262329	-2.172664	-1.318735
O	-0.519657	0.709688	2.092768
H	0.054993	1.400461	2.478036
H	-0.538040	0.023455	2.788822
O	2.181228	-0.107013	-0.355770
H	2.701586	-0.631127	0.284660
H	2.468128	-0.468495	-1.217881
Na	-0.049413	0.063742	-0.024412

13

O	1.120090	1.389871	0.414528
H	0.787168	0.986177	1.264559
H	0.953583	2.345632	0.529328
O	0.005910	0.087174	-3.384937
H	-0.804926	-0.188688	-3.856645
H	0.703306	-0.450009	-3.810663
O	0.034330	-0.063472	2.433139
H	0.646329	-0.595127	2.981674
H	-0.567817	0.358751	3.079207
O	-1.133450	-1.139968	0.228692

H -0.761967 -0.895784 1.122078
H -0.947759 -2.095931 0.152021
Na -0.034797 0.261375 -1.159511
13

O -1.060419 -1.193433 -0.574377
H -0.619155 -1.583250 0.231000
H -2.010361 -1.367801 -0.429343
O 0.483255 -1.835989 1.562195
H 0.084200 -1.997123 2.441293
H 1.135517 -2.558001 1.454565
O 1.153879 0.744092 1.054657
H 1.068588 -0.210738 1.332735
H 2.114329 0.867043 0.925413
O -0.829477 2.434305 -2.208478
H -0.836855 3.385331 -1.981421
H -0.443777 2.423062 -3.106997
Na -0.241250 0.898471 -0.706449
13

O -0.881326 1.972404 -0.588453
H -0.353805 2.771222 -0.389293
H -1.140818 2.109090 -1.521151
O -1.445099 -1.687244 -0.591108
H -1.208340 -2.570625 -0.244689
H -2.371502 -1.580581 -0.296466
O 0.333601 -0.191732 2.197987
H -0.468534 -0.306584 2.744860
H 0.792788 0.550630 2.638576
O 1.980146 -0.469941 -1.037447
H 2.745904 0.122334 -0.902271
H 1.999038 -0.644642 -1.998950
Na 0.006529 -0.030451 -0.040055
13

O -2.015466 -0.239326 -1.357387
H -2.600254 0.461425 -1.711807
H -2.416976 -1.072699 -1.678036
O 2.767456 0.198261 1.968313
H 3.543830 -0.331128 1.698372
H 3.154986 1.071197 2.177526
O 0.673454 0.104128 -1.492305
H -0.303992 -0.044808 -1.629136
H 1.094578 -0.583603 -2.043148
O -1.289564 -0.111212 1.250827
H -1.741441 0.636820 1.687385
H -1.728198 -0.165511 0.355016
Na 0.901262 0.078409 0.749452

Na – 8 water molecules

25

O -1.338896 0.853762 -1.302322
H -2.026960 1.013723 -1.965613
H -0.472791 0.907309 -1.781019
O -0.923037 2.132547 0.995969
H -1.196995 1.874411 0.077789
H -1.273346 3.026234 1.134910
O -0.783060 -2.764185 1.588747
H -0.648183 -3.709973 1.427572
H 0.122420 -2.399654 1.644551
O -2.232166 -0.169286 1.710197
H -1.853304 -0.641988 2.466250
H -1.814566 0.720057 1.722626
O 0.173974 -1.896252 -1.872291
H 0.715774 -1.107096 -2.092099
H 0.794770 -2.638980 -1.900975
O 1.285368 -1.065952 0.837873
H 1.569644 -0.119884 0.867376
H 1.732307 -1.428363 0.058848
O 1.652421 1.566470 0.546963
H 0.773178 1.943831 0.812021
H 2.326690 2.170698 0.892589
O 1.233141 0.668059 -2.009331
H 1.545412 1.080400 -1.166233
H 1.621467 1.200259 -2.720767
Na -1.003506 -1.112485 -0.044749
25

O 0.695458 -1.246681 2.058031
H 1.467880 -1.230642 2.642698
H 0.030063 -0.684312 2.521443
O -1.192051 0.543361 2.860007
H -1.972765 0.255381 2.323547
H -1.516063 0.666231 3.765073
O 1.512110 -1.696094 -1.407303
H 1.535830 -1.273474 -2.294574
H 1.047931 -2.534930 -1.540965
O 2.150771 1.307680 -1.247586

H	1.668786	2.147933	-1.219456
H	1.999410	0.974623	-2.158201
O	0.356791	1.977152	1.193880
H	-0.225560	1.623776	1.905758
H	1.116208	2.341354	1.672506
O	-1.159305	-0.221685	-0.947201
H	-1.061592	-1.102466	-1.338427
H	-1.890413	-0.317626	-0.297327
O	-3.040997	-0.289384	1.102701
H	-3.428427	-1.159491	1.294837
H	-3.807079	0.292478	0.969659
O	1.627845	-0.078182	-3.609281
H	0.786503	-0.010065	-4.088598
H	2.286236	-0.264105	-4.297666
Na	0.868903	-0.038538	0.096292

25

O	-1.756247	-0.950349	0.936482
H	-1.872222	-0.875933	-0.040206
H	-2.648313	-0.827196	1.292876
O	-0.526227	0.542411	3.880424
H	-1.198926	1.151183	4.222664
H	-0.778218	-0.311501	4.265292
O	-0.165593	2.912669	1.450833
H	0.674718	3.324547	1.701737
H	-0.056901	2.679854	0.503184
O	-0.029590	1.424031	-0.838496
H	-0.740735	0.884042	-1.251362
H	0.789661	0.932948	-1.077253
O	2.002610	-0.366594	-1.323514
H	2.816307	-0.144974	-1.801549
H	1.513161	-1.002421	-1.899974
O	-1.724843	-0.536397	-1.750841
H	-2.480158	-0.461889	-2.353275
H	-1.068646	-1.117998	-2.206405
O	0.349090	-1.934703	-2.787636
H	0.382021	-2.890374	-2.614779
H	0.477684	-1.854631	-3.747237
O	1.757075	-0.590013	1.369786
H	2.532741	-0.215851	1.813062
H	1.985906	-0.565082	0.410982
Na	-0.198552	0.564245	1.605371

25

O	-1.092431	-0.524092	3.812845
H	-1.868932	-0.980516	4.175877
H	-0.590658	-0.237136	4.592716
O	1.921236	1.008019	0.888536
H	2.297303	1.154372	-0.008045
H	2.550533	0.411084	1.319128
O	0.198846	-1.752272	1.753557
H	-0.195071	-1.418714	2.590534
H	1.109625	-1.978401	1.991772
O	-1.573417	-0.355205	-3.265787
H	-1.338741	-0.453250	-4.202273
H	-2.540587	-0.432614	-3.243072
O	2.402862	1.281533	-1.806744
H	2.957679	2.001941	-2.146034
H	2.776138	0.479491	-2.206482
O	-1.377726	1.201269	1.649820
H	-1.383897	0.685436	2.486766
H	-2.314339	1.275774	1.413964
O	-0.116930	-1.619786	-1.328651
H	-0.574055	-2.386293	-0.952014
H	-0.681998	-1.332423	-2.079165
O	-0.347282	1.510958	-1.599790
H	0.601281	1.505711	-1.845902
H	-0.782387	0.958891	-2.281953
Na	-0.034367	0.019574	0.243629

25

O	0.631027	-0.192051	-2.376986
H	0.629364	0.689534	-1.946780
H	1.127333	-0.764881	-1.747971
O	-3.341494	0.340119	1.440280
H	-3.781733	0.973978	0.852762
H	-3.210382	0.844077	2.258399
O	0.365458	2.063871	-0.772862
H	0.155697	2.983474	-0.998557
H	-0.070453	1.888758	0.087908
O	1.871608	-1.575889	-0.332999
H	2.644529	-2.106483	-0.581954
H	2.238505	-0.738608	0.048201
O	2.373956	0.915496	0.573984
H	3.176491	1.358842	0.890248
H	1.936857	1.545968	-0.042601
O	-0.118578	0.826070	1.675883
H	0.862530	0.849810	1.587858
H	-0.330621	1.442953	2.392448
O	-1.910233	-0.575513	-1.641708
H	-1.005268	-0.471711	-2.044004
H	-2.244817	-1.400557	-2.023662

O	-0.306742	-2.499932	0.994394
H	0.558386	-2.283029	0.567898
H	-0.584987	-3.318363	0.557248
Na	-1.489937	-0.615209	0.568227

25

O	-1.262781	0.467204	-1.217255
H	-1.993419	0.495341	-1.865087
H	-0.418870	0.638955	-1.746097
O	-1.026259	2.145659	0.768178
H	-1.260895	1.656066	-0.089539
H	-1.496503	3.001759	0.723837
O	-1.199754	-3.387715	0.765490
H	-1.709171	-3.462652	1.596530
H	-1.832067	-3.713458	0.094607
O	-1.837095	-0.183237	1.919268
H	-1.410689	-0.292043	2.791303
H	-1.632751	0.763750	1.683974
O	0.895426	-1.895642	-1.527055
H	1.176400	-0.995924	-1.848483
H	1.729520	-2.299885	-1.220402
O	1.454099	-0.607729	1.437283
H	1.623386	0.319841	1.100952
H	2.221818	-1.106596	1.097655
O	1.542593	1.832312	0.290031
H	0.609454	2.141026	0.534823
H	2.148447	2.551745	0.555711
O	1.204673	0.739296	-2.085318
H	1.479050	1.268999	-1.269825
H	1.455383	1.276779	-2.861676
Na	-0.480240	-1.250188	0.299978

25

O	1.116520	-0.730744	0.936313
H	1.954266	-1.028935	1.339331
H	0.465196	-0.652050	1.700382
O	-0.800757	-0.081681	2.646722
H	-1.682150	-0.281184	2.200924
H	-0.894350	-0.378567	3.572884
O	0.076667	-1.907854	-1.272934
H	0.740374	-1.589941	-1.943553
H	0.504436	-1.653547	-0.406360
O	1.830887	1.732923	-1.866552
H	2.754678	1.985806	-1.675972
H	1.918590	0.872308	-2.368593
O	-0.221529	2.381714	1.724332
H	-0.460855	1.570419	2.259824
H	0.462588	2.819638	2.267152
O	-1.425994	0.303827	-1.061004
H	-0.978575	-0.585779	-1.224033
H	-2.094265	0.087420	-0.361536
O	-2.964902	-0.403769	1.147415
H	-3.349723	-1.302638	1.092248
H	-3.723379	0.162732	1.398640
O	1.860748	-0.719458	-3.013249
H	1.570246	-0.742337	-3.948622
H	2.746648	-1.136705	-3.034332
Na	0.451106	1.260693	-0.149580

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O	-1.913386	-0.745103	0.965804
H	-1.914155	-0.600251	-0.027139
H	-2.789803	-0.414904	1.243059
O	-0.305678	0.325216	4.091511
H	-1.091980	0.748530	4.489537
H	-0.327805	-0.575014	4.472133
O	-0.032924	2.539562	1.105699
H	-0.867829	3.044634	1.153129
H	0.063857	2.324076	0.115910
O	0.233450	1.746918	-1.389575
H	-0.538038	1.135939	-1.561922
H	1.002620	1.108954	-1.389157
O	2.034966	-0.297813	-1.258200
H	2.920039	-0.266369	-1.672603
H	1.518780	-0.982642	-1.779759
O	-1.618331	-0.231008	-1.647565
H	-2.401082	-0.180550	-2.231708
H	-1.029004	-0.935449	-2.052582
O	0.292404	-1.896934	-2.520435
H	0.251864	-2.839884	-2.256585
H	0.407611	-1.925304	-3.493293
O	1.764758	-0.727957	1.370302
H	2.548499	-0.358790	1.821140
H	1.980589	-0.616910	0.397125
Na	-0.153620	0.391077	1.815340

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O	-1.973784	-1.218752	2.761520
H	-2.240044	-2.135462	2.544669
H	-2.461511	-1.015013	3.585777
O	2.827156	0.762925	0.253630
H	2.883264	0.839514	-0.738790

H	3.338655	-0.045817	0.448696
O	0.651317	-0.459412	2.612885
H	-0.248394	-0.836939	2.805408
H	1.251224	-1.219482	2.737773
O	-1.813786	-0.001243	-1.759674
H	-2.639025	-0.202782	-2.241521
H	-2.081715	0.198988	-0.810094
O	2.531293	1.074630	-2.431595
H	3.100498	1.709804	-2.912084
H	2.535571	0.274432	-2.995027
O	-1.859801	0.601878	0.804727
H	-2.084989	-0.049042	1.532648
H	-2.285317	1.439810	1.070831
O	0.233848	-1.499244	-0.906264
H	-0.081753	-2.328900	-0.500728
H	-0.583284	-1.132711	-1.352440
O	0.132506	1.894834	-1.366026
H	0.932535	1.653282	-1.901050
H	-0.594687	1.342558	-1.751886
Na	0.532904	0.375498	0.461849

25

O	0.060319	0.026997	-1.700541
H	0.477473	0.928618	-1.689441
H	0.780599	-0.570971	-1.347358
O	-3.424100	-0.515637	1.515563
H	-3.941079	0.314660	1.512846
H	-3.296447	-0.687196	2.469501
O	1.501734	2.330394	-1.312703
H	2.216826	2.516576	-1.955657
H	1.060421	3.195617	-1.187489
O	1.866910	-1.362935	-0.262505
H	2.687571	-1.764564	-0.608323
H	2.146770	-0.529115	0.231945
O	2.139089	0.998042	0.895662
H	2.910282	1.328334	1.397992
H	2.041122	1.610965	0.102901
O	-0.418254	1.107514	1.761257
H	0.563844	1.107908	1.570363
H	-0.469211	0.736114	2.663325
O	-2.508271	-0.642764	-1.816767
H	-1.557908	-0.459571	-2.056911
H	-2.623268	-1.587892	-2.033408
O	-0.403479	-2.333817	0.803256
H	0.515242	-2.136748	0.462928
H	-0.691198	-3.088317	0.254174
Na	-1.458490	-0.341493	0.315044

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O	-2.033666	-2.586266	-0.324274
H	-1.527338	-2.631934	-1.168672
H	-1.364894	-2.775070	0.369584
O	-1.709177	-0.050836	0.442001
H	-2.053400	-0.904926	0.072295
H	-1.995768	0.672000	-0.159735
O	-0.023637	-2.346948	1.552545
H	0.595269	-2.959555	1.976603
H	-0.380500	-1.782366	2.278727
O	1.881892	-2.103700	-1.340537
H	1.163105	-2.456605	-1.912410
H	2.198880	-2.874120	-0.846134
O	0.259422	2.919011	0.236484
H	0.359660	2.530477	1.146577
H	0.361100	3.876484	0.354146
O	2.109231	1.714489	-1.340148
H	2.721324	2.309096	-1.799765
H	1.507442	2.303960	-0.818611
O	2.378889	0.194850	0.954226
H	1.933023	0.756278	1.627274
H	2.559478	0.797022	0.202279
O	0.682429	1.615733	2.560477
H	0.998137	2.067594	3.357871
H	-0.008020	0.969012	2.863267
O	-1.782423	2.007881	-1.287176
H	-2.417511	2.664121	-1.610142
H	-1.125542	2.499283	-0.731972
O	0.012713	0.246688	-2.287525
H	-0.706073	0.895825	-2.108418
H	0.843820	0.768722	-2.207180
O	-1.118055	-0.313632	2.975046
H	-1.808482	-0.328152	3.655321
H	-1.571652	-0.122986	2.110240
O	-0.468918	-2.375178	-2.583998
H	-0.386316	-1.396285	-2.699394
H	-0.730313	-2.734232	-3.445091
Na	0.546251	-0.751960	-0.074462

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O	-2.151606	-2.691149	1.562479
H	-2.382002	-2.651111	0.603141
H	-2.839980	-3.225587	1.985904
O	0.473037	-3.042388	0.770177
H	1.009836	-2.308907	1.132059
H	-0.376129	-3.016544	1.256905
O	0.227450	1.140384	2.705309
H	-0.620530	0.767952	2.339685
H	0.129832	1.188559	3.667905
O	1.595856	-0.591750	1.105387
H	1.219345	-0.025217	1.816952
H	2.289754	-0.031706	0.687404
O	3.044179	1.342125	-0.145847
H	2.399294	2.002145	0.223037
H	3.920405	1.651076	0.132828
O	2.043427	1.159285	-2.624162
H	2.444836	1.719207	-3.305626
H	2.581543	1.290168	-1.802185
O	0.981969	-1.318833	-2.467777
H	1.652457	-2.016334	-2.435827
H	1.487524	-0.496733	-2.665992
O	0.983387	2.747643	0.759931
H	0.927159	3.706203	0.892658
H	0.702938	2.324918	1.614564
O	-2.867844	0.657298	-0.980250
H	-2.024181	1.105030	-1.238533
H	-3.580390	1.289839	-1.155269
O	-0.297329	1.367394	-1.204804
H	0.400114	1.428705	-1.896510
H	0.040847	1.959457	-0.490433
O	-1.727057	-0.017682	1.386708
H	-2.320885	0.330519	0.683606
H	-2.050629	-0.919773	1.612329
O	-2.224853	-1.989964	-1.039551
H	-2.336933	-2.518474	-1.843463
H	-2.696634	-1.141194	-1.204541
Na	-0.136420	-0.917651	-0.474559

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O	0.271081	1.258832	-2.906790
H	0.342035	1.881005	-3.646872
H	1.095200	1.376005	-2.371938
O	1.484091	-1.293712	-0.887834
H	1.107683	-1.456580	-1.781997
H	1.943373	-0.425360	-0.967451
O	-0.518333	2.644044	1.571299
H	-0.561792	3.600235	1.725145
H	0.443338	2.406782	1.600150
O	0.664725	-3.120572	0.941748
H	-0.113850	-3.301602	0.378828
H	1.205673	-2.571435	0.330021
O	2.351336	1.261315	-1.163018
H	3.282211	1.396027	-1.398330
H	2.277852	1.479454	-0.196624
O	-1.693818	0.681612	3.042740
H	-1.875509	0.921638	3.963648
H	-1.341913	1.500986	2.610619
O	1.942584	1.524540	1.462363
H	1.564531	0.653148	1.756572
H	2.662203	1.731841	2.078168
O	-1.283633	-2.726234	-1.084587
H	-0.964427	-2.427617	-1.965500
H	-2.227907	-2.908469	-1.197007
O	-0.055032	-1.413493	-3.154172
H	0.349738	-1.775130	-3.957037
H	0.030034	-0.428641	-3.228039
O	-2.826560	-0.976235	1.207913
H	-2.631568	-0.338163	1.931656
H	-3.511375	-0.535837	0.682526
O	-1.307274	1.354417	-0.674170
H	-1.016568	1.994882	0.012417
H	-0.804387	1.559303	-1.490546
O	0.472283	-0.601119	2.084465
H	0.513060	-1.580050	2.003661
H	-0.277559	-0.349932	2.671092
Na	-0.789240	-0.714258	0.037196

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O	-1.608488	-2.230561	-0.912964
H	-1.222593	-2.479280	-1.782555
H	-1.737511	-3.056483	-0.424244
O	-2.826843	0.137287	-1.182326
H	-2.619514	-0.826230	-1.105668
H	-3.763069	0.195598	-1.423912
O	0.175948	-2.356849	1.845245
H	1.101701	-2.548516	2.056975
H	-0.089723	-1.695187	2.524512
O	1.611958	-2.343777	-1.229660
H	1.137694	-2.425954	-2.086396
H	2.407651	-1.833965	-1.440462
O	0.158708	2.966823	0.648921

H	0.605741	2.699244	1.494990
H	-0.245040	3.832764	0.813107
O	1.623518	2.030370	-1.362918
H	2.198496	2.641613	-1.847946
H	1.130026	2.578271	-0.700990
O	2.192832	0.201108	0.618344
H	2.193608	0.866667	-0.104101
H	2.044355	0.738789	1.425292
O	1.291785	1.745357	2.740275
H	1.724106	2.180345	3.490483
H	0.634991	1.107778	3.121094
O	-1.324845	0.715864	0.901770
H	-2.056660	0.611773	0.246898
H	-0.931654	1.605925	0.741358
O	-0.198486	0.232377	-2.165651
H	-1.113124	0.532034	-1.997411
H	0.411858	0.997660	-2.043439
O	-0.579706	-0.133202	3.258814
H	-1.199497	-0.048236	3.999910
H	-1.070521	0.191210	2.454295
O	-0.150545	-2.179849	-3.234525
H	-0.129708	-1.200998	-3.086174
H	-0.181033	-2.326881	-4.190857
Na	0.236587	-0.930087	-0.005912
37			
O	-2.787632	-2.276666	-0.250656
H	-3.342013	-3.037415	-0.017691
H	-1.917986	-2.422621	0.203732
O	-3.051394	0.153726	0.883554
H	-3.148576	-0.752172	0.489672
H	-3.948370	0.498202	1.011076
O	-0.324580	-2.010581	0.742617
H	0.576024	-2.413531	0.838601
H	-0.444994	-1.399602	1.506537
O	2.274269	-2.716996	0.709561
H	2.635166	-2.842368	1.600661
H	2.507515	-1.786864	0.476071
O	0.512252	2.960733	-0.131744
H	0.732897	2.531248	0.736121
H	0.331713	3.892478	0.066404
O	2.607319	2.077929	-1.514341
H	3.332625	2.704707	-1.654760
H	1.884042	2.579948	-1.055712
O	2.317036	-0.108816	0.074228
H	1.977034	0.381469	0.862895
H	2.680303	0.605801	-0.497556
O	1.122227	1.397710	1.954610
H	0.308049	0.927197	2.281359
H	1.588867	1.721237	2.740165
O	-1.284608	1.083890	-1.016737
H	-1.979915	0.906840	-0.347107
H	-0.797128	1.872379	-0.692658
O	1.287667	0.288529	-3.007097
H	0.631533	0.716059	-3.576293
H	1.824893	1.031556	-2.646138
O	-0.992621	-0.077906	2.530855
H	-1.243704	-0.321398	3.435178
H	-1.843624	0.092421	2.043649
O	-1.074367	-1.936075	-2.412251
H	-1.831347	-2.114006	-1.812207
H	-1.467957	-1.458661	-3.157149
Na	0.243248	-0.575261	-1.124033
37			
O	-1.566107	-2.223742	-0.511513
H	-1.338376	-2.332913	-1.485463
H	-1.777321	-3.121035	-0.189864
O	-2.713911	-0.107747	0.673339
H	-2.415037	-0.922806	0.172592
H	-2.436183	0.652350	0.082471
O	0.295018	-2.290872	2.213249
H	1.113597	-2.205308	2.739499
H	-0.279128	-1.542256	2.554165
O	1.614117	-2.991326	-1.263980
H	0.982035	-2.876428	-2.025994
H	2.469114	-2.697948	-1.634152
O	0.318220	3.058792	0.181174
H	0.443575	2.605932	1.087859
H	0.288568	4.019617	0.361126
O	2.128990	1.775064	-1.283410
H	2.770882	2.312988	-1.786591
H	1.538615	2.429062	-0.794692
O	2.337123	0.039611	0.808149
H	1.887976	0.619814	1.482818
H	2.469391	0.668041	0.047273
O	0.726091	1.632173	2.321372
H	0.987152	2.074678	3.152817
H	-0.060089	1.022861	2.558009
O	-1.693643	1.785131	-0.934923
H	-2.203695	2.338406	-1.558981
H	-1.014716	2.402103	-0.504560

O	0.150772	0.076804	-1.825619
H	-0.606607	0.709870	-1.631270
H	0.951432	0.676588	-1.869263
O	-1.176225	-0.095829	2.711542
H	-1.711314	-0.022133	3.526480
H	-1.855514	-0.081446	1.917040
O	-0.402265	-2.216094	-2.884781
H	-0.178808	-1.241626	-2.715033
H	-0.745023	-2.275746	-3.797115
Na	0.601675	-1.340856	0.095550

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O	-2.040407	-2.555331	1.392248
H	-2.263358	-2.456683	0.414253
H	-2.750467	-3.107431	1.775206
O	0.566305	-3.139174	0.734105
H	1.100902	-2.412624	1.143229
H	-0.325273	-3.055008	1.164401
O	0.150253	1.071112	2.556370
H	-0.781466	0.702433	2.309673
H	0.144498	1.239830	3.518857
O	1.672624	-0.667486	1.198491
H	1.197876	-0.066257	1.843958
H	2.306494	-0.058978	0.724593
O	2.931159	1.279411	-0.253310
H	2.315923	1.964439	0.160925
H	3.836856	1.596772	-0.064643
O	1.852319	1.108846	-2.667633
H	2.245857	1.663214	-3.369347
H	2.414537	1.251529	-1.841057
O	1.305994	-1.490470	-2.405481
H	2.144354	-1.956247	-2.222697
H	1.596890	-0.570969	-2.674390
O	0.930668	2.704624	0.710891
H	0.823772	3.661348	0.878703
H	0.608609	2.219018	1.546413
O	-2.832094	0.709435	-0.742685
H	-1.956603	1.104775	-1.062939
H	-3.547341	1.293928	-1.060120
O	-0.341887	1.279309	-1.155200
H	0.312341	1.349759	-1.909265
H	0.024812	1.923475	-0.475291
O	-2.114000	0.111801	1.810197
H	-2.465077	0.416301	0.924544
H	-2.140648	-0.889758	1.763745
O	-2.111132	-1.776363	-1.112485
H	-2.356118	-2.262828	-1.922762
H	-2.599708	-0.895512	-1.147858
Na	0.064325	-1.033329	-0.520000

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O	0.394281	1.112910	-2.643030
H	0.529594	1.795706	-3.329625
H	1.238828	1.116777	-2.076040
O	2.056545	-1.857534	-1.188990
H	1.463282	-1.828096	-1.996403
H	2.324544	-0.896625	-1.092282
O	-0.769828	2.451571	1.426327
H	-0.881281	3.408750	1.592438
H	0.233073	2.284634	1.406922
O	0.335103	-2.039756	0.714870
H	0.250147	-2.979205	0.971632
H	1.055855	-2.029894	-0.030949
O	2.424616	0.814218	-1.026261
H	3.299824	1.176412	-1.268578
H	2.214952	1.184712	-0.099831
O	-1.401504	0.584911	3.166253
H	-1.658799	0.917606	4.048782
H	-1.256543	1.409115	2.593654
O	1.714073	1.614370	1.356473
H	1.533351	0.758152	1.936683
H	2.381053	2.132507	1.851205
O	-1.964654	-2.287253	-1.969546
H	-1.187351	-2.024779	-2.547837
H	-2.742974	-2.005140	-2.488076
O	0.270082	-1.458153	-3.186630
H	0.520644	-1.687305	-4.103536
H	0.302135	-0.445060	-3.140314
O	-2.944603	-1.088284	1.755944
H	-2.465328	-0.452282	2.367909
H	-3.809717	-0.657726	1.612584
O	-1.561493	1.075978	-0.769437
H	-1.305044	1.702530	-0.037619
H	-0.886095	1.233428	-1.485962
O	1.068825	-0.438949	2.725488
H	0.843848	-1.122874	2.018720
H	0.166241	-0.128916	3.032137
Na	-1.583394	-1.064830	-0.076767

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O	-1.708252	-2.238292	-1.149336
H	-1.127022	-2.408227	-1.953718

H	-2.054110	-3.109907	-0.878828
O	-2.810528	0.153641	-1.249687
H	-2.635192	-0.838421	-1.268829
H	-3.688796	0.288680	-1.654796
O	0.035051	-2.221872	1.999334
H	0.945421	-2.491589	2.226739
H	-0.179677	-1.516506	2.671223
O	1.905941	-2.455313	-0.884846
H	1.502140	-2.369513	-1.786405
H	2.265487	-1.556829	-0.674063
O	0.129140	2.886194	0.864398
H	0.741142	2.468767	1.557874
H	-0.119883	3.766233	1.208777
O	1.293736	2.195144	-1.377600
H	1.821673	2.870860	-1.845811
H	0.867298	2.659549	-0.589240
O	2.188801	0.104405	0.096086
H	2.034072	0.895886	-0.493781
H	2.136935	0.483440	1.016073
O	1.566919	1.355803	2.441327
H	2.168400	1.688997	3.136281
H	0.821059	0.872984	2.928176
O	-1.409727	0.693658	0.940184
H	-2.146732	0.623978	0.269458
H	-1.005464	1.603814	0.831515
O	-0.306756	0.272817	-2.268018
H	-1.256916	0.456769	-2.032251
H	0.237400	1.085719	-2.051820
O	-0.559719	0.047662	3.300705
H	-1.060373	0.291999	4.103534
H	-1.123100	0.324858	2.507199
O	0.183293	-2.156514	-3.007448
H	0.056447	-1.154968	-2.920323
H	0.098893	-2.360536	-3.959127
Na	0.026005	-1.020568	0.001216

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O	-2.484214	-2.372430	-0.020541
H	-3.149704	-3.055099	0.198110
H	-1.681328	-2.540624	0.622912
O	-2.832362	0.116245	0.715454
H	-2.860341	-0.861022	0.429357
H	-3.756556	0.364008	0.917906
O	-0.457005	-2.526808	1.545438
H	0.289390	-2.263529	0.921742
H	-0.619833	-1.679294	2.052864
O	1.358539	-1.620248	-0.210032
H	1.922630	-2.355455	-0.522507
H	2.017980	-0.958728	0.238321
O	0.572900	2.791216	-0.163627
H	0.679516	2.428067	0.780713
H	0.416578	3.751508	-0.066556
O	2.727528	1.777578	-1.283696
H	3.421460	2.435399	-1.489198
H	1.948912	2.313074	-0.916438
O	2.906513	0.139543	0.869582
H	2.255433	0.632132	1.450655
H	3.009161	0.760264	0.090187
O	0.960144	1.553359	2.105483
H	0.163932	0.969994	2.360794
H	1.166158	2.088017	2.897598
O	-1.252166	1.120884	-1.253508
H	-1.915034	0.884471	-0.549011
H	-0.683331	1.831582	-0.844856
O	1.683659	0.209910	-3.188455
H	1.378360	0.769095	-3.928492
H	2.148685	0.855201	-2.575447
O	-1.023628	-0.075467	2.583638
H	-1.404441	-0.063011	3.484752
H	-1.808768	0.087573	1.954306
O	-1.357661	-2.297902	-2.452390
H	-1.861177	-2.428690	-1.592571
H	-2.046060	-1.989911	-3.073567
Na	0.059992	-0.617781	-1.815500

Na – 16 water molecules

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O	2.494293	-2.368457	-1.010515
H	2.130511	-1.801244	-1.739274
H	3.170405	-2.930597	-1.420489
O	1.241773	-0.498598	-2.451119
H	1.872357	0.258907	-2.463869
H	0.762147	-0.333454	-1.594919
O	0.359016	2.791983	-0.890310
H	-0.363170	2.669956	-1.557542
H	-0.107375	3.061686	-0.060201
O	-1.960282	-1.967737	-0.807432
H	-1.780622	-1.512871	-1.659088

H	-1.160039	-2.516019	-0.636424
O	-2.541597	-0.790584	2.878770
H	-3.329638	-1.111454	3.340724
H	-1.881544	-1.533491	2.889490
O	2.850202	-0.176239	0.556398
H	3.028522	0.538178	-0.101154
H	2.920358	-1.017595	0.042930
O	-1.192825	3.024175	1.318397
H	-0.962828	2.380570	2.048338
H	-1.453766	3.845080	1.763167
O	2.757976	1.621320	-1.533836
H	2.016363	2.230862	-1.307516
H	3.460457	2.183326	-1.894922
O	-0.659880	1.189289	3.151967
H	-1.396552	0.552755	3.281936
H	0.158503	0.641283	3.112705
O	-2.951282	1.471299	-0.068078
H	-2.673101	1.689919	-0.986095
H	-2.468099	2.148639	0.460515
O	0.207367	-3.372068	0.043117
H	0.156305	-4.334662	-0.063271
H	1.080626	-3.108479	-0.346381
O	-1.715730	2.081594	-2.439026
H	-1.614836	1.163537	-2.806496
H	-2.116591	2.609447	-3.146164
O	-0.428158	-2.317674	2.474393
H	0.332539	-1.720626	2.663838
H	-0.185094	-2.769872	1.632178
O	-1.353855	-0.480553	-3.103001
H	-1.685605	-0.828779	-3.945453
H	-0.369311	-0.534378	-3.157157
O	0.244392	0.219512	-0.081233
H	0.263221	1.177495	-0.345150
H	1.135968	0.070769	0.316225
O	1.546062	-0.448403	2.915386
H	2.135602	-0.555020	3.677965
H	2.137454	-0.289593	2.141550
Na	-1.758044	-0.340303	0.751876

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O	2.365300	-2.342356	-0.978972
H	2.308563	-1.805975	-1.815063
H	3.138082	-2.918597	-1.088515
O	2.111220	-0.567792	-2.988760
H	2.698743	-0.629163	-3.757865
H	2.334050	0.293163	-2.552149
O	0.171105	2.837954	-1.002923
H	-0.551000	2.632794	-1.648537
H	-0.299662	3.073492	-0.163126
O	-2.122946	-2.193041	-0.811518
H	-1.802293	-1.803867	-1.648028
H	-1.361107	-2.760270	-0.544922
O	-2.741344	-0.674140	3.015596
H	-3.392849	-0.884496	3.700372
H	-2.069406	-1.392872	3.033587
O	2.563070	-0.139750	0.550082
H	2.751901	0.577966	-0.104213
H	2.663910	-0.992077	0.057376
O	-1.352836	2.998971	1.208916
H	-1.132096	2.401410	1.984148
H	-1.654941	3.833916	1.598284
O	2.554628	1.661370	-1.446837
H	1.749590	2.220863	-1.300617
H	3.279773	2.281510	-1.621067
O	-0.823265	1.328260	3.172509
H	-1.538597	0.665042	3.289251
H	0.015582	0.811825	3.136645
O	-3.103801	1.361892	-0.078734
H	-2.809913	1.495225	-1.007106
H	-2.600570	2.056931	0.407496
O	0.129296	-3.441137	0.076464
H	0.232101	-4.402741	0.142230
H	0.957236	-3.107637	-0.355981
O	-1.804571	1.769242	-2.482351
H	-1.397266	0.901422	-2.744790
H	-2.166229	2.155598	-3.294306
O	-0.561543	-1.888073	2.184243
H	0.235112	-1.405583	2.504536
H	-0.242863	-2.550753	1.528316
O	-0.601233	-0.623628	-2.632713
H	0.282289	-0.679300	-3.061215
H	-0.350099	-0.422462	-1.694038
O	-0.018403	0.233825	-0.165530
H	0.038405	1.181833	-0.431635
H	0.886647	0.018081	0.169632
O	1.445746	-0.200681	2.952651
H	2.063639	-0.373627	3.679140
H	1.996341	-0.116433	2.134508
Na	-1.940114	-0.470934	0.786892

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O	2.580184	-1.850861	-1.381479

H	2.173580	-1.215745	-2.032544
H	3.300403	-2.294731	-1.855671
O	1.466359	0.066552	-2.853343
H	1.812059	0.164014	-3.754893
H	1.798288	0.863452	-2.357041
O	-0.128010	2.908147	-0.865356
H	-0.897279	2.650655	-1.431860
H	-0.516131	3.016642	0.037191
O	-1.778336	-2.297770	-0.783293
H	-1.598815	-1.686510	-1.534184
H	-0.915531	-2.754879	-0.654806
O	-2.480114	-1.227881	3.016381
H	-3.179361	-1.590198	3.580074
H	-1.774944	-1.913491	2.976965
O	2.914425	0.057691	0.505532
H	2.927769	0.873961	-0.044473
H	2.977644	-0.684408	-0.145722
O	-1.391272	2.791586	1.548922
H	-1.754040	3.528312	2.064058
H	-1.095254	2.114010	2.222352
O	2.379399	2.073815	-1.319570
H	1.523064	2.541611	-1.137305
H	2.973985	2.733686	-1.707700
O	-0.694917	0.880738	3.236987
H	-1.359983	0.171888	3.374566
H	0.176825	0.431358	3.146143
O	-3.063894	0.969604	0.335119
H	-2.961593	1.265497	-0.597080
H	-2.615153	1.698168	0.823550
O	0.685154	-3.350597	-0.187494
H	0.858873	-4.277541	-0.412062
H	1.398994	-2.830975	-0.641471
O	-2.292193	1.887525	-2.127223
H	-1.944010	1.034661	-2.504280
H	-2.782143	2.324344	-2.839992
O	-0.202834	-2.328300	2.193575
H	0.547354	-1.753559	2.474176
H	0.139048	-2.820313	1.412105
O	-1.203716	-0.445142	-2.785656
H	-1.361971	-0.772077	-3.685507
H	-0.229705	-0.252318	-2.754634
O	0.196561	0.183498	-0.074188
H	0.101953	1.112894	-0.363396
H	1.128280	0.105460	0.210182
O	1.688704	-0.467545	2.852486
H	2.329800	-0.657459	3.554300
H	2.221118	-0.237627	2.051017
Na	-1.591409	-0.722066	0.876947
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O	2.435346	-2.519622	-0.875958
H	2.197725	-1.931144	-1.646086
H	3.140304	-3.102111	-1.199145
O	1.798436	-0.715411	-2.717364
H	2.209304	-0.806981	-3.591306
H	2.186640	0.110949	-2.325133
O	0.452565	2.749931	-0.901273
H	-0.284465	2.487911	-1.513800
H	-0.018357	3.061376	-0.090579
O	-1.791916	-2.114545	-0.553225
H	-2.585481	-2.651826	-0.693062
H	-1.070739	-2.758356	-0.326704
O	-3.885700	-0.387224	1.127368
H	-3.767584	0.495283	0.683744
H	-4.311747	-0.172484	1.970188
O	2.901082	-0.376452	0.718717
H	3.037249	0.325598	0.040026
H	2.886214	-1.224732	0.210067
O	-1.204166	3.254419	1.230566
H	-1.029990	2.558560	1.920457
H	-1.285463	4.089305	1.717186
O	2.763285	1.420135	-1.368719
H	2.011310	2.042793	-1.198779
H	3.490700	1.965295	-1.705937
O	-0.883442	1.146005	2.787326
H	-1.319422	1.135137	3.652829
H	0.042252	0.839477	2.951330
O	-3.195596	1.895659	-0.057678
H	-2.599872	2.468131	0.478941
H	-2.704445	1.805619	-0.911023
O	0.264876	-3.588837	0.282797
H	0.237474	-4.555473	0.220306
H	1.082624	-3.298773	-0.200464
O	-1.609569	1.724488	-2.239103
H	-1.362851	0.769734	-2.471296
H	-1.936444	2.126741	-3.058173
O	-0.328968	-1.917388	2.425010
H	0.439330	-1.361864	2.676784
H	0.010177	-2.574990	1.781246
O	-0.955897	-0.742797	-2.739516
H	0.024801	-0.718185	-2.661537
H	-1.257073	-1.232561	-1.935426

O	0.261210	0.109954	-0.055658
H	0.365739	1.039290	-0.344863
H	1.135841	-0.133487	0.302856
O	1.583098	-0.002530	3.017052
H	2.145133	-0.171043	3.788225
H	2.165612	-0.100966	2.222068
Na	-1.569028	-0.466704	1.106614

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O	2.149331	-2.385633	-0.550341
H	2.612997	-1.628551	-0.097620
H	2.833908	-3.054076	-0.709470
O	1.429487	-0.728130	-2.582996
H	1.960664	0.081497	-2.395680
H	1.792738	-1.428537	-1.989822
O	0.389259	2.808105	-0.985442
H	-0.348053	2.637022	-1.625680
H	-0.070407	3.086030	-0.154707
O	-2.335159	-1.819967	-0.837232
H	-2.009464	-1.433472	-1.681697
H	-1.615518	-2.438981	-0.572228
O	-2.394200	-0.759151	2.814600
H	-3.181206	-1.021728	3.313429
H	-1.727311	-1.503198	2.913488
O	3.179427	-0.150179	0.459774
H	3.062134	0.542980	-0.240977
H	4.117127	-0.121049	0.705749
O	-1.168620	3.098137	1.214083
H	-0.927819	2.457475	1.946207
H	-1.369631	3.938673	1.653406
O	2.666037	1.519205	-1.612975
H	1.925217	2.136133	-1.383372
H	3.346026	2.060979	-2.042419
O	-0.600030	1.282154	3.037962
H	-1.322634	0.627926	3.169775
H	0.205802	0.729305	2.889123
O	-3.043407	1.660965	-0.125409
H	-2.511112	2.316390	0.383713
H	-2.727019	1.803803	-1.046528
O	-0.265830	-3.288552	0.186502
H	-0.280458	-4.240716	0.002326
H	0.638448	-2.983471	-0.089921
O	-1.694093	2.029530	-2.480467
H	-1.535611	1.103474	-2.807945
H	-2.040797	2.525932	-3.237452
O	-0.392995	-2.460494	2.763497
H	0.342276	-1.803719	2.721153
H	-0.388871	-2.868671	1.863984
O	-1.217410	-0.541911	-3.035760
H	-1.453477	-0.882901	-3.912653
H	-0.233833	-0.660277	-2.959923
O	0.221757	0.173249	-0.088445
H	0.306025	1.121411	-0.337509
H	0.512419	-0.279504	-0.901305
O	1.478837	-0.443751	2.609496
H	2.157538	-0.448553	3.302709
H	1.974538	-0.263569	1.773080
Na	-1.871465	-0.177206	0.665820

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O	2.372331	-2.343946	-0.847708
H	2.040299	-1.798062	-1.632076
H	3.026386	-2.972898	-1.213379
O	1.184063	-0.582004	-2.410561
H	1.820254	0.192732	-2.398314
H	0.695991	-0.405749	-1.536110
O	0.323562	2.645423	-0.822497
H	-0.419470	2.540438	-1.497525
H	-0.147082	2.955706	0.018534
O	-2.105236	-1.978964	-1.207428
H	-1.832721	-1.505224	-2.039192
H	-1.299175	-2.496595	-0.929658
O	-2.191775	-0.886211	2.714601
H	-2.914311	-1.190504	3.296365
H	-1.437900	-1.582532	2.798149
O	2.807668	-0.165577	0.650236
H	2.950662	0.523877	-0.066571
H	2.840598	-1.043503	0.163668
O	-1.155001	3.002387	1.325341
H	-0.938477	2.358620	2.105372
H	-1.388628	3.858291	1.734742
O	2.647663	1.486848	-1.476745
H	1.894403	2.111097	-1.251562
H	3.359566	2.049250	-1.840447
O	-0.686448	1.310182	3.214853
H	-1.345380	0.557806	3.154114
H	0.191217	0.837854	3.124638
O	-2.981947	1.497697	-0.008425
H	-2.692940	1.714127	-0.938388
H	-2.442109	2.147722	0.527321
O	0.006311	-3.195356	0.048564
H	-0.041345	-4.172300	0.023009

H	0.930396	-2.981159	-0.296637
O	-1.748443	2.029941	-2.379310
H	-1.599254	1.149025	-2.856367
H	-2.117720	2.637935	-3.049535
O	-0.110318	-2.413500	2.655390
H	0.572535	-1.684787	2.741313
H	-0.038364	-2.735315	1.707973
O	-1.284244	-0.396557	-3.325327
H	-1.484242	-0.639911	-4.251038
H	-0.285275	-0.484665	-3.225486
O	0.206430	0.118718	-0.050100
H	0.226461	1.100966	-0.310474
H	1.107932	-0.022704	0.364143
O	1.515326	-0.259063	2.955117
H	2.112539	-0.325937	3.726453
H	2.116667	-0.138476	2.158986
Na	-1.908862	-0.462316	0.497724

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O	2.258565	-2.293299	-0.980888
H	2.207075	-1.746027	-1.835148
H	2.984682	-2.933360	-1.122139
O	1.986846	-0.588409	-2.972061
H	2.534389	-0.647397	-3.779849
H	2.248461	0.278037	-2.521982
O	0.206425	2.708795	-0.899938
H	-0.510427	2.558824	-1.595157
H	-0.303237	3.004590	-0.076286
O	-2.182078	-2.199271	-0.995336
H	-1.761523	-1.768705	-1.783793
H	-1.402700	-2.693154	-0.605927
O	-2.346784	-0.862174	2.738649
H	-3.031940	-1.170525	3.362088
H	-1.559697	-1.523412	2.823227
O	2.522018	-0.201528	0.614254
H	2.713262	0.511115	-0.068053
H	2.588365	-1.067356	0.102160
O	-1.380176	3.029195	1.174420
H	-1.177380	2.412671	1.980542
H	-1.650094	3.888619	1.553046
O	2.520402	1.521012	-1.434492
H	1.718761	2.104727	-1.245521
H	3.251521	2.133382	-1.650717
O	-0.919798	1.412824	3.132231
H	-1.551695	0.636031	3.107044
H	-0.027589	0.964687	3.058242
O	-3.153177	1.494562	-0.203760
H	-2.815182	1.656829	-1.127136
H	-2.623146	2.157400	0.327174
O	0.039515	-3.224549	0.178858
H	0.092078	-4.201459	0.185881
H	0.873990	-2.929603	-0.306989
O	-1.731758	1.865152	-2.508334
H	-1.347861	0.949720	-2.720976
H	-1.987851	2.261209	-3.364337
O	-0.210387	-2.309739	2.729348
H	0.447983	-1.557485	2.813009
H	-0.079320	-2.670010	1.803293
O	-0.644377	-0.531867	-2.561592
H	0.254182	-0.615153	-2.996241
H	-0.367878	-0.362803	-1.603432
O	-0.053853	0.169464	-0.063958
H	0.030677	1.139296	-0.326369
H	0.870633	-0.061927	0.255554
O	1.324652	-0.097043	2.953565
H	1.953914	-0.102344	3.701682
H	1.889238	-0.055934	2.121103
Na	-2.164342	-0.438405	0.526399

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O	2.372985	-1.893454	-1.158352
H	2.061885	-1.283347	-1.908187
H	3.101312	-2.425050	-1.537558
O	1.489660	-0.090743	-2.863942
H	1.923104	-0.052466	-3.740468
H	1.794418	0.750135	-2.376733
O	-0.096526	2.849037	-0.633143
H	-0.851850	2.598629	-1.255162
H	-0.540842	2.915615	0.273123
O	-1.971727	-2.247195	-1.174579
H	-1.684413	-1.631677	-1.905341
H	-1.119007	-2.694680	-0.908832
O	-1.975029	-1.353667	2.736165
H	-2.611517	-1.777169	3.343403
H	-1.130043	-1.943806	2.745204
O	2.884738	0.101342	0.543733
H	2.818801	0.880383	-0.082393
H	2.853053	-0.702891	-0.060664
O	-1.495470	2.701353	1.601074
H	-1.812880	3.489971	2.083114
H	-1.163513	2.041053	2.325264
O	2.253124	1.927593	-1.352661

H	1.407248	2.409362	-1.064912
H	2.841932	2.611419	-1.728881
O	-0.727179	0.972936	3.354092
H	-1.292559	0.151504	3.252595
H	0.191746	0.625001	3.160024
O	-3.237456	1.088159	0.276521
H	-2.997101	1.395429	-0.641835
H	-2.735833	1.746836	0.837951
O	0.335857	-3.222512	-0.111161
H	0.500095	-4.179529	-0.227398
H	1.133314	-2.770235	-0.542657
O	-2.117390	1.889958	-2.065647
H	-1.773532	1.044586	-2.514372
H	-2.532544	2.420431	-2.773880
O	0.284220	-2.584809	2.519198
H	0.870811	-1.775964	2.605430
H	0.346808	-2.847785	1.552043
O	-1.142741	-0.365250	-2.991995
H	-1.344431	-0.553509	-3.930569
H	-0.134115	-0.258267	-2.954908
O	0.124426	0.167235	-0.021288
H	0.055420	1.134481	-0.241973
H	1.057732	0.070932	0.284568
O	1.634309	-0.253353	2.829825
H	2.285199	-0.294675	3.558178
H	2.170498	-0.040260	1.999017
Na	-1.817785	-0.723315	0.549367

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O	2.477789	-2.302123	-0.733355
H	2.237694	-1.758137	-1.563146
H	3.204754	-2.896362	-1.007780
O	1.806243	-0.667899	-2.656841
H	2.257115	-0.761290	-3.519818
H	2.175382	0.185427	-2.251781
O	0.377222	2.626035	-1.046703
H	-0.393054	2.335299	-1.638120
H	-0.065744	2.914251	-0.188439
O	-1.835167	-2.093088	-0.655745
H	-2.585787	-2.693755	-0.828324
H	-1.067063	-2.704032	-0.413936
O	-3.827060	-0.124593	1.368808
H	-3.675904	0.704571	0.802025
H	-4.061948	0.239313	2.243914
O	2.905752	-0.190214	0.841271
H	2.983894	0.520530	0.139281
H	2.895575	-1.047449	0.313839
O	-1.048656	3.103909	1.143347
H	-0.869115	2.406307	1.861429
H	-1.074932	3.967705	1.599883
O	2.686153	1.432580	-1.307819
H	1.856144	2.013503	-1.218739
H	3.380808	2.003485	-1.691029
O	-0.798386	1.073932	2.752690
H	-1.216329	1.169480	3.630560
H	0.110844	0.664653	2.933349
O	-3.196095	1.980857	-0.088775
H	-2.495133	2.478737	0.421741
H	-2.731811	1.778871	-0.955066
O	0.284201	-3.441070	0.193920
H	0.361654	-4.410491	0.096358
H	1.142436	-3.060068	-0.188090
O	-1.704409	1.610351	-2.304451
H	-1.404861	0.644161	-2.561222
H	-2.028030	2.020605	-3.130419
O	-0.465303	-2.195056	2.498391
H	0.309083	-1.636989	2.775644
H	-0.104926	-2.750724	1.754051
O	-0.927599	-0.769124	-2.831891
H	0.063256	-0.716343	-2.709137
H	-1.250181	-1.270157	-2.022638
O	0.248311	0.006420	-0.082821
H	0.289219	0.933689	-0.431957
H	1.138717	-0.103312	0.332468
O	1.441340	-0.281360	3.031178
H	1.995703	-0.192943	3.830886
H	2.067112	-0.183788	2.242457
Na	-1.558801	-0.569000	1.150447

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O	2.130552	-2.398597	-0.719993
H	2.574526	-1.669303	-0.167573
H	2.828920	-3.057709	-0.905388
O	1.298356	-0.707109	-2.597636
H	1.848402	0.091808	-2.343426
H	1.669168	-1.453986	-2.033972
O	0.408849	2.735155	-0.902788
H	-0.334731	2.540071	-1.554836
H	-0.077538	3.011336	-0.059636
O	-2.316087	-1.979939	-1.046674
H	-1.961108	-1.552639	-1.875032
H	-1.554796	-2.539578	-0.724261

O	-2.290152	-0.713163	2.702871
H	-3.014931	-0.971177	3.303593
H	-1.553065	-1.428604	2.808008
O	3.072119	-0.303340	0.570954
H	2.955399	0.418467	-0.132958
H	4.022798	-0.292767	0.802613
O	-1.126424	3.116261	1.210569
H	-0.912560	2.468728	1.989921
H	-1.294667	3.988599	1.617548
O	2.592138	1.362726	-1.428942
H	1.846675	2.015883	-1.220634
H	3.317142	1.887743	-1.821818
O	-0.652856	1.407390	3.070466
H	-1.354706	0.692476	3.066226
H	0.190791	0.892298	2.895266
O	-3.038686	1.668304	-0.059986
H	-2.467790	2.305730	0.458094
H	-2.697069	1.810217	-0.987722
O	-0.225590	-3.238202	0.170838
H	-0.223220	-4.216188	0.161956
H	0.690230	-2.975433	-0.166676
O	-1.680362	1.979313	-2.393176
H	-1.543822	1.050841	-2.779775
H	-2.026730	2.524589	-3.126628
O	-0.257520	-2.293859	2.707542
H	0.449452	-1.580400	2.683242
H	-0.231944	-2.690215	1.785561
O	-1.261408	-0.521914	-3.116484
H	-1.450061	-0.785599	-4.038917
H	-0.257777	-0.626790	-3.002196
O	0.159997	0.099513	-0.102748
H	0.268106	1.070742	-0.297727
H	0.437381	-0.301532	-0.962447
O	1.461186	-0.213976	2.689813
H	2.095763	-0.226570	3.434064
H	2.033910	-0.171130	1.858972
Na	-1.970699	-0.304042	0.485830

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O	3.249398	-0.435490	-0.954015
H	3.353233	0.462949	-1.359352
H	2.897555	-0.997798	-1.685117
O	3.602345	0.001817	1.792029
H	3.679654	-0.266015	0.848609
H	4.479695	-0.141024	2.179254
O	-0.804960	2.866160	-0.950257
H	0.099598	3.222060	-0.818764
H	-1.194663	2.918930	-0.049443
O	3.081337	2.039853	-1.950726
H	3.730612	2.499894	-2.504163
H	2.681765	2.736295	-1.361751
O	-2.161067	-1.912302	1.587289
H	-1.371307	-2.332389	1.162032
H	-2.303279	-1.052313	1.098367
O	-1.845154	2.715293	1.562568
H	-2.563883	3.241340	1.945180
H	-1.263105	2.448424	2.337061
O	1.877891	-1.584952	-3.049642
H	2.139134	-2.196537	-3.754056
H	0.963818	-1.853015	-2.769531
O	-3.179015	-2.318204	-2.397668
H	-3.479633	-2.728894	-1.536255
H	-3.531953	-2.880940	-3.103459
O	-2.547379	0.376739	0.375465
H	-2.393573	1.253795	0.802636
H	-2.946594	0.509759	-0.512978
O	-2.961833	0.343576	-2.277243
H	-3.190998	-0.607759	-2.431453
H	-3.634405	0.860452	-2.743182
O	-0.546454	-1.791061	-1.981975
H	-0.323747	-2.236379	-1.130228
H	-1.436685	-2.131581	-2.235575
O	1.362439	-1.510460	2.202865
H	0.725363	-1.219551	2.902604
H	2.214539	-1.025544	2.295178
O	-3.865103	-3.315059	-0.022735
H	-3.315741	-2.847246	0.654463
H	-4.772986	-3.045008	0.186558
O	0.060835	-2.928927	0.418511
H	0.704454	-2.530640	1.059276
H	0.168488	-3.889866	0.491358
O	-0.769463	-0.791476	3.598180
H	-1.396175	-1.234109	2.963539
H	-0.935621	-1.203986	4.460478
O	1.782395	3.686052	-0.345017
H	1.912081	3.251977	0.538619
H	2.055213	4.610345	-0.237579

O	0.847780	0.206864	0.128335
H	1.706514	-0.020229	-0.317055
H	0.825007	-0.455168	0.857131
O	0.843157	0.964014	-3.205001
H	1.608223	1.465613	-2.844380
H	1.228430	0.071850	-3.346882
O	1.822003	2.063346	1.768552
H	1.326762	1.460266	1.149594
H	2.636425	1.530703	1.927301
O	-0.264505	1.909652	3.513213
H	0.589708	1.967845	3.025337
H	-0.466021	0.947610	3.573974
Na	-0.717837	0.581305	-1.482952

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O	2.948141	-0.422974	-1.051043
H	2.984701	0.479330	-1.466655
H	2.626291	-0.989105	-1.795754
O	3.625164	-0.145039	1.616642
H	3.592097	-0.359244	0.655755
H	4.533888	-0.328589	1.899809
O	-0.862504	2.804125	-0.805812
H	0.046507	3.120268	-0.613310
H	-1.309959	2.882298	0.063240
O	2.611830	1.989840	-2.113034
H	3.294006	2.436381	-2.637599
H	2.360698	2.628430	-1.389760
O	-1.870725	-1.951254	1.703872
H	-1.135486	-2.461895	1.284507
H	-1.488772	-1.538665	2.515856
O	-2.018617	2.673985	1.712357
H	-2.806523	3.188940	1.945995
H	-2.361724	1.812329	1.355843
O	1.664813	-1.455465	-3.199440
H	1.912123	-2.145815	-3.833120
H	0.832582	-1.774887	-2.748720
O	-3.023205	-2.159599	-2.697880
H	-3.408506	-2.181127	-1.783381
H	-3.395338	-2.924301	-3.162364
O	-2.505855	0.373868	0.457272
H	-3.351000	0.013246	0.129287
H	-2.154051	-0.407820	0.955018
O	-2.459126	0.557301	-3.109276
H	-2.679686	-0.396832	-3.160714
H	-1.593426	0.654245	-3.547932
O	-0.517629	-1.859173	-1.797918
H	-0.306120	-2.414414	-1.013776
H	-1.373743	-2.175492	-2.175017
O	1.478644	-1.720796	2.284210
H	0.875476	-1.293264	2.944406
H	2.318921	-1.208405	2.241824
O	-3.873382	-1.959195	-0.154229
H	-3.256632	-2.135015	0.590299
H	-4.711619	-2.365506	0.115663
O	0.215052	-3.169060	0.473358
H	0.844093	-2.767477	1.125655
H	0.249135	-4.127358	0.616342
O	-0.527527	-0.626636	3.662969
H	-0.469852	0.378240	3.717576
H	-0.615649	-0.928817	4.580437
O	1.729648	3.484371	-0.134276
H	1.886180	3.016663	0.730268
H	2.076264	4.383533	-0.028231
O	0.690167	0.078196	0.311116
H	1.505082	-0.100507	-0.235432
H	0.744834	-0.641579	0.976813
O	0.372922	0.950957	-3.396221
H	1.100749	1.496820	-3.023053
H	0.820108	0.085826	-3.532631
O	1.823383	1.866169	1.949754
H	1.268733	1.283187	1.364532
H	2.647710	1.328684	2.010465
O	-0.296174	1.997606	3.698690
H	-0.960025	2.295940	3.029325
H	0.559530	2.056643	3.217395
Na	-0.894054	0.501464	-1.270967

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O	3.336901	0.064060	-0.901547
H	3.429558	0.978962	-1.269841
H	2.975554	-0.476548	-1.646147
O	3.545201	-0.088256	1.764072
H	3.626303	-0.133846	0.778125
H	4.420833	-0.314451	2.114247
O	-1.069807	2.807479	-0.713034
H	-0.179282	3.090655	-0.406912
H	-1.633001	2.871342	0.085226
O	3.086730	2.577211	-1.777319
H	3.691414	3.231078	-2.158725
H	2.572959	3.044536	-1.061653
O	-2.264161	-2.323118	1.546502
H	-1.446384	-2.642854	1.088612

H	-2.446381	-1.442267	1.111783
O	-2.476808	2.456064	1.648856
H	-3.032099	2.909782	2.300456
H	-1.620148	2.248475	2.108394
O	2.034408	-1.082310	-2.990032
H	2.367260	-1.581585	-3.750677
H	1.139828	-1.457363	-2.774017
O	-2.969469	-2.407771	-2.525926
H	-3.281664	-2.918183	-1.723801
H	-3.287104	-2.902113	-3.296955
O	-2.558470	0.032530	0.431336
H	-2.688946	0.878747	0.917936
H	-2.931086	0.165435	-0.470580
O	-2.918082	0.254525	-2.218739
H	-3.096381	-0.693911	-2.444025
H	-3.667746	0.759836	-2.565132
O	-0.388393	-1.645750	-2.062835
H	-0.203348	-2.148183	-1.230519
H	-1.238708	-2.024851	-2.387452
O	1.416222	-1.733046	2.044403
H	0.759681	-1.428153	2.716118
H	2.243220	-1.199361	2.131914
O	-3.725940	-3.702656	-0.329766
H	-3.278521	-3.269537	0.438111
H	-4.667085	-3.512239	-0.192927
O	0.006060	-2.987897	0.219871
H	0.680157	-2.627850	0.854411
H	0.223275	-3.926370	0.104364
O	-0.778859	-0.913745	3.366310
H	-1.411309	-1.462021	2.833774
H	-0.914655	-1.184692	4.287975
O	1.515236	3.502111	0.128131
H	1.917527	3.101219	0.956606
H	1.582884	4.460775	0.263188
O	0.836877	0.314612	0.251113
H	1.730726	0.372578	-0.163182
H	0.915746	-0.492984	0.805177
O	0.884873	1.415709	-3.015340
H	1.613432	1.966211	-2.654908
H	1.336537	0.564161	-3.203766
O	-0.097839	1.586810	2.487893
H	-0.375685	0.743432	2.922490
H	0.226425	1.283324	1.603591
O	2.544465	2.417001	2.313597
H	2.982982	1.554690	2.115906
H	1.673611	2.148644	2.678000
Na	-0.710249	0.628729	-1.406387
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O	3.244290	0.132695	-0.608792
H	3.008035	-0.566796	-1.268638
H	3.186609	0.968730	-1.140880
O	3.342265	0.061019	2.130684
H	3.503812	0.004630	1.158218
H	4.201810	-0.103060	2.549255
O	-0.847979	2.617469	-0.993420
H	-0.015102	2.977650	-0.612206
H	-1.489471	2.725239	-0.260249
O	2.605936	2.296999	-2.062413
H	3.275636	2.829471	-2.518530
H	2.252777	2.873981	-1.328930
O	-2.475164	-2.179255	1.633879
H	-1.661297	-2.659270	1.339087
H	-2.160742	-1.709709	2.440625
O	-2.414967	2.444297	1.289368
H	-3.202102	2.876673	1.653316
H	-2.706070	1.552184	0.963504
O	2.230524	-1.441299	-2.579265
H	2.647599	-2.128741	-3.119694
H	1.374838	-1.826402	-2.239263
O	-2.451432	-2.394866	-2.879058
H	-3.127935	-2.362131	-2.155508
H	-2.783967	-3.035540	-3.525283
O	-2.667527	0.049075	0.158149
H	-3.415676	-0.257231	-0.389742
H	-2.534526	-0.735580	0.755052
O	-1.935917	0.348675	-3.234791
H	-2.128820	-0.610382	-3.303743
H	-1.006990	0.458968	-3.533816
O	-0.143375	-1.985221	-1.577801
H	-0.137780	-2.509959	-0.740796
H	-0.899368	-2.317766	-2.118254
O	1.277761	-1.683910	2.463567
H	0.561100	-1.339764	3.051964
H	2.071269	-1.103340	2.544877
O	-4.141178	-2.025986	-0.802835
H	-3.821684	-2.339182	0.066602
H	-5.062246	-2.325969	-0.855828
O	-0.111103	-3.203632	0.829138
H	0.543770	-2.756629	1.425242
H	0.068450	-4.154279	0.897238
O	-1.006509	-0.748378	3.510475

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H	-1.165426	-0.742520	4.467469
O	1.523998	3.555020	-0.024113
H	1.896689	3.213707	0.844907
H	1.616383	4.519802	0.011447
O	0.785406	0.227902	0.504103
H	1.690939	0.293795	0.105166
H	0.862241	-0.560665	1.087053
O	0.801515	0.740343	-3.466111
H	1.342231	1.441906	-3.037026
H	1.343499	-0.066508	-3.313106
O	2.386093	2.650544	2.296301
H	1.493179	2.453268	2.652067
H	2.810273	1.760743	2.251535
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H	-1.019072	2.084104	2.243582
H	0.196651	1.236310	1.782358
Na	-0.731558	0.307574	-1.191550

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O	3.549958	-0.146390	-0.423591
H	3.648257	0.803246	-0.692054
H	3.280422	-0.583023	-1.267811
O	3.183680	-0.421939	2.386864
H	3.500078	-0.394907	1.455472
H	3.961749	-0.654478	2.916261
O	-0.805642	2.968271	-0.498919
H	0.060459	3.228259	-0.117109
H	-1.381660	2.838302	0.285006
O	3.340606	2.427193	-1.187101
H	4.031998	3.032446	-1.494958
H	2.831592	2.918337	-0.488987
O	-2.311382	-2.751958	1.054717
H	-3.048295	-2.529572	0.442987
H	-1.549481	-2.997786	0.476085
O	-2.387780	2.247345	1.632176
H	-3.253741	2.609624	1.873767
H	-1.963009	1.933204	2.486402
O	2.399011	-0.846988	-2.819663
H	2.807654	-1.308580	-3.567714
H	1.465898	-1.184441	-2.776141
O	-2.751343	-1.715827	-3.192970
H	-3.318071	-1.784294	-2.381135
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O	-0.163163	-1.377076	-2.364016
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O	-3.980099	-1.644030	-0.837246
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O	-0.003064	-3.136732	-0.300806
H	0.557709	-2.888277	0.475602
H	0.255887	-4.039698	-0.542420
O	-1.244895	-1.492467	3.107690
H	-1.780220	-1.973964	2.417647
H	-1.431861	-1.955031	3.940201
O	1.718292	3.465521	0.649232
H	1.647313	2.859350	1.432108
H	1.887536	4.346533	1.018108
O	0.941662	0.071683	0.243805
H	1.889699	0.025333	-0.041533
H	0.830787	-0.769034	0.745616
O	1.232837	1.671765	-2.892208
H	1.924716	2.096704	-2.340755
H	1.652986	0.805545	-3.081595
O	1.255447	1.519121	2.431994
H	0.989685	1.042970	1.597190
H	2.047385	0.993775	2.688486
O	-1.133610	1.205623	3.709829
H	-0.211345	1.368963	3.398432
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Na	-0.517925	0.807929	-1.403496

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O	3.113497	-0.163397	-0.913885
H	3.194734	0.723753	-1.395577
H	2.821805	-0.803669	-1.637137
O	3.528359	-0.077144	1.737546
H	3.583455	-0.192199	0.741714
H	4.427663	-0.258726	2.074685
O	-0.701596	2.861100	-0.989918
H	0.199289	3.225273	-0.779986
H	-1.140849	2.822017	-0.092847

O	2.949845	2.159725	-2.157919
H	3.722953	2.571306	-2.591659
H	2.633855	2.824368	-1.457097
O	-2.148287	-1.873411	1.648914
H	-1.371958	-2.325699	1.198918
H	-2.372209	-1.020899	1.115972
O	-1.900502	2.497722	1.402186
H	-2.562149	3.145858	1.714796
H	-1.299322	2.293619	2.220234
O	1.952058	-1.492827	-2.902235
H	2.293347	-2.199207	-3.484466
H	1.024761	-1.784410	-2.604670
O	-3.000213	-2.280009	-2.285527
H	-3.407731	-2.595231	-1.400377
H	-3.418391	-2.821969	-2.983020
O	-2.997218	0.250943	0.495542
H	-2.604043	1.111161	0.843502
H	-3.033585	0.343055	-0.500500
O	-2.830212	0.335169	-2.185614
H	-3.041188	-0.637081	-2.363712
H	-3.523700	0.851248	-2.638838
O	-0.411510	-1.806975	-1.887936
H	-0.241287	-2.297698	-1.030312
H	-1.313664	-2.132241	-2.178453
O	1.437151	-1.713927	2.121997
H	0.799339	-1.352810	2.813651
H	2.285505	-1.175278	2.143645
O	-3.976800	-3.022955	0.033734
H	-3.360267	-2.661938	0.744707
H	-4.787411	-2.488213	0.152564
O	-0.043322	-3.041900	0.442692
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H	0.000260	-4.016352	0.511373
O	-0.618072	-0.780242	3.513269
H	-1.308945	-1.207432	2.897499
H	-0.785275	-1.168688	4.395413
O	1.856607	3.627141	-0.300507
H	1.949973	3.123433	0.576741
H	2.115244	4.551151	-0.114858
O	0.766883	0.160060	0.266026
H	1.644257	0.043163	-0.237308
H	0.841935	-0.582667	0.933816
O	0.831053	0.953592	-3.387791
H	1.574923	1.522067	-3.046779
H	1.272199	0.062890	-3.436511
O	1.803761	2.029180	1.776684
H	1.274480	1.373901	1.202135
H	2.615006	1.471631	1.947425
O	-0.366919	1.916478	3.394892
H	0.526643	2.015374	2.958345
H	-0.474314	0.924706	3.489512
Na	-0.600135	0.594747	-1.533584

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O	3.059027	-0.115550	-1.004448
H	3.004125	0.765437	-1.497252
H	2.729181	-0.775636	-1.692654
O	3.575460	-0.136736	1.652658
H	3.589267	-0.189335	0.651241
H	4.489443	-0.336081	1.936068
O	-0.815997	2.882892	-0.832361
H	0.098263	3.224087	-0.639838
H	-1.233556	2.871030	0.071705
O	2.486008	2.141407	-2.280835
H	3.166242	2.569229	-2.837843
H	2.289743	2.799061	-1.532773
O	-2.088070	-1.950322	1.736756
H	-1.372416	-2.515393	1.311003
H	-1.625982	-1.570291	2.547169
O	-1.932333	2.478997	1.647138
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H	-2.291167	1.621056	1.234795
O	1.779213	-1.484123	-2.882083
H	2.066687	-2.171969	-3.513413
H	0.895953	-1.805436	-2.477916
O	-2.967065	-2.006461	-2.473351
H	-3.470385	-2.031216	-1.597252
H	-3.316304	-2.750889	-3.001340
O	-2.492170	0.275533	0.386773
H	-3.393220	0.010594	0.090233
H	-2.227063	-0.541827	0.931316
O	-2.343944	0.610720	-3.167479
H	-2.583641	-0.347876	-3.072080
H	-1.408969	0.620253	-3.497490
O	-0.454699	-1.878218	-1.686870
H	-0.325726	-2.456935	-0.881216
H	-1.366755	-2.096520	-2.050746
O	1.490636	-1.791951	2.080834
H	0.877003	-1.433989	2.801819
H	2.343869	-1.262891	2.077917
O	-4.155519	-1.834703	-0.090288
H	-3.573570	-2.076287	0.679388

H	-5.003526	-2.291125	0.075830
O	-0.058450	-3.245886	0.573204
H	0.682902	-2.828613	1.117344
H	0.031278	-4.214075	0.673489
O	-0.468151	-0.868553	3.569678
H	-0.395441	0.173621	3.586009
H	-0.522289	-1.137685	4.508359
O	1.769312	3.592694	-0.229196
H	1.927277	3.083220	0.634504
H	2.053123	4.512884	-0.063963
O	0.787770	0.155586	0.339610
H	1.632111	0.055571	-0.216409
H	0.873082	-0.625325	0.962453
O	0.410191	0.794228	-3.430602
H	1.082882	1.448001	-3.090072
H	0.929749	-0.058644	-3.413125
O	1.860553	1.986906	1.848900
H	1.315706	1.337496	1.278767
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H	2.791315	-0.357800	-1.576310
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H	4.398710	-0.211150	2.036742
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H	-0.009301	3.109352	-0.364541
H	-1.480736	2.796443	0.043191
O	2.711969	2.630960	-1.928104
H	3.479727	3.150340	-2.237741
H	2.347980	3.111056	-1.106072
O	-2.043698	-2.078088	1.474694
H	-1.265065	-2.457204	0.964827
H	-2.346360	-1.219205	0.998812
O	-2.330428	2.311689	1.472842
H	-2.880779	2.887958	2.038476
H	-1.528632	2.034766	2.034166
O	2.077008	-1.094989	-2.901059
H	2.522147	-1.711055	-3.514740
H	1.178843	-1.508544	-2.666537
O	-2.798000	-2.350080	-2.507744
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H	-3.158970	-2.892971	-3.235755
O	-3.119939	-0.002752	0.396203
H	-2.900859	0.890352	0.797971
H	-3.115868	0.135357	-0.595942
O	-2.816632	0.258297	-2.260570
H	-2.953659	-0.710600	-2.512652
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O	-0.263858	-1.723000	-1.992540
H	-0.079809	-2.282036	-1.180995
H	-1.129730	-2.085902	-2.343243
O	1.561973	-1.886584	2.005248
H	0.911113	-1.611530	2.720617
H	2.356589	-1.269708	2.042962
O	-3.829600	-3.176054	-0.233672
H	-3.220091	-2.870325	0.506728
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O	0.106571	-3.122705	0.241658
H	0.811639	-2.785016	0.882637
H	0.167006	-4.098545	0.250211
O	-0.550243	-1.088630	3.425620
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O	1.589585	3.558997	0.222798
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H	1.658411	4.519607	0.391853
O	0.670665	0.160517	0.394156
H	1.566805	0.318740	-0.057265
H	0.864067	-0.678125	0.899275
O	0.755158	1.256617	-3.264799
H	1.432109	1.888054	-2.900160
H	1.286460	0.419417	-3.354577
O	-0.136163	1.406903	2.573018
H	-0.342211	0.555219	3.069478
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H	1.481642	2.079168	2.698913
Na	-0.639189	0.615153	-1.460479

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H	2.867661	-0.594907	-1.220872
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H	0.063873	3.077735	-0.594079
H	-1.438635	2.846846	-0.264927
O	2.604244	2.259322	-2.022851
H	3.339797	2.734037	-2.457753
H	2.298649	2.857553	-1.257215
O	-2.252183	-1.998605	1.549709
H	-1.474159	-2.556269	1.240132
H	-1.920272	-1.598412	2.408549
O	-2.426721	2.501027	1.163493
H	-3.246482	2.908240	1.504990
H	-2.687544	1.592690	0.791176
O	2.165042	-1.438698	-2.482088
H	2.608141	-2.136222	-3.003247
H	1.254443	-1.811531	-2.202183
O	-2.539197	-2.259132	-2.793807
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H	-2.757157	-3.054150	-3.318566
O	-2.600484	0.154393	0.062719
H	-3.401786	-0.229760	-0.367598
H	-2.363359	-0.605695	0.694067
O	-1.943654	0.386306	-3.423846
H	-2.141897	-0.583462	-3.365659
H	-0.974363	0.446269	-3.628343
O	-0.191743	-1.971691	-1.620292
H	-0.155652	-2.537924	-0.795595
H	-1.021030	-2.244806	-2.121035
O	1.306921	-1.773578	2.346518
H	0.601034	-1.409175	2.964048
H	2.103840	-1.162671	2.398563
O	-4.023059	-2.065825	-0.583994
H	-3.568407	-2.262107	0.277187
H	-4.908113	-2.473240	-0.508762
O	-0.056674	-3.278495	0.701400
H	0.616950	-2.840222	1.311579
H	0.038203	-4.243159	0.827976
O	-0.884812	-0.779057	3.510064
H	-0.762208	0.200066	3.247703
H	-1.051302	-0.780942	4.473466
O	1.629907	3.532979	0.024972
H	1.899813	3.153991	0.946495
H	1.768384	4.498512	0.090643
O	0.662966	0.165265	0.535347
H	1.588313	0.257032	0.132968
H	0.767322	-0.658410	1.090643
O	0.792926	0.715547	-3.367090
H	1.361624	1.436206	-2.978643
H	1.358135	-0.095396	-3.220937
O	2.183596	2.585845	2.376906
H	1.243422	2.348639	2.614784
H	2.629486	1.691998	2.306225
O	-0.341620	1.580582	2.507957
H	-1.156492	2.041725	2.127965
H	0.070613	1.131729	1.696438
Na	-0.696735	0.408696	-1.288562
61			
O	3.219904	0.021085	-0.491630
H	3.223785	0.982439	-0.804523
H	3.010137	-0.488698	-1.335527
O	3.235732	-0.518349	2.180804
H	3.424506	-0.378578	1.206777
H	4.089844	-0.791709	2.569984
O	-0.780048	2.982794	-0.393128
H	0.083442	3.271040	0.006759
H	-1.347364	2.805453	0.406578
O	2.800802	2.490130	-1.369036
H	3.552844	3.022524	-1.696248
H	2.439324	2.991996	-0.563957
O	-2.318526	-2.388289	1.044264
H	-3.057657	-2.385589	0.378755
H	-1.549630	-2.842712	0.578542
O	-2.303625	2.161469	1.717118
H	-3.097060	2.596862	2.085229
H	-1.772783	1.804667	2.529559
O	2.258562	-0.952680	-2.772233
H	2.649038	-1.506971	-3.475806
H	1.326483	-1.329316	-2.581048
O	-2.431300	-1.440677	-3.378999
H	-3.068825	-1.605908	-2.612454
H	-2.703823	-2.054661	-4.088666
O	-2.490157	0.155480	0.043683
H	-2.574774	0.903054	0.721241
H	-2.229914	-0.647316	0.572662
O	-1.771912	1.253345	-3.353863
H	-1.995063	0.301267	-3.523659
H	-0.792100	1.320146	-3.493549
O	-0.142391	-1.528933	-2.061417
H	-0.145626	-2.265573	-1.384528
H	-0.945333	-1.663917	-2.650373

O	1.116071	-2.151995	1.918874
H	0.397799	-1.931144	2.587801
H	1.958711	-1.664974	2.171438
O	-3.871452	-1.698516	-1.138871
H	-3.584827	-0.808787	-0.754451
H	-4.846952	-1.651280	-1.198582
O	-0.098377	-3.324538	-0.079430
H	0.518558	-3.012384	0.655768
H	0.049458	-4.285754	-0.178046
O	-1.111618	-1.493724	3.232195
H	-1.733577	-1.827187	2.515374
H	-1.340561	-2.013276	4.029086
O	1.666320	3.534886	0.745978
H	1.709822	2.873797	1.515289
H	1.906925	4.405909	1.117799
O	0.754882	0.089446	0.466879
H	1.683309	0.077303	0.053661
H	0.739511	-0.797889	0.934854
O	0.974654	1.417519	-3.078797
H	1.581774	1.985250	-2.526195
H	1.492909	0.565951	-3.141995
O	1.471526	1.566633	2.472848
H	1.083997	1.037644	1.685116
H	2.272067	1.003300	2.657526
O	-0.924626	1.187198	3.674598
H	0.017284	1.349528	3.376773
H	-1.037788	0.200794	3.554583
Na	-0.616986	0.748935	-1.221307

K – 1 water molecule

4

O	0.068743	-0.078384	-0.282167
H	0.522936	-0.927429	-0.396377
H	-0.773794	-0.205505	-0.747103
K	0.229273	1.481672	1.738081

4

O	0.132597	0.088456	-0.206816
H	-0.342497	0.760620	-0.721247
H	1.037552	0.435185	-0.165450
K	-1.014255	-1.581583	1.322028

4

O	0.187953	0.117464	-0.201409
H	-0.281345	0.758161	-0.759997
H	0.485335	-0.552798	-0.837576
K	-0.485051	-0.408507	2.198847

4

O	0.000605	0.319383	0.159335
H	0.921167	0.621536	0.098074
H	-0.071568	0.031016	1.084339
K	-1.022213	-1.201905	-1.645786

4

O	0.198293	0.228601	0.059328
H	1.083758	-0.025660	-0.245249
H	-0.017506	0.995369	-0.494767
K	-1.547648	-1.457971	0.865036

4

O	-0.019080	-0.136379	-0.181637
H	0.556799	-0.889400	-0.420412
H	-0.752645	-0.203631	-0.824430
K	0.262086	1.499764	1.738913

4

O	0.102330	0.170506	-0.110551
H	-0.327731	0.742278	-0.776849
H	1.048652	0.399753	-0.199479
K	-1.009853	-1.609860	1.315395

4

O	0.145447	0.098172	-0.201152
H	-0.262242	0.775756	-0.776327
H	0.503047	-0.548280	-0.841784
K	-0.479359	-0.411328	2.219129

4

O	0.030859	0.234386	0.152470
H	0.914068	0.651288	0.099933
H	-0.079845	0.080713	1.112181
K	-1.037092	-1.196358	-1.668622

4

O	0.147120	0.132566	-0.113566
H	1.115261	0.014228	-0.185790
H	0.009619	1.049408	-0.424832

K -1.555104 -1.455863 0.908536

K – 2 water molecules

7

O -0.015270 -0.010772 -2.547139
H 0.501942 -0.574421 -3.143548
H -0.485178 0.588617 -3.147478
O 0.000988 -0.000484 2.546868
H 0.573699 0.506470 3.143245
H -0.569345 -0.504143 3.148242
K -0.006849 -0.005270 -0.000190
7

O 1.830680 0.884144 1.426433
H 2.234758 1.765886 1.453917
H 1.920544 0.567199 2.339169
O -1.817158 -1.005092 -1.448805
H -1.741031 -1.968111 -1.536272
H -2.045736 -0.715840 -2.346785
K -0.384453 0.472199 0.114549
7

O -0.639211 -1.327204 -1.002217
H -0.648757 -1.807465 -0.159474
H -0.830901 -2.013818 -1.658635
O 0.615847 1.258611 1.069034
H 1.392678 0.686862 1.173575
H 0.847935 2.044049 1.589510
K -0.786694 1.229938 -1.084243
7

O -1.473741 0.361120 2.116914
H -1.244458 0.903191 2.887232
H -1.910998 -0.412211 2.508786
O 1.249466 -0.395781 -2.258973
H 2.146554 -0.766380 -2.250651
H 1.292881 0.276217 -2.957724
K -0.059704 0.033841 -0.045586
7

O 1.727101 1.815972 0.764044
H 1.614055 2.189570 1.653364
H 1.895522 2.600311 0.217653
O -1.547159 -1.898079 -0.719419
H -1.322449 -2.829992 -0.866536
H -2.469715 -1.837406 -1.009943
K 0.150920 -0.100399 -0.010519
7

O 0.000625 -0.002035 -2.571088
H 0.338224 -0.701487 -3.164887
H -0.312878 0.683124 -3.194016
O -0.091538 0.060811 2.586241
H 0.473197 0.601499 3.173343
H -0.367261 -0.675934 3.166829
K -0.040383 0.034017 0.003578
7

O 1.737761 1.135501 1.560050
H 2.658997 0.830161 1.679479
H 1.528701 1.535547 2.427537
O -1.702915 -1.044167 -1.614986
H -1.552352 -1.439057 -2.496546
H -2.676881 -1.060819 -1.530323
K 0.004292 0.043220 -0.023006
7

O -1.334900 0.326925 2.100944
H -0.818699 0.469932 2.918686
H -2.219497 0.085898 2.440097
O 1.355203 -0.432074 -2.125490
H 2.282859 -0.145983 -2.008736
H 1.170688 -0.189773 -3.054768
K -0.435656 -0.114928 -0.270733
7

O -1.302671 -1.657682 -0.999801
H -1.661245 -2.051316 -1.819565
H -1.032617 -2.440587 -0.480329
O 1.215165 1.808455 0.988197
H 0.870545 2.240763 1.794817
H 2.094256 1.488446 1.271932
K -0.232536 0.682890 -0.827700
7

O 1.481398 1.836666 0.695432
H 2.394546 1.884105 0.350091
H 1.367767 2.701560 1.136812

O	-1.442763	-1.921975	-0.683822
H	-2.376639	-2.167957	-0.531677
H	-1.295431	-2.185022	-1.613734
K	-0.080603	-0.207400	0.675541

K – 4 water molecules

13

O	1.076680	2.302284	0.476703
H	0.720760	3.133295	0.101104
H	1.895235	2.579832	0.936323
O	-0.646990	0.593398	1.707970
H	-0.051758	1.328988	1.396908
H	-1.057944	0.946670	2.518967
O	-1.818546	-3.458394	-0.747940
H	-1.381848	-4.323955	-0.619648
H	-2.270532	-3.575002	-1.607258
O	1.360676	0.176099	-1.210526
H	1.402101	0.459517	-2.143841
H	1.335817	1.033889	-0.704015
K	-0.581441	-1.233427	-0.113010

13

O	1.131924	-0.154556	1.734126
H	0.588139	0.679146	1.782266
H	2.006543	0.124565	2.066455
O	0.665198	-3.131053	-2.258451
H	1.234075	-3.147560	-3.053579
H	-0.161412	-3.542990	-2.579165
O	-0.552939	1.979883	1.506181
H	-1.207440	2.113406	2.222187
H	-0.151611	2.864447	1.384576
O	-1.392432	0.657678	-0.726711
H	-1.204836	1.243683	0.057405
H	-1.588487	1.289819	-1.444607
K	0.641205	-1.010003	-0.715864

13

O	2.078721	0.732049	-1.433002
H	2.923239	0.476700	-1.011323
H	2.265302	1.638062	-1.749551
O	-2.049683	1.955548	0.123048
H	-2.005505	2.791222	-0.382270
H	-2.991519	1.705026	0.044339
O	-0.563475	-2.269945	-1.142521
H	-0.331169	-3.070371	-0.631472
H	-1.421487	-2.513759	-1.542424
O	0.803855	-0.309565	2.281434
H	0.279321	-0.083576	3.074881
H	1.165710	-1.188837	2.508525
K	-0.153308	0.137446	-0.139663

13

O	1.326041	2.099011	-0.633707
H	1.574879	2.282392	-1.561008
H	1.094991	2.985549	-0.292646
O	0.958218	-2.258857	-0.520743
H	1.924928	-2.372490	-0.610868
H	0.686686	-3.079450	-0.063866
O	-2.244895	-0.044692	-1.674144
H	-3.140837	0.242366	-1.407551
H	-2.415114	-0.919812	-2.076214
O	-0.046036	0.116137	2.659386
H	0.854374	0.004908	3.024330
H	-0.377348	0.895961	3.147598
K	-0.195395	0.046983	0.009396

13

O	-0.041995	0.010124	-3.870728
H	0.422641	0.807442	-4.193906
H	0.155598	-0.648491	-4.566089
O	1.728262	-0.454354	0.553445
H	1.220710	-0.196136	1.371350
H	2.254079	-1.224400	0.843723
O	-1.761685	0.463702	0.433085
H	-2.620856	0.082846	0.697784
H	-1.239564	0.474781	1.281882
O	0.004335	0.343868	2.511428
H	0.224168	1.173287	2.982830
H	-0.204381	-0.289940	3.227892
K	-0.116763	-0.596231	-1.323976

K – 8 water molecules

25

O	0.611684	0.653830	-1.950947

H	-0.372408	0.771997	-2.008107
H	0.964169	1.016145	-2.777636
O	-1.516529	-2.064980	-1.979644
H	-2.204645	-2.592317	-1.547501
H	-1.862004	-1.145425	-1.929779
O	-0.626486	-0.789043	1.410931
H	0.248795	-0.507919	1.784628
H	-1.050551	-1.308071	2.111544
O	-1.614489	1.615626	0.743798
H	-2.225839	2.028284	1.373518
H	-1.386639	0.728318	1.127497
O	1.080126	2.120275	0.324305
H	0.131539	2.156823	0.583631
H	1.025471	1.714942	-0.574045
O	2.631777	-2.545005	1.102570
H	3.557256	-2.669519	0.843346
H	2.596000	-1.617069	1.420106
O	1.897681	0.041425	1.742818
H	1.696821	0.884506	1.233572
H	2.200084	0.340035	2.614849
O	-2.052573	0.653992	-1.728634
H	-2.081947	1.078900	-0.831808
H	-2.570693	1.234811	-2.306665
K	0.793650	-1.728942	-0.724847

25

O	0.212828	0.302339	-3.460460
H	-0.673045	0.255894	-3.029829
H	0.314316	1.236319	-3.696859
O	-0.732519	-2.053738	-0.329813
H	-0.942721	-1.689438	0.556921
H	-1.319206	-1.516785	-0.907697
O	-1.213686	-0.468051	1.894397
H	-0.266716	-0.396983	2.177597
H	-1.715939	-0.710269	2.687345
O	-1.548331	1.579350	0.234550
H	-2.088593	2.319431	0.552221
H	-1.575243	0.893132	0.954409
O	1.138020	1.500538	0.075043
H	0.177750	1.741341	0.126321
H	1.623093	2.338549	0.038960
O	3.214845	-1.547761	0.435065
H	2.709191	-1.154721	1.181639
H	3.267220	-2.490201	0.654750
O	1.477415	-0.197245	2.105708
H	1.446979	0.569322	1.472811
H	1.841711	0.164942	2.928823
O	-1.953683	-0.097724	-1.838013
H	-1.963099	0.609185	-1.143655
H	-2.869477	-0.173452	-2.147157
K	1.422048	-0.778135	-1.372276

25

O	2.484408	-2.310201	-2.602286
H	2.080239	-2.876877	-3.278155
H	3.149817	-2.888704	-2.197825
O	-0.172730	-1.416212	1.275525
H	0.193484	-0.633565	1.764313
H	-0.071263	-2.171691	1.874480
O	-2.501326	-0.339860	0.693698
H	-3.274436	-0.569179	1.231236
H	-1.743346	-0.880580	1.041006
O	-1.812971	-0.627054	-1.993193
H	-2.232214	-0.592227	-1.107738
H	-1.399947	0.257961	-2.084273
O	-0.130277	1.573974	-1.788464
H	-0.554686	1.950344	-0.979351
H	-0.118409	2.293669	-2.436503
O	2.922775	0.175200	0.642081
H	2.245208	0.575337	1.232080
H	3.298396	-0.543941	1.172584
O	0.729727	0.966598	2.023314
H	0.014305	1.507235	1.593080
H	0.777338	1.268421	2.943588
O	-1.268735	2.011757	0.606085
H	-1.769686	2.793859	0.885574
H	-1.889112	1.237543	0.691660
K	0.983840	-0.775325	-1.096072

25

O	0.979709	1.224074	-1.870745
H	0.000490	1.241986	-1.980555
H	1.329235	1.787676	-2.577447
O	-2.045546	-2.208837	-1.614824
H	-2.539584	-2.541450	-0.850399
H	-2.225275	-1.244559	-1.615375
O	-0.754161	-1.034310	1.302641
H	0.109317	-0.899739	1.772524
H	-1.237124	-1.689395	1.828976
O	-1.568945	1.463237	0.854269
H	-2.241657	1.860755	1.428239
H	-1.420353	0.543059	1.198547

O	1.148314	1.889232	0.760249
H	0.174444	1.920906	0.898811
H	1.224111	1.768240	-0.215343
O	2.738455	-2.007011	-0.009560
H	3.555384	-1.661607	-0.400026
H	2.578440	-1.430725	0.774695
O	1.758160	-0.393429	1.935022
H	1.628960	0.528267	1.558396
H	2.145217	-0.277014	2.816008
O	-1.707549	0.576267	-1.682866
H	-1.862717	0.992819	-0.795432
H	-2.318806	1.027820	-2.284910
K	0.438113	-1.353812	-1.147645

25

O	-1.024430	0.626626	-2.237084
H	-0.956753	1.483497	-1.746498
H	-1.319689	0.861200	-3.129478
O	-0.630536	-2.648416	-1.283269
H	-0.480542	-3.329023	-0.610702
H	-1.403536	-2.140456	-0.946895
O	-0.498309	0.347043	0.901184
H	-0.138854	0.006976	1.750446
H	-1.325861	-0.139443	0.695172
O	-0.496055	2.583636	-0.469929
H	-1.052668	3.318803	-0.172456
H	-0.549262	1.883840	0.234978
O	1.987784	1.929377	-1.431577
H	2.713820	2.286123	-0.898098
H	1.189602	2.361022	-1.053595
O	2.476442	-1.790805	0.991924
H	3.398643	-1.531837	1.139557
H	1.998356	-1.422608	1.768266
O	0.915917	-0.696602	2.973225
H	1.385550	-0.073641	3.551980
H	0.547361	-1.360080	3.578787
O	-2.459065	-0.808477	-0.505180
H	-3.424579	-0.841700	-0.572186
H	-2.135338	-0.241776	-1.253077
K	1.178361	-0.632336	-1.088025

25

O	0.855459	0.399480	-1.889400
H	-0.110894	0.627774	-2.071775
H	1.339730	0.700386	-2.682904
O	-2.005806	-2.019476	-1.812459
H	-2.744722	-2.271869	-1.225767
H	-2.116681	-1.032285	-1.914168
O	-0.664271	-0.913916	1.641590
H	0.211471	-0.584329	2.032606
H	-1.141630	-1.338411	2.381052
O	-1.524707	1.347413	0.632648
H	-2.193904	1.825301	1.161831
H	-1.339471	0.478232	1.126849
O	1.129955	1.878515	0.359998
H	0.143940	1.894370	0.525585
H	1.169677	1.404766	-0.524910
O	2.821268	-1.928520	0.566895
H	3.532399	-1.535174	0.024754
H	2.595948	-1.199496	1.213375
O	1.740737	0.031914	2.072632
H	1.588892	0.832330	1.438295
H	2.058901	0.406299	2.917309
O	-1.778905	0.676888	-1.895016
H	-1.835683	1.016467	-0.942085
H	-2.272944	1.322406	-2.437817
K	0.411498	-1.947447	-0.641621

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O	0.098334	0.227436	-3.493523
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H	0.222450	1.161832	-3.749289
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H	-0.872386	-1.665649	0.400673
H	-1.346259	-1.433134	-1.055703
O	-1.014804	-0.631780	1.845522
H	-0.073513	-0.434339	2.164321
H	-1.543691	-0.819036	2.645765
O	-1.454434	1.388599	0.240237
H	-1.958515	2.131104	0.628984
H	-1.422962	0.663681	0.953810
O	1.181539	1.534655	0.088763
H	0.176062	1.644629	0.076457
H	1.539798	2.443581	0.061932
O	3.076370	-1.584313	0.617237
H	2.586613	-1.106435	1.343012
H	2.982714	-2.525687	0.860541
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K – 12 water molecules

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H	1.537037	0.583191	-2.059559
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O	-0.678949	3.223595	1.906646
H	-0.542435	3.087203	0.931047
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O	-1.943773	-0.649396	0.043006
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O	1.420347	1.826262	2.871358
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H	2.245836	2.321737	2.762680
O	3.065852	-1.175229	-0.203230
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O	0.480368	-0.572591	-2.765850
H	0.593929	-1.422496	-2.256708
H	0.766399	-0.764019	-3.672936
O	-1.179153	-3.111432	0.462233
H	-1.811636	-3.821272	0.275016
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H	1.231464	-3.446639	-1.574100
H	0.123723	-2.930079	-0.593345
K	0.664560	0.027077	0.986798

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O	2.331684	1.542796	-1.003871
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H	1.320370	-2.552926	1.715487
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H	-0.341345	3.106601	0.328259
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O	1.573128	2.118327	2.861464
H	0.924543	2.683033	2.384577
H	2.407097	2.607395	2.801307
O	1.818015	-1.019514	-1.461915
H	1.010728	-1.168466	-2.008213
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H	-1.868218	-3.580640	-0.373616
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K	0.843701	0.303973	0.985888

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H	-2.479321	0.846048	-3.537061
H	-2.048522	-0.247568	-2.519952
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H	-0.900240	1.417576	2.793105
H	-2.024105	0.499485	2.292847
O	1.598792	-2.075711	0.682659
H	1.111108	-2.096107	1.544670
H	2.490126	-2.402696	0.880674
O	0.913096	0.358801	-3.208127
H	0.910688	-0.520791	-2.745263
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H	1.041507	-2.081162	-0.997662
H	-0.304510	-2.008079	-1.735193
K	-1.184861	1.145378	-0.282193

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O	1.437121	2.298982	-2.147931
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H	1.327868	-2.750451	0.619537
H	1.704414	-3.170173	2.082652
O	-3.460929	0.945385	0.010768
H	-3.063371	0.926010	0.910566
H	-3.692531	1.876494	-0.123114
O	1.805442	-0.247920	-1.337321
H	2.161951	-0.098522	-0.427975
H	1.852433	0.637402	-1.766039
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H	0.171003	2.621853	0.821323
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O	0.607887	1.835495	2.223917
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O	2.372682	-0.037376	1.290531
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H	2.102953	-0.965370	1.522999
O	-0.806777	1.143483	-3.263832
H	-1.469635	1.813054	-3.489487
H	0.003454	1.667803	-3.071809
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H	1.428964	-1.907163	-1.391653
H	1.534591	-3.456408	-1.602159
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O	-1.596253	-2.256699	-1.170872
H	-0.696469	-2.650315	-1.280679
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K	-0.908168	0.314629	-0.668622

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O	-2.300980	1.464280	-1.905555
H	-2.351540	0.491560	-1.700994
H	-3.125361	1.692557	-2.360467
O	-2.042328	-1.124023	-1.282152
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H	-1.255265	-1.550995	-1.688070
O	1.225289	2.578920	0.704133
H	0.275702	2.854862	0.591683
H	1.727156	3.389004	0.876133
O	-1.687114	-1.842376	1.366674
H	-1.888253	-0.970326	1.793182
H	-2.223452	-2.497209	1.839701
O	0.857570	0.770593	2.599797
H	1.127010	1.539343	2.025446
H	1.238595	0.942881	3.474687
O	2.444720	-2.671131	-0.495238
H	1.989367	-2.477144	0.366274
H	2.882519	-3.529710	-0.393046
O	-1.819053	0.709498	2.231079
H	-2.376137	0.934347	2.992851
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O	0.220939	1.601598	-2.865998
H	-0.754622	1.600890	-2.723994
H	0.351496	1.033306	-3.639045
O	-1.429887	2.726632	0.400151
H	-1.709049	2.069560	1.078406
H	-1.821731	2.387284	-0.437832
O	0.457703	-1.893096	-2.135539
H	1.171383	-2.366406	-1.641176
H	0.763521	-1.854264	-3.053681

O	1.039980	-1.777068	1.581392
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O	3.264091	-0.090285	-0.596356
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H	3.655574	0.136083	-1.453082
K	0.586543	0.313082	-0.534579

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O	2.185364	1.188456	-1.823833
H	2.746454	1.728859	-2.414158
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H	-0.361155	-2.704941	1.948342
H	0.787798	-3.081104	2.919891
O	-0.716214	3.127261	1.761489
H	-0.406820	2.846428	0.834897
H	-1.081746	4.028655	1.673732
O	-2.630976	-0.788927	0.073025
H	-2.488042	-0.152176	0.835632
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O	1.422612	2.045055	3.025396
H	0.699532	2.630556	2.664358
H	2.238851	2.465076	2.691400
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H	2.281265	-1.478013	-0.466450
H	2.775637	-0.026535	-0.652879
O	-1.947061	0.796079	2.127269
H	-1.675715	1.761323	2.042430
H	-2.397667	0.725849	2.990619
O	0.054856	1.896245	-0.369128
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O	-1.631818	0.606194	-1.992737
H	-2.178978	1.077671	-2.651436
H	-0.897735	0.144618	-2.516536
O	0.519247	-0.510476	-3.013914
H	0.683836	-1.344519	-2.447860
H	0.566397	-0.801298	-3.946304
O	-1.005215	-2.740965	0.335824
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H	-1.713277	-1.981137	0.219174
O	0.999322	-2.408601	-1.303179
H	1.303085	-3.276967	-1.634354
H	0.189311	-2.609034	-0.712542
K	0.616441	-0.099391	1.530794

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O	2.247193	1.161286	-0.884173
H	2.237313	0.284521	-1.409603
H	3.123197	1.559117	-1.048385
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H	1.083678	-2.382415	2.015324
H	1.488032	-1.882838	3.424562
O	-0.534081	3.157874	1.431955
H	-0.328375	3.042765	0.425572
H	-0.830620	4.081244	1.548903
O	-2.162458	-0.626064	0.308416
H	-2.222009	-0.029058	1.115340
H	-2.153938	-0.010290	-0.483137
O	1.562576	2.028330	2.680210
H	0.865326	2.635675	2.298220
H	2.400649	2.424785	2.372857
O	2.025453	-1.190456	-1.980846
H	1.120584	-1.252914	-2.407049
H	1.946801	-1.806926	-1.199959
O	-2.069045	1.154300	2.258329
H	-1.584279	1.999189	1.992679
H	-1.785433	0.969708	3.174647
O	0.052618	2.671853	-1.034285
H	0.929951	2.181335	-1.096200
H	-0.617634	2.048186	-1.441396
O	-1.730241	0.839870	-1.896627
H	-2.507120	1.110175	-2.425472
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O	-0.554316	-1.352824	-2.769788
H	-0.850833	-2.018449	-2.066439
H	-0.801963	-1.748097	-3.629612
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H	-1.643921	-3.560895	-0.577684
H	-1.590945	-2.021461	-0.124928
O	1.414343	-2.690464	0.260304
H	1.888114	-3.545785	0.237682
H	0.471189	-2.906084	-0.037264
K	0.623832	0.114253	0.998937

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O	-2.214058	-1.222747	1.307431
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H	-2.971511	-1.643124	1.761483
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H	3.505040	2.192461	-1.842481

H	2.140881	1.400870	-2.091631
O	-2.028399	-1.816201	-1.249383
H	-2.152024	-1.709600	-0.247876
H	-2.521903	-2.626440	-1.485018
O	-2.938211	0.600114	-2.093650
H	-3.791610	0.778975	-1.653209
H	-2.762374	-0.358450	-1.873861
O	1.764779	0.736660	0.688614
H	2.289405	1.230623	-0.007359
H	1.973077	-0.237738	0.577647
O	0.072740	-1.666777	2.524806
H	0.273951	-0.715621	2.839229
H	0.102080	-2.225247	3.327624
O	0.508645	0.877248	2.930459
H	1.137654	0.983114	2.139058
H	0.998883	1.187429	3.717072
O	0.452894	3.609421	-0.993223
H	0.127567	4.000147	-1.827300
H	1.326554	3.204397	-1.255946
O	-1.940047	1.490742	1.824753
H	-1.107719	1.427453	2.364111
H	-2.206311	0.536971	1.745865
O	1.811865	-1.923378	0.549472
H	1.205141	-1.980041	1.355816
H	2.603130	-2.450703	0.776647
O	0.980668	0.450944	-2.726590
H	0.899527	-0.539934	-2.472539
H	0.758996	0.510329	-3.675341
O	0.616875	-1.976472	-1.873083
H	1.062770	-2.052906	-0.980390
H	-0.361181	-2.008223	-1.663770
K	-0.692956	1.129224	-0.632100

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O	1.504297	2.183639	-2.363569
H	1.075521	2.638042	-1.564400
H	2.206419	2.782512	-2.683860
O	1.301351	-2.469850	1.502582
H	1.322864	-2.700717	0.515473
H	1.717938	-3.226479	1.961118
O	-3.481549	1.088188	0.176123
H	-3.047206	0.897895	1.056293
H	-4.281225	1.593797	0.414439
O	1.627552	-0.144145	-1.090641
H	2.040086	0.005468	-0.188359
H	1.800216	0.679769	-1.634511
O	0.084416	2.920295	-0.305333
H	0.285595	2.592299	0.646171
H	-0.341070	3.793131	-0.208558
O	0.471237	1.850870	2.029656
H	1.184485	1.156300	1.925717
H	-0.365153	1.325519	2.201152
O	-1.829974	0.421635	2.230001
H	-2.218398	0.488335	3.124182
H	-1.672789	-0.588331	2.077154
O	2.320116	-0.037934	1.476954
H	3.249376	0.014874	1.775197
H	2.037720	-0.998616	1.621448
O	-0.806108	1.199113	-3.397812
H	-1.396147	1.948377	-3.608518
H	0.067509	1.643858	-3.210119
O	1.075942	-2.648926	-1.117284
H	1.406487	-1.700856	-1.297744
H	1.590905	-3.239963	-1.701091
O	-1.373602	-2.056580	1.664783
H	-1.565536	-2.213946	0.691181
H	-0.392979	-2.250168	1.730093
O	-1.544454	-2.195722	-1.020772
H	-0.615157	-2.532611	-1.205622
H	-2.142146	-2.836062	-1.452682
K	-1.108390	0.470798	-0.769252

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O	-2.053866	1.276925	-1.821334
H	-2.112853	0.256746	-1.658557
H	-2.908096	1.535542	-2.218322
O	-2.014277	-1.255763	-1.356145
H	-2.011520	-1.436636	-0.370593
H	-1.138452	-1.618285	-1.684048
O	1.056523	2.554739	0.897502
H	0.052552	2.687794	0.726285
H	1.422718	3.446672	1.054130
O	-1.778766	-1.622995	1.300526
H	-1.930670	-0.778066	1.837568
H	-2.228068	-2.337845	1.793563
O	0.831007	0.808138	2.832136
H	1.032716	1.578428	2.195554
H	1.260158	1.034629	3.680563
O	2.329592	-2.654140	-0.464642
H	1.832419	-2.305031	0.345766
H	2.657404	-3.542773	-0.226423
O	-1.779363	0.716700	2.499016

H	-2.320536	0.927240	3.285853
H	-0.813157	0.774771	2.804302
O	0.256607	1.862681	-3.086233
H	-0.682695	1.681341	-2.792238
H	0.332505	1.367668	-3.924389
O	-1.501819	2.521553	0.497195
H	-1.756786	1.882896	1.222838
H	-1.793431	2.080151	-0.358424
O	0.460087	-1.886071	-2.185645
H	1.138141	-2.380098	-1.629815
H	0.605581	-2.192051	-3.101275
O	0.876897	-1.383619	1.270468
H	1.026075	-0.696038	1.978270
H	-0.096992	-1.617716	1.343226
O	3.563397	-0.288361	-0.946883
H	3.307695	-1.238598	-0.779412
H	3.902935	-0.306825	-1.862682
K	0.941917	0.486148	-0.855190

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O	-1.262614	-3.258388	0.342818
H	-1.715386	-4.115552	0.353990
H	-1.946169	-2.572256	0.596832
O	-2.332552	0.426556	3.032595
H	-1.353073	0.266418	3.096290
H	-2.683042	0.396144	3.935476
O	-1.279497	1.230230	-2.823797
H	-0.683446	1.958900	-2.523498
H	-0.661601	0.557290	-3.200428
O	2.497675	0.221151	-0.044354
H	2.674652	0.539584	-0.971037
H	2.721594	-0.737889	-0.028896
O	0.224872	-0.022424	2.635539
H	1.024717	0.554104	2.670468
H	0.524393	-0.958731	2.593202
O	-3.033622	0.608620	-0.965004
H	-2.451260	0.809741	-1.755783
H	-3.942767	0.767058	-1.261388
O	0.432483	3.277277	0.715307
H	1.060559	2.803446	1.308010
H	-0.475430	2.964323	0.944524
O	-2.060958	2.234598	1.001338
H	-2.570818	1.801887	0.280284
H	-2.282255	1.719583	1.810241
O	0.647207	-0.540451	-3.531552
H	0.642014	-0.905071	-4.429697
H	0.491895	-1.306545	-2.917734
O	2.525589	-2.471509	0.006415
H	2.009492	-2.645696	0.835794
H	3.227674	-3.138669	-0.026984
O	0.741661	-2.659911	2.019430
H	0.909700	-3.319652	2.710021
H	-0.029672	-3.007944	1.496393
O	0.624994	2.935457	-1.896921
H	0.618881	3.798483	-2.338592
H	0.600198	3.134904	-0.914038
O	-2.849637	-1.292031	1.001650
H	-3.043234	-0.659241	0.275953
H	-2.759294	-0.739252	1.815711
O	0.319913	-2.261184	-1.582978
H	-0.352290	-2.759954	-1.061622
H	1.176337	-2.458406	-1.133354
O	2.209988	1.690376	2.130402
H	2.987990	1.976276	2.632062
H	2.541425	1.184366	1.340420
O	2.583610	1.121171	-2.566631
H	1.978952	1.878010	-2.381223
H	1.986972	0.470285	-3.003602
K	-0.217555	0.150006	-0.097589

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O	-1.454109	-3.016468	1.635978
H	-2.018055	-3.717512	1.996322
H	-2.064995	-2.311148	1.289257
O	-2.854092	1.555627	1.822248
H	-1.961334	1.506013	2.268219
H	-3.447643	2.018584	2.432108
O	2.398114	0.044296	-1.674627
H	2.135222	0.760384	-2.297326
H	2.145987	-0.799753	-2.115772
O	3.287636	0.191428	0.784429
H	4.238367	0.358849	0.873675
H	3.115181	0.118773	-0.194122
O	-0.423770	1.198080	2.706144
H	0.389786	1.626102	2.334128
H	-0.201112	0.278022	2.977361
O	-3.003082	-0.014430	-1.884093

H	-2.161159	-0.164732	-2.393379
H	-3.721032	0.015139	-2.534001
O	0.472260	3.215341	-0.908342
H	0.452801	4.184019	-0.951703
H	-0.480118	2.929285	-0.821673
O	-1.916258	2.127172	-0.639207
H	-2.408793	1.482360	-1.200325
H	-2.351351	2.080396	0.245283
O	1.192213	-2.214809	-2.596780
H	1.473203	-2.941183	-3.172436
H	1.006593	-2.609245	-1.704634
O	2.433677	-2.157525	1.963211
H	1.671290	-1.887485	2.525570
H	2.806097	-1.312513	1.618801
O	0.064473	-1.462345	3.178684
H	0.010766	-1.684255	4.121332
H	-0.556051	-2.095577	2.725113
O	1.129632	1.907682	-3.155436
H	1.287814	2.451872	-3.941702
H	0.906630	2.535342	-2.419070
O	-2.643890	-0.882059	0.679465
H	-2.952841	-0.703984	-0.238368
H	-2.900993	-0.084453	1.199092
O	0.733787	-2.764036	-0.035183
H	1.447121	-2.663836	0.651025
H	-0.051359	-3.081068	0.463800
O	1.655411	2.291326	1.405979
H	1.345470	2.693349	0.562206
H	2.349870	1.631638	1.169798
O	-0.575002	-0.185340	-2.809120
H	-0.035461	0.587105	-3.097335
H	-0.011269	-0.984797	-2.923049
K	0.004411	-0.008943	0.001099

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O	-1.094125	-3.319271	-0.145756
H	-1.480180	-4.206917	-0.099038
H	-1.800705	-2.687287	0.165422
O	-2.160810	-0.220486	3.123984
H	-1.201564	-0.354218	3.346304
H	-2.632501	-0.115266	3.963702
O	-1.501207	1.197301	-2.422551
H	-0.930481	1.951685	-2.117112
H	-0.880042	0.617239	-2.921722
O	2.526525	0.571145	-0.097067
H	2.833522	-0.349719	-0.273418
H	2.672980	1.038072	-0.952729
O	0.496320	-0.610291	3.291845
H	1.063735	0.179823	3.023399
H	0.847782	-0.909269	4.144826
O	-3.445456	0.651784	-0.724372
H	-2.811819	0.824797	-1.474499
H	-4.315554	0.955930	-1.022800
O	0.290114	3.189475	1.191027
H	0.209199	4.093820	1.530905
H	-0.607589	2.771794	1.291465
O	-1.844188	1.682495	1.266460
H	-2.557519	1.530457	0.605824
H	-2.067633	1.110107	2.040650
O	0.546022	-0.276094	-3.389789
H	0.524271	-0.410945	-4.349732
H	0.541482	-1.193524	-2.985350
O	2.788681	-2.087878	-0.567239
H	2.252606	-2.288635	0.248079
H	3.574185	-2.654240	-0.528144
O	0.999237	-2.382923	1.284641
H	0.784784	-1.868857	2.099197
H	0.198869	-2.868204	0.977907
O	0.259584	2.988619	-1.524917
H	1.110367	2.637622	-1.869792
H	0.374022	3.130068	-0.556287
O	-2.624779	-1.424868	0.735073
H	-3.098779	-0.744900	0.199815
H	-2.601553	-1.093412	1.661338
O	0.611023	-2.578899	-2.125301
H	-0.057555	-2.925285	-1.488070
H	1.460292	-2.534222	-1.624780
O	1.931704	1.392961	2.400618
H	1.343317	2.129671	2.107706
H	2.327360	1.096361	1.546169
O	2.379523	1.562409	-2.566367
H	3.003576	1.865651	-3.242744
H	1.821379	0.862198	-2.989693
K	-0.121128	-0.069695	-0.116157

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O	-1.377133	-3.157181	0.653444
H	-2.006193	-3.879740	0.801540
H	-1.874655	-2.309912	0.817446
O	-1.609588	0.917125	3.121597
H	-0.665855	0.610313	3.042265
H	-1.877945	0.762718	4.039949

O	-1.716242	0.805907	-2.291949
H	-1.108245	1.556830	-2.492326
H	-1.363498	0.042742	-2.807797
O	3.126457	0.072989	-0.385973
H	4.090607	0.039742	-0.486484
H	2.772515	0.214946	-1.309999
O	0.749505	0.005453	2.402853
H	1.575532	0.537767	2.376579
H	0.949563	-0.943207	2.565526
O	-3.412014	1.258905	-0.343921
H	-2.905908	1.077016	-1.180832
H	-4.346163	1.319481	-0.594858
O	0.449101	2.876599	0.157290
H	1.177219	2.700696	0.792095
H	-0.407766	2.949735	0.660144
O	-1.972594	2.917823	1.292247
H	-2.550399	2.429135	0.661189
H	-1.897768	2.296342	2.052974
O	-0.264404	-1.204003	-3.347837
H	-0.313237	-1.610806	-4.225894
H	-0.117587	-1.952813	-2.694502
O	2.400758	-2.579435	0.040774
H	1.973209	-2.632557	0.927043
H	2.756761	-1.666788	-0.040171
O	0.793184	-2.705656	2.278714
H	0.954685	-3.393026	2.942794
H	-0.030263	-2.981083	1.801411
O	0.303327	2.589959	-2.473607
H	0.343386	3.405930	-2.994056
H	0.419231	2.854693	-1.520211
O	-2.225434	-0.705096	1.027257
H	-2.844890	-0.125997	0.519923
H	-2.117408	-0.232005	1.887144
O	0.235158	-2.949376	-1.496991
H	-0.433854	-3.116440	-0.790678
H	1.097733	-2.869590	-1.010606
O	2.557190	1.817029	1.623213
H	3.322208	2.231676	2.049266
H	2.915378	1.264816	0.886492
O	1.865967	0.373060	-2.723229
H	1.409698	1.246589	-2.770956
H	1.197908	-0.265725	-3.071663
K	0.120309	0.007727	-0.233150

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O	-1.563956	-3.478455	0.282765
H	-2.102870	-4.276819	0.386967
H	-2.151787	-2.706916	0.511002
O	-1.921470	0.303993	2.950614
H	-0.975183	0.064306	3.183602
H	-2.417205	0.296810	3.783323
O	-0.714021	1.054082	-2.124337
H	-0.255459	1.926540	-2.085873
H	-0.224182	0.477756	-2.756090
O	2.895340	2.027690	-0.908116
H	3.688736	2.584038	-0.941342
H	2.162142	2.590742	-1.269041
O	0.615646	-0.381224	3.314221
H	1.149567	0.220321	2.747266
H	0.684607	-1.267715	2.887017
O	-3.056421	0.679956	-0.998744
H	-2.282439	0.846630	-1.601121
H	-3.853546	0.915298	-1.497085
O	0.033135	3.539230	1.000435
H	0.015918	4.355208	1.523671
H	-0.884677	3.138908	1.059170
O	-2.265548	2.273792	1.113874
H	-2.636607	1.791905	0.340089
H	-2.215434	1.610791	1.843066
O	0.745431	-0.875201	-3.305347
H	0.858951	-1.106159	-4.239652
H	0.420561	-1.696432	-2.851282
O	2.462219	-3.022339	-0.080053
H	3.201306	-3.618582	-0.272267
H	2.706560	-2.143622	-0.469558
O	0.594711	-2.719426	1.859800
H	-0.182581	-3.140459	1.428762
H	1.355585	-2.938236	1.274275
O	0.672906	3.345359	-1.597056
H	0.633911	4.163009	-2.116934
H	0.400557	3.591049	-0.671987
O	-2.807144	-1.246529	0.888604
H	-3.051034	-0.582026	0.204052
H	-2.597004	-0.742101	1.710838
O	0.188370	-2.932298	-1.676366
H	-0.542345	-3.222372	-1.079580
H	1.013458	-3.131393	-1.179301
O	1.578008	1.362800	1.448302
H	1.047791	2.196857	1.463039
H	2.242445	1.546993	0.746500
O	2.500990	-0.628971	-1.258443
H	2.795810	0.308633	-1.185030

H	2.055363	-0.687354	-2.134436
K	-0.044194	-0.416392	0.082102
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O	-1.123589	-3.173118	0.461328
H	-1.573746	-4.040542	0.443728
H	-1.861679	-2.465153	0.574548
O	-2.296055	0.341054	2.816821
H	-1.312848	0.102475	2.915182
H	-2.686141	0.327515	3.712417
O	-1.336861	1.333344	-2.714668
H	-0.671954	2.052125	-2.484454
H	-0.784236	0.590123	-3.101418
O	2.798604	0.244040	0.050709
H	2.729943	0.502059	-0.929217
H	2.877327	-0.752329	0.082525
O	0.194695	-0.241753	2.573611
H	0.955700	0.410196	2.604475
H	0.558809	-1.173660	2.579066
O	-3.105697	0.828996	-0.918185
H	-2.479064	1.024470	-1.707879
H	-4.007733	1.041245	-1.227157
O	0.390437	3.278049	0.591159
H	1.006543	2.767256	1.194626
H	-0.542624	2.970860	0.826216
O	-2.052817	2.358595	1.050663
H	-2.546743	1.925309	0.294336
H	-2.194456	1.724641	1.812879
O	0.401887	-0.569150	-3.446875
H	0.428926	-0.947072	-4.347434
H	0.368589	-1.354063	-2.805279
O	2.580733	-2.429658	0.072225
H	2.065378	-2.660767	0.912635
H	3.293825	-3.094768	0.003558
O	0.909107	-2.769887	2.081796
H	1.030304	-3.453003	2.770993
H	0.076440	-3.038027	1.563607
O	0.640928	2.960528	-1.945416
H	0.753910	3.821909	-2.392677
H	0.583626	3.165060	-0.933733
O	-2.834498	-1.272499	0.751457
H	-3.036507	-0.588566	0.049687
H	-2.743430	-0.740076	1.598741
O	0.432293	-2.276150	-1.503628
H	-0.233333	-2.746591	-0.919493
H	1.313085	-2.440653	-1.050874
O	1.988935	1.644711	2.053437
H	2.698674	2.013971	2.614281
H	2.453649	1.139715	1.296075
O	2.396066	0.982784	-2.443316
H	1.835722	1.804081	-2.310251
H	1.766839	0.357683	-2.906061
K	-0.107701	0.160180	-0.140302
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O	-1.367019	-2.855692	1.571754
H	-1.906556	-3.598834	1.905399
H	-2.015078	-2.176564	1.172706
O	-2.656912	1.457967	1.782853
H	-1.821048	1.412680	2.394486
H	-3.387944	1.809466	2.327353
O	2.660057	-0.097062	-1.711253
H	2.234786	0.627707	-2.259096
H	2.247806	-0.946062	-2.052802
O	3.243534	0.350489	0.757979
H	4.191646	0.552109	0.883061
H	3.119602	0.183553	-0.244712
O	-0.484382	1.253583	3.129186
H	0.241608	1.640642	2.547976
H	-0.247810	0.284126	3.208648
O	-2.991566	0.211014	-1.845120
H	-2.162109	-0.071243	-2.359290
H	-3.744114	0.153522	-2.465394
O	0.454904	3.123981	-0.942954
H	0.522524	4.095351	-1.034729
H	-0.549630	2.919788	-0.839401
O	-1.983506	2.388428	-0.619434
H	-2.432308	1.690082	-1.180729
H	-2.281835	2.181411	0.318001
O	1.183362	-2.185712	-2.533935
H	1.504164	-2.882469	-3.138585
H	0.964841	-2.637869	-1.644442
O	2.338174	-2.018633	1.691453
H	1.631588	-1.770898	2.353882
H	2.754622	-1.147992	1.422173
O	0.137094	-1.386315	3.151592
H	0.177628	-1.710475	4.073421
H	-0.513819	-2.007906	2.679793
O	1.140909	1.673925	-3.018846
H	1.411831	2.179965	-3.809564
H	0.898650	2.356368	-2.307546
O	-2.681602	-0.896046	0.558431

H	-2.948949	-0.635008	-0.372122
H	-2.821804	-0.064251	1.107429
O	0.719461	-2.993046	-0.137971
H	1.416257	-2.681489	0.534260
H	-0.111761	-3.117123	0.401284
O	1.353731	2.134589	1.421078
H	1.116268	2.625134	0.583202
H	2.169553	1.592580	1.207823
O	-0.656904	-0.295718	-2.807696
H	-0.068749	0.474573	-3.059799
H	-0.065105	-1.103099	-2.872255
K	0.025959	-0.052838	-0.004899

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O	-0.932594	-3.330103	-0.125526
H	-1.343516	-4.216165	-0.142813
H	-1.673359	-2.668470	0.090823
O	-2.044899	-0.165040	2.887148
H	-1.094002	-0.380669	3.179596
H	-2.609296	-0.325925	3.668650
O	-1.492205	1.233420	-2.217489
H	-0.916572	2.059904	-2.065677
H	-0.945022	0.653071	-2.820700
O	2.860261	0.438540	-0.052068
H	3.039926	-0.534797	-0.202891
H	2.731979	0.833725	-0.962959
O	0.477254	-0.699157	3.310930
H	1.032815	0.105267	2.966361
H	0.772718	-0.866240	4.227518
O	-3.415075	0.801967	-0.574313
H	-2.757991	0.961450	-1.338781
H	-4.306477	1.003853	-0.919234
O	0.173880	2.993347	0.999138
H	0.277165	3.885963	1.384140
H	-0.798530	2.717218	1.202793
O	-2.189102	2.088605	1.438212
H	-2.735746	1.730938	0.674853
H	-2.170407	1.332496	2.096632
O	0.403253	-0.199369	-3.457976
H	0.388502	-0.411117	-4.412036
H	0.493552	-1.093891	-2.965178
O	2.865574	-2.202563	-0.427042
H	2.287461	-2.383203	0.392668
H	3.607260	-2.837929	-0.390974
O	1.082974	-2.482209	1.410698
H	0.841262	-1.946172	2.221456
H	0.262563	-2.917412	1.039952
O	0.193204	3.181788	-1.710702
H	1.017012	2.688037	-1.990058
H	0.241724	3.196711	-0.710328
O	-2.517021	-1.420054	0.576562
H	-3.004525	-0.699948	0.075348
H	-2.437030	-1.068935	1.513596
O	0.693569	-2.286346	-1.992303
H	0.029969	-2.767901	-1.415610
H	1.571650	-2.360671	-1.512908
O	1.792501	1.234188	2.251189
H	1.218124	1.980400	1.903735
H	2.316245	0.955940	1.437406
O	2.168792	1.473572	-2.439588
H	2.882570	1.743718	-3.050391
H	1.601962	0.810529	-2.956389
K	-0.005057	0.015815	-0.024541

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O	-1.248606	-3.083400	1.029345
H	-1.755663	-3.895596	1.224978
H	-1.897327	-2.300161	1.164693
O	-1.763680	0.755019	3.108799
H	-0.790331	0.468374	3.044938
H	-1.979972	0.830819	4.058678
O	-1.787160	1.032955	-2.738772
H	-1.072309	1.737126	-2.700609
H	-1.308564	0.216303	-3.074273
O	3.127239	-0.055621	-0.430693
H	4.090901	-0.070194	-0.597425
H	2.700265	0.185241	-1.340027
O	0.594877	-0.023366	2.428975
H	1.405094	0.551934	2.305685
H	0.883598	-0.978558	2.538675
O	-3.078166	0.943361	-0.515324
H	-2.647337	0.969725	-1.450684
H	-4.015538	1.184343	-0.649630
O	0.575333	3.063244	0.096451
H	1.301417	2.654585	0.650855
H	-0.297454	2.952584	0.599687
O	-1.784849	2.638882	1.189641
H	-2.353221	2.143869	0.533155
H	-1.811721	2.053818	2.003502
O	-0.178803	-1.017861	-3.372794
H	-0.219739	-1.487391	-4.228591
H	-0.203843	-1.728311	-2.643291

O	2.325249	-2.639266	-0.111233
H	1.982386	-2.690367	0.827452
H	2.691682	-1.711748	-0.191831
O	1.038844	-2.629252	2.270597
H	1.238589	-3.245437	3.002811
H	0.127112	-2.900366	1.918805
O	0.336458	2.645951	-2.421812
H	0.493104	3.451746	-2.951583
H	0.464757	2.911712	-1.435646
O	-2.733827	-0.994696	1.328750
H	-2.976827	-0.363590	0.591422
H	-2.470387	-0.400259	2.093689
O	-0.022165	-2.481830	-1.269685
H	-0.611265	-2.847692	-0.548418
H	0.922300	-2.610367	-0.906524
O	2.427313	1.634397	1.469284
H	3.182130	2.090731	1.889609
H	2.825749	1.043971	0.746722
O	1.900703	0.509299	-2.612433
H	1.416717	1.392094	-2.618226
H	1.232741	-0.132150	-2.999921
K	-0.158256	0.128702	-0.174296

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O	-1.379012	-3.358914	0.343847
H	-1.826596	-4.203373	0.545573
H	-2.064879	-2.619085	0.516587
O	-1.922800	0.176440	2.816745
H	-0.949076	-0.035573	3.107869
H	-2.454312	0.158093	3.636893
O	-0.883419	1.090031	-2.226829
H	-0.261278	1.867309	-2.101690
H	-0.387365	0.398340	-2.759252
O	3.048708	1.898123	-0.602703
H	3.882425	2.389419	-0.738889
H	2.324933	2.439631	-1.055441
O	0.542849	-0.354827	3.333321
H	1.035478	0.327282	2.790936
H	0.679666	-1.219886	2.836065
O	-3.054111	0.799487	-0.854397
H	-2.296081	0.940232	-1.519717
H	-3.881582	1.032622	-1.318622
O	-0.046638	3.490242	0.808342
H	-0.043839	4.372739	1.227339
H	-0.983120	3.075889	0.980346
O	-2.264669	2.310222	1.229001
H	-2.641581	1.842445	0.424904
H	-2.157144	1.580928	1.911778
O	0.586339	-0.889274	-3.227492
H	0.732943	-1.101846	-4.169734
H	0.326271	-1.768087	-2.773182
O	2.363711	-2.927466	-0.253345
H	3.162738	-3.478464	-0.364971
H	2.587762	-2.010772	-0.625493
O	0.732401	-2.561059	1.845193
H	-0.076406	-2.975716	1.424940
H	1.462492	-2.754184	1.187521
O	0.861569	3.034312	-1.585096
H	0.930674	3.827969	-2.152849
H	0.466243	3.362268	-0.704299
O	-2.883677	-1.317643	0.807375
H	-3.068869	-0.612687	0.121638
H	-2.605466	-0.816239	1.632864
O	0.155644	-3.040433	-1.827214
H	-0.544151	-3.214635	-1.129690
H	1.009178	-3.149040	-1.314805
O	1.506076	1.461934	1.593029
H	0.955552	2.290538	1.453516
H	2.263516	1.593939	0.957952
O	2.384297	-0.562478	-1.273333
H	2.784159	0.348781	-1.142534
H	1.925171	-0.582876	-2.160435
K	-0.059812	-0.302982	0.082750

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O	-2.872894	-0.770707	2.558530
H	-2.924669	-0.562569	1.589165
H	-2.413836	0.018612	2.930560
O	-1.109955	2.315955	0.876683
H	-1.884048	2.447388	0.278231
H	-0.437363	2.978765	0.584460
O	-1.639782	1.724508	-3.053370
H	-1.892219	2.091218	-3.914655
H	-1.602900	0.723291	-3.175085
O	-2.851406	-2.403493	-1.605507
H	-3.442550	-3.157025	-1.747828
H	-2.069709	-2.738064	-1.083776

O	3.356984	-2.141088	1.276919
H	3.887787	-2.688902	1.873590
H	2.546911	-1.848262	1.789709
O	-0.727576	-2.818131	-0.144522
H	0.201785	-3.102718	-0.310282
H	-0.876318	-2.904037	0.827381
O	1.898311	-3.212618	-0.669948
H	2.506752	-2.909594	0.058018
H	2.234800	-4.076495	-0.953008
O	-1.481422	1.495745	3.311614
H	-1.925544	2.151996	3.870873
H	-1.412325	1.918109	2.402367
O	2.543157	2.230050	1.263197
H	2.737862	1.423385	0.718140
H	2.056120	1.898542	2.053527
O	0.927871	3.684904	-0.142872
H	1.612489	3.196944	0.417753
H	1.169947	4.622954	-0.124031
O	-2.744933	-0.207992	-0.062934
H	-3.097849	0.637563	-0.417059
H	-3.018891	-0.932982	-0.667438
O	0.919148	1.991445	-2.240405
H	0.009517	1.998217	-2.621338
H	0.941674	2.713553	-1.568534
O	-3.084596	2.341995	-0.915886
H	-3.849547	2.911758	-1.084324
H	-2.627114	2.205434	-1.789425
O	1.191185	-1.457246	-2.647518
H	1.546942	-2.085011	-1.978180
H	1.911401	-0.820888	-2.843607
O	-1.363790	-0.853759	-3.307929
H	-1.950661	-1.444781	-2.781921
H	-0.439056	-1.131593	-3.090062
O	1.157296	1.201235	3.396870
H	1.537248	1.301364	4.283013
H	0.181838	1.372708	3.496631
O	3.012941	0.551327	-2.903565
H	2.274694	1.208782	-2.772977
H	3.650990	0.960583	-3.506143
O	1.119241	-1.218546	2.210816
H	0.373554	-1.788663	2.513901
H	1.141742	-0.414434	2.782906
O	2.849839	0.069189	-0.244838
H	3.304767	-0.703215	0.145474
H	3.159360	0.186543	-1.170754
O	-1.093814	-2.691316	2.532355
H	-1.349071	-3.417354	3.120772
H	-1.818362	-1.993229	2.605930
K	0.053567	-0.051037	-0.208222
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O	-3.054757	-0.381421	2.196857
H	-3.104419	-0.255223	1.215979
H	-2.704875	0.483488	2.515658
O	-1.505718	2.788052	0.250748
H	-2.037775	2.712586	-0.575228
H	-0.643841	3.198443	0.009149
O	-0.891840	0.974410	-3.264919
H	-0.994520	-0.031152	-3.306643
H	-0.938665	1.257439	-4.192236
O	-2.788328	-2.514907	-1.428468
H	-2.077052	-2.727644	-0.761517
H	-3.345266	-3.303393	-1.507148
O	3.072795	-2.029233	1.673945
H	3.991861	-2.195717	1.932440
H	3.059974	-1.148095	1.194426
O	-0.799421	-2.640213	0.296026
H	0.075675	-3.076600	0.177757
H	-1.023774	-2.694787	1.256989
O	1.771105	-3.379028	-0.152368
H	2.180403	-4.217789	-0.413724
H	2.361915	-2.984305	0.546392
O	-1.873328	2.022174	2.771105
H	-2.254958	2.720351	3.323376
H	-1.824068	2.390876	1.846926
O	2.379701	2.505019	1.713729
H	2.908134	2.948790	2.393789
H	1.692893	1.946432	2.186219
O	1.065053	3.573942	-0.330526
H	1.607412	3.284396	0.454181
H	1.240117	4.522643	-0.431073
O	-2.935138	-0.031996	-0.450628
H	-3.178864	0.709010	-1.045775
H	-3.097768	-0.877176	-0.926386
O	1.486817	2.265470	-2.653870
H	0.638833	1.807053	-2.850557
H	1.346601	2.763795	-1.811865
O	-2.898910	2.168490	-1.987628
H	-3.438490	2.731039	-2.563137
H	-2.198765	1.759606	-2.564485
O	1.289149	-1.484420	-2.016345
H	1.592132	-2.191992	-1.400308

H	2.075023	-0.932577	-2.235394
O	-1.014298	-1.645485	-3.338704
H	-1.675799	-2.019926	-2.711670
H	-0.134942	-1.733075	-2.889717
O	0.532404	0.858984	2.504392
H	-0.302283	1.238388	2.859405
H	0.736109	0.010596	2.984333
O	3.212600	0.338491	-2.282232
H	4.002695	0.422103	-2.836425
H	2.618061	1.120486	-2.495040
O	1.086128	-1.548638	3.509450
H	1.759671	-1.856184	2.862012
H	0.232351	-1.979366	3.281465
O	2.698592	0.181830	0.356402
H	2.816584	1.043093	0.816229
H	3.082514	0.282977	-0.546635
O	-1.462643	-2.367816	2.894681
H	-2.012611	-3.063488	3.286120
H	-2.090179	-1.611976	2.675219
K	-0.138015	0.089295	-0.100728

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O	-2.995651	-0.685771	2.386958
H	-2.987259	-0.464768	1.420166
H	-2.574916	0.102242	2.803009
O	-1.175027	2.400480	0.886134
H	-1.861890	2.536197	0.193699
H	-0.421386	2.992128	0.634049
O	-1.187569	1.603550	-3.145451
H	-1.381354	2.053728	-3.982834
H	-1.258533	0.615849	-3.352575
O	-2.693348	-2.302886	-1.772089
H	-3.341030	-3.015227	-1.878310
H	-1.982368	-2.647559	-1.159081
O	3.117173	-2.246112	1.313208
H	3.708193	-2.698140	1.933330
H	2.318327	-1.941613	1.835186
O	-0.778013	-2.809474	-0.088267
H	0.135240	-3.144734	-0.248754
H	-0.979529	-2.932525	0.868919
O	1.798173	-3.334936	-0.692884
H	2.376519	-3.047253	0.064815
H	2.130902	-4.200889	-0.973391
O	-1.668078	1.563524	3.282407
H	-2.107846	2.223337	3.840692
H	-1.558648	1.997782	2.383616
O	2.550419	2.117423	1.588106
H	2.747633	1.345473	0.996406
H	1.982737	1.765504	2.312770
O	1.050395	3.578391	0.059451
H	1.683292	3.080730	0.671023
H	1.260250	4.519335	0.161894
O	-2.722098	-0.107840	-0.214505
H	-2.973796	0.741188	-0.642341
H	-2.923415	-0.838557	-0.843449
O	1.304023	2.495731	-2.439294
H	0.404234	2.184135	-2.692572
H	1.212232	2.931093	-1.558193
O	-2.834276	2.413840	-1.232256
H	-3.615379	2.868965	-1.580420
H	-2.271570	2.174885	-2.018402
O	1.109822	-1.287633	-2.369109
H	1.463604	-2.059062	-1.869526
H	1.884861	-0.730155	-2.611456
O	-1.218763	-0.977715	-3.642353
H	-1.830203	-1.484346	-3.056733
H	-0.323596	-1.189852	-3.274470
O	0.928083	1.081923	3.548557
H	1.241565	1.164035	4.462218
H	-0.037362	1.328835	3.566305
O	3.053668	0.522119	-2.724945
H	2.457392	1.325296	-2.683679
H	3.712090	0.688192	-3.415232
O	0.906050	-1.272241	2.284143
H	0.160524	-1.847128	2.575284
H	0.925911	-0.489217	2.887319
O	2.826303	0.086762	-0.081643
H	3.172534	-0.751716	0.291009
H	3.156908	0.187176	-1.002284
O	-1.345903	-2.712390	2.562824
H	-1.705878	-3.412578	3.127123
H	-2.030476	-1.973095	2.548917
K	0.031081	-0.024684	-0.108429

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O	-2.883674	-0.798430	2.511848
H	-2.923402	-0.600863	1.540921
H	-2.430757	-0.003617	2.881658
O	-1.193645	2.363585	0.842918
H	-1.919026	2.436872	0.180228
H	-0.517110	3.022658	0.552616
O	-1.518506	1.386637	-3.197306

H	-1.693689	1.793995	-4.059811
H	-1.486796	0.390656	-3.364332
O	-2.745496	-2.474005	-1.611272
H	-3.382132	-3.201241	-1.673401
H	-2.012074	-2.778651	-1.002039
O	3.230599	-2.034988	1.153809
H	3.903145	-2.407836	1.743681
H	2.430198	-1.825233	1.725178
O	-0.776342	-2.854371	0.027483
H	0.141888	-3.167001	-0.147102
H	-0.931346	-2.955364	0.997442
O	1.796640	-3.345032	-0.614668
H	2.438538	-2.967160	0.046673
H	2.163183	-4.198257	-0.892064
O	-1.475041	1.445879	3.268177
H	-1.905928	2.084204	3.857265
H	-1.442293	1.892551	2.373138
O	2.420451	2.550126	1.491903
H	2.692829	1.764076	0.929058
H	3.246186	2.981753	1.760643
O	0.810708	3.797212	-0.177293
H	1.497770	3.454807	0.459312
H	0.889676	4.763076	-0.175804
O	-2.735798	-0.230340	-0.106900
H	-3.063357	0.601484	-0.516038
H	-2.950353	-0.973821	-0.715446
O	0.916025	1.991888	-2.202685
H	0.026019	1.856872	-2.606569
H	0.852098	2.743072	-1.570553
O	-2.996079	2.250865	-1.159484
H	-3.803667	2.713658	-1.427524
H	-2.521279	1.991213	-1.994202
O	1.106546	-1.350023	-2.315926
H	1.450414	-2.128530	-1.818343
H	1.887054	-0.811885	-2.565278
O	-1.295418	-1.212584	-3.540874
H	-1.883631	-1.705961	-2.921092
H	-0.385682	-1.338604	-3.171844
O	1.228264	1.063212	3.493608
H	1.643623	1.654845	2.824693
H	0.268954	1.293945	3.492882
O	3.030100	0.549900	-2.654853
H	2.276096	1.204423	-2.613052
H	3.716457	0.945839	-3.211758
O	1.037604	-1.266500	2.268291
H	0.337022	-1.848590	2.636392
H	1.109084	-0.447045	2.831911
O	2.804737	0.446909	0.035508
H	3.160577	-0.393217	0.401623
H	3.067470	0.486184	-0.914884
O	-1.168802	-2.770692	2.700248
H	-1.544695	-3.502347	3.211950
H	-1.866009	-2.042442	2.690993
K	0.012270	-0.057650	-0.071154

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H	-2.386529	0.262044	2.595725
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H	-0.775694	3.114242	0.286765
O	-1.231560	1.221007	-3.331145
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H	-1.200301	0.235729	-3.364548
O	-2.769455	-2.504164	-1.535793
H	-3.282195	-3.313093	-1.684086
H	-2.018836	-2.745699	-0.918198
O	3.397122	-1.976055	1.212518
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H	2.623646	-1.810520	1.828993
O	-0.738881	-2.710655	0.078383
H	0.171485	-3.052800	-0.086626
H	-0.909293	-2.848983	1.042135
O	1.851098	-3.263098	-0.481830
H	2.526596	-2.882669	0.143518
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O	-1.647878	1.788847	3.007969
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O	2.378543	2.703146	1.612610
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H	3.169602	3.147800	1.954237
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O	1.299227	-1.238415	-2.195216
H	0.477469	-1.442665	-2.699562
H	1.539025	-2.050513	-1.689631
O	-1.130933	-1.493894	-3.360127
H	-1.807115	-1.939572	-2.781908
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O	0.973609	1.138237	3.362395
H	1.483087	1.764854	2.797312
H	0.037614	1.446083	3.312526
O	3.065884	0.675373	-2.420161
H	2.477466	-0.124420	-2.511237
H	3.789608	0.579308	-3.056061
O	1.218458	-1.333713	2.440139
H	0.452402	-1.878934	2.724582
H	1.130394	-0.439046	2.868950
O	2.897056	0.559841	0.254346
H	3.261865	-0.286099	0.596847
H	3.137058	0.605395	-0.701636
O	-1.130577	-2.642875	2.730495
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H	-1.587909	-3.317429	3.254211
K	0.030694	0.007391	0.103878

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H	-2.280457	0.128326	2.951541
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H	-1.985714	-2.713112	-1.081500
O	3.118406	-2.135138	0.957472
H	3.801875	-2.537570	1.528016
H	2.361578	-1.811619	1.578676
O	-0.811865	-2.976440	-0.090134
H	0.127322	-3.247674	-0.308550
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O	-1.359430	1.555263	3.221951
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H	2.077141	2.031258	2.270555
O	0.950537	3.680395	-0.037735
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H	1.109752	4.643885	-0.007954
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H	1.455243	-2.297746	-2.165826
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O	-1.263231	-0.814401	-3.354548
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H	0.219803	1.386796	3.498024
O	2.838295	0.457401	-2.704986
H	2.110053	1.167774	-2.589560
H	3.477317	0.808562	-3.355169
O	1.106716	-1.141550	2.166457
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H	1.189689	-0.347326	2.775765
O	2.933201	0.343347	-0.057318
H	3.205873	-0.558416	0.267404
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O	-1.053411	-2.577941	2.546968
H	-1.213677	-3.237623	3.249325
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O	1.731535	-3.562112	-0.224288
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O	2.358494	2.524195	1.448896
H	3.074229	2.994857	1.920308
H	1.709520	2.171638	2.195496
O	0.985146	3.759524	-0.398990
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O	0.817881	1.554542	3.215860
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H	0.847092	0.538312	3.222047
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H	3.915714	0.517730	-2.719699
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O	2.898728	0.104597	0.486316
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H	3.579858	-2.641324	1.650280
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H	-0.003995	-3.292613	-0.352642
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O	1.620307	-3.496242	-0.778715
H	2.223564	-3.107091	-0.058819
H	1.977222	-4.381062	-0.988492
O	-1.528281	1.577877	3.147748
H	-1.979083	2.250661	3.695801
H	-1.437292	1.996581	2.209672
O	2.447550	2.252073	1.583377
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O	1.007079	3.669427	0.035790
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H	-3.745309	2.758555	-1.466273
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H	1.435498	-2.283047	-1.941108
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O	1.007356	1.087428	3.567109
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O	3.113849	-2.076969	1.010939
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H	0.796319	2.713322	-1.439178
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H -3.044945 -3.303604 -1.842377
H -1.782079 -2.762589 -0.995820
O 3.030254 -1.918674 1.150051
H 3.840202 -2.237018 1.595195
H 2.329166 -1.749685 1.907961
O -0.665651 -2.757397 0.055005
H 0.228157 -3.178720 -0.108757
H -0.871020 -2.813994 1.037710
O 1.812160 -3.426111 -0.605374
H 2.378265 -2.947840 0.091594
H 2.199864 -4.314814 -0.721592
O -1.723653 1.754112 2.998028
H -2.133418 2.433026 3.569161
H -1.657971 2.168617 2.063056
O 2.284147 2.670543 1.599937
H 2.660355 1.866637 1.080148
H 3.057320 3.117347 1.997869
O 0.807620 3.904837 -0.178364
H 1.453103 3.548982 0.521634
H 0.975750 4.864646 -0.248009
O -2.777345 -0.338229 -0.133339
H -3.052479 0.480576 -0.642912
H -2.899306 -1.120277 -0.738352
O 0.698589 1.977983 -2.030986
H 0.828165 2.790960 -1.465426
H 1.604315 1.640924 -2.275314
O -3.006308 1.965967 -1.406060
H -3.821428 2.405527 -1.715566
H -2.448159 1.733830 -2.251307
O 1.310617 -1.323861 -2.186365
H 0.474345 -1.426403 -2.732977
H 1.522242 -2.203998 -1.765757
O -1.030399 -1.314104 -3.472348
H -1.658858 -1.848410 -2.874395
H -1.061023 -1.755585 -4.344145
O 0.857634 1.139292 3.325207
H 1.367581 1.766419 2.736228
H -0.102302 1.424015 3.256723
O 2.967108 0.609687 -2.375062
H 2.390602 -0.233752 -2.436439
H 3.681573 0.517897 -3.034294
O 1.281995 -1.409031 2.914989
H 0.371932 -1.830059 2.857359
H 1.118341 -0.417637 3.074782
O 2.949717 0.598175 0.271546
H 3.123621 -0.335734 0.595993
H 3.117211 0.602619 -0.717936
O -1.154856 -2.463471 2.629954
H -1.893819 -1.727149 2.634189
H -1.456014 -3.168270 3.235876
K 0.029519 0.033343 0.050751

F -1 water molecule

4

O 0.702201 -0.106922 -0.055033
H -0.253247 0.271803 -0.218555
H 0.533451 -0.753811 0.645615
F -1.581619 0.750767 -0.397205
4

O -0.185685 0.685846 0.000539
H 0.152289 -0.244523 0.331336
H -0.390557 0.493609 -0.925264
F 0.606891 -1.525827 0.692841
4

O -0.579230 -0.130458 -0.393939
H 0.406045 0.083497 -0.130281
H -1.000633 -0.185190 0.475582
F 1.727452 0.358294 0.303631
4

O 0.483990 -0.517288 -0.048593
H -0.239818 -1.076820 0.266755
H 0.033551 0.417087 -0.079508

F -0.628028 1.693611 -0.122455
4

O -0.488880 -0.441010 -0.274210
H 0.144976 0.376621 -0.158877
H -0.309577 -0.932341 0.540009
F 1.066155 1.444978 0.049715
4

O 0.708558 -0.106328 -0.057142
H -0.279946 0.279514 -0.220179
H 0.531268 -0.756364 0.648741
F -1.559094 0.745015 -0.396598
4

O -0.186586 0.693885 0.002449
H 0.158283 -0.268430 0.331360
H -0.393353 0.497834 -0.930957
F 0.604593 -1.514184 0.696600
4

O -0.583711 -0.132906 -0.400604
H 0.428621 0.090969 -0.119301
H -1.000461 -0.185892 0.480134
F 1.709187 0.353973 0.294763
4

O 0.491754 -0.522789 -0.052239
H -0.255278 -1.062444 0.268588
H 0.030444 0.447230 -0.081492
F -0.617226 1.654593 -0.118657
4

O -0.496600 -0.437367 -0.275215
H 0.176232 0.389864 -0.152947
H -0.312858 -0.938697 0.541623
F 1.045901 1.434448 0.043175

F -2 water molecules

7

O 1.420191 -0.371459 -0.491020
H 1.155414 0.044070 0.346295
H 0.523135 -0.726858 -0.770478
O -0.916979 0.661162 0.889307
H -0.689942 1.382457 0.283842
H -1.007488 -0.113046 0.238939
F -0.975819 -1.134275 -0.866069
7

O 0.088805 -0.602953 -1.313191
H 0.497465 0.271117 -1.395984
H 0.422242 -0.892236 -0.400636
O -0.548694 1.012081 1.005271
H -0.956053 0.740595 0.167774
H 0.078795 0.236477 1.133444
F 0.886098 -1.095717 1.031752
7

O -0.504020 -1.204017 0.649165
H 0.311286 -0.955754 1.110425
H -0.902761 -0.289476 0.470609
O 0.953451 0.794903 -0.953964
H 0.087947 1.055985 -0.513595
H 0.873607 -0.170751 -0.916682
F -1.264384 1.163267 0.255711
7

O 0.549543 -0.223795 1.260623
H 0.740243 0.456487 0.530278
H 0.876247 -1.038294 0.848670
O -1.145950 -0.176653 -1.015684
H -0.365803 0.453665 -1.056874
H -1.059446 -0.434716 -0.082186
F 0.883045 1.320084 -0.699248
7

O 0.682689 0.303463 1.182036
H 0.977415 1.107460 0.728316
H 0.813998 -0.391628 0.453021
O -1.300213 0.044886 -0.867717
H -1.092619 0.405366 0.011272
H -0.480102 -0.521694 -0.983665
F 0.880515 -1.265444 -0.775894
7

O 1.420114 -0.386184 -0.460232
H 1.077969 0.089594 0.329698
H 0.516395 -0.742726 -0.775221

O -0.864594 0.646759 0.900073
H -0.694283 1.385692 0.283723
H -0.971587 -0.133759 0.223059
F -0.975502 -1.117326 -0.870285
7

O 0.021408 -0.566569 -1.289017
H 0.557990 0.236981 -1.433655
H 0.386515 -0.863137 -0.361769
O -0.599537 0.981980 1.027151
H -0.877108 0.716447 0.122141
H 0.065730 0.220467 1.168149
F 0.913659 -1.056806 0.995430
7

O -0.499967 -1.190108 0.686761
H 0.383645 -0.896713 0.983530
H -0.918803 -0.269377 0.478666
O 0.989618 0.756837 -0.846627
H 0.090636 1.045676 -0.442352
H 0.792959 -0.197883 -0.940254
F -1.282963 1.145724 0.181946
7

O 0.532123 -0.226417 1.263595
H 0.722132 0.470344 0.515877
H 0.876437 -1.036016 0.838153
O -1.153974 -0.176790 -1.014678
H -0.356623 0.458870 -1.056482
H -1.025492 -0.436035 -0.073813
F 0.883276 1.302823 -0.687073
7

O 0.666247 0.302560 1.177218
H 0.934918 1.113146 0.702039
H 0.805908 -0.406097 0.429579
O -1.287251 0.073445 -0.856603
H -1.039017 0.386950 0.043543
H -0.465823 -0.517662 -0.987806
F 0.866700 -1.269932 -0.760601

F -4 water molecules

13

O -0.418084 -0.668141 1.756654
H 0.064949 -1.319150 1.213603
H -1.000351 -0.280625 1.046951
O 0.019118 -1.912318 -0.812279
H -0.761946 -1.321741 -0.708193
H 0.658415 -1.240579 -1.125997
O 0.785337 0.640262 -1.650014
H 1.113503 1.077796 -0.839376
H -0.165966 0.539488 -1.383981
O 0.467484 1.775540 0.906724
H -0.364036 1.624101 0.410852
H 0.474838 0.939545 1.422817
F -1.473981 0.283629 -0.396141
13

O -0.378018 -0.479051 -1.670768
H -0.833120 -1.208704 -1.209325
H 0.405307 -0.397203 -1.072783
O 1.660141 2.039376 -0.227826
H 1.731570 1.082160 -0.011693
H 0.751800 2.213457 0.071888
O -0.866439 0.952270 0.769092
H -1.072618 0.758786 -0.165155
H -0.031812 0.425311 0.854138
O -0.847131 -2.089259 0.671315
H 0.049151 -1.665832 0.643234
H -1.386601 -1.347825 0.990769
F 1.244172 -0.536219 0.400961
13

O 0.005849 1.201398 1.307655
H 0.409057 0.297457 1.329201
H -0.401621 1.218041 0.418335
O -0.873776 0.703042 -1.359513
H -1.200719 -0.117563 -0.917374
H 0.090716 0.512825 -1.432915
O 1.815236 0.166490 -0.956796
H 1.545222 -0.456855 -0.217739
H 1.886623 1.009609 -0.480800
O -1.454623 -1.450614 0.249766
H -0.490336 -1.446461 0.536055
H -1.879408 -0.928454 0.947590
F 0.971844 -1.223726 1.020349
13

O	0.102160	0.563766	-1.492686
H	0.337741	0.816129	-0.564967
H	-0.268403	-0.323677	-1.321750
O	2.544811	-0.559180	-0.196829
H	1.962905	-0.076371	0.435518
H	2.067118	-0.385003	-1.025602
O	-0.636865	-1.559907	0.244524
H	0.022582	-0.935173	0.623032
H	-1.447999	-1.046284	0.429628
O	-1.991980	0.846511	0.845766
H	-1.029261	0.866182	1.090836
H	-1.957773	1.090107	-0.093002
F	0.588573	0.678689	1.068159

13

O	0.427360	-0.346732	2.134258
H	0.544482	-1.031693	1.446074
H	-0.453312	-0.001316	1.834422
O	-0.436399	-1.696441	-0.221507
H	0.071424	-1.227885	-0.919133
H	-1.024478	-0.969303	0.117378
O	0.722520	0.022406	-2.123112
H	0.660515	0.688148	-1.385359
H	-0.102130	0.159781	-2.614668
O	0.372140	1.652762	0.023228
H	-0.529050	1.258753	0.246589
H	0.900350	1.193379	0.703163
F	-1.668810	0.367965	0.773498

13

O	-0.374220	-0.719311	1.769951
H	0.064650	-1.309614	1.098972
H	-1.012340	-0.279296	1.133317
O	0.016247	-1.825316	-0.710659
H	-0.764780	-1.200696	-0.638422
H	0.663505	-1.157275	-1.064461
O	0.835519	0.621646	-1.650310
H	1.090220	1.043857	-0.784684
H	-0.142625	0.541850	-1.449579
O	0.434165	1.718734	0.826838
H	-0.405177	1.487387	0.334256
H	0.480101	0.881731	1.366087
F	-1.485986	0.334110	-0.389688

13

O	-0.416805	-0.431663	-1.621577
H	-0.845463	-1.179288	-1.129981
H	0.405719	-0.372177	-1.050633
O	1.664091	2.007071	-0.223500
H	1.730148	1.035156	-0.002206
H	0.733530	2.161437	0.047779
O	-0.911721	0.899284	0.776481
H	-1.046259	0.674910	-0.182194
H	-0.025555	0.443837	0.883987
O	-0.842334	-2.052115	0.601969
H	0.070170	-1.630837	0.600748
H	-1.362393	-1.294764	0.951240
F	1.273275	-0.513586	0.391735

13

O	-0.081940	1.113161	1.310639
H	0.373622	0.219648	1.313959
H	-0.435003	1.134197	0.380443
O	-0.839260	0.664823	-1.348965
H	-1.164547	-0.169758	-0.896938
H	0.144665	0.477400	-1.406735
O	1.826401	0.233414	-0.957684
H	1.541312	-0.443054	-0.242295
H	1.823432	1.059418	-0.431197
O	-1.491049	-1.394963	0.322781
H	-0.492387	-1.458575	0.539629
H	-1.756290	-0.691470	0.951867
F	0.975108	-1.259051	0.908311

13

O	-0.030366	0.388838	-1.474151
H	0.288069	0.746492	-0.594287
H	-0.315679	-0.504169	-1.143718
O	2.591688	-0.359873	-0.297785
H	1.983978	0.068515	0.369390
H	2.011491	-0.303793	-1.088089
O	-0.623371	-1.561604	0.413204
H	0.045417	-0.896902	0.753186
H	-1.429828	-1.001026	0.552305
O	-1.977199	0.860138	0.717591
H	-1.019623	0.914028	1.021141
H	-1.838937	0.944579	-0.251847
F	0.607970	0.680567	1.065684

13

O	0.280426	-0.263679	1.969993

H	0.409762	-1.002756	1.309127
H	-0.564320	0.089734	1.582670
O	-0.190831	-1.877957	-0.160680
H	0.287939	-1.422404	-0.903855
H	-0.892241	-1.164391	-0.029296
O	0.229782	0.131843	-1.990396
H	0.748523	0.721963	-1.376223
H	-0.634491	0.186597	-1.493161
O	0.676300	1.762032	0.156090
H	-0.274522	1.446260	0.060403
H	0.934083	1.114716	0.866269
F	-1.525797	0.347865	0.023889

F -8 water molecules

25

O	1.753605	2.265481	1.331198
H	2.234612	2.623369	0.568558
H	0.920397	1.918510	0.923659
O	-1.736271	-0.281565	-1.770211
H	-1.202446	0.357722	-1.248737
H	-2.147074	-0.830182	-1.058144
O	2.045237	0.476121	-1.356507
H	1.210128	0.848033	-0.998913
H	2.478428	0.139105	-0.534464
O	-2.758880	1.230048	0.923339
H	-1.801624	1.289254	0.679589
H	-3.209058	1.419543	0.085185
O	0.581258	-1.823758	-1.727353
H	-0.276294	-1.372508	-1.913083
H	1.217046	-1.068774	-1.753811
O	-2.591729	-1.493159	0.536896
H	-2.775602	-0.571697	0.838299
H	-1.666095	-1.629516	0.836796
O	2.791497	-0.302643	1.187713
H	2.510503	0.613871	1.422628
H	1.954755	-0.809787	1.280028
O	0.186907	-1.312224	0.929711
H	0.373929	-1.698203	0.034568
H	0.002804	-0.367445	0.686296
F	-0.251679	1.118070	0.038672

25

O	-0.160312	0.058572	2.687256
H	-0.228448	-0.763056	2.151680
H	-0.913344	0.590243	2.329802
O	1.098982	-0.781731	-2.378351
H	0.392788	-1.446199	-2.519509
H	0.579490	-0.105506	-1.885644
O	-0.339265	3.164949	-0.097201
H	0.467207	2.850317	0.354082
H	-0.535295	2.402674	-0.675996
O	1.466920	1.059648	0.724426
H	1.039013	0.780674	1.573676
H	0.735109	0.876775	0.087789
O	-1.463150	-1.941729	-2.094447
H	-1.205368	-2.321885	-1.233282
H	-1.543503	-0.996520	-1.865082
O	-2.076241	1.390986	1.231497
H	-1.750049	0.905931	0.440041
H	-1.623726	2.247413	1.081445
O	2.303692	-1.532054	-0.036352
H	2.251490	-0.623710	0.335471
H	2.008815	-1.372914	-0.967531
O	-0.335293	-1.803859	0.596224
H	-0.524648	-0.976105	0.095889
H	0.638955	-1.902157	0.442100
F	-0.622841	0.475618	-0.806952

25

O	1.672303	2.272266	1.186210
H	0.893274	1.921946	0.684406
H	1.346391	2.338250	2.097200
O	-1.794054	-0.439388	-1.727298
H	-1.269896	0.261739	-1.279009
H	-2.176709	-0.915015	-0.950711
O	1.978806	0.466384	-1.633408
H	1.158364	0.842652	-1.249332
H	2.478055	0.207692	-0.819371
O	-2.631758	1.271949	1.073937
H	-3.223341	1.501909	0.340520
H	-1.731331	1.328874	0.668117
O	0.576578	-1.890041	-1.746080
H	-0.309263	-1.477225	-1.889238
H	1.180689	-1.114884	-1.849409
O	-2.490019	-1.445327	0.738738
H	-2.658685	-0.504854	0.988804
H	-1.537710	-1.553868	0.949562
O	2.917424	-0.157610	0.870541

H	2.601675	0.748090	1.113020
H	2.119867	-0.703283	1.047737
O	0.334190	-1.265671	0.902637
H	0.462860	-1.691933	0.015063
H	0.104185	-0.341385	0.621877
F	-0.264854	1.087499	-0.111264

25

O	0.150510	0.744852	-2.673939
H	0.232141	-0.204930	-2.906301
H	0.591585	0.726249	-1.797014
O	-1.145832	-1.547908	-0.107999
H	-1.334774	-1.362103	0.845361
H	-0.307041	-1.051093	-0.232932
O	-0.774375	1.644539	0.636020
H	-0.053365	1.056895	0.319426
H	-1.467971	1.486386	-0.051273
O	2.102850	1.802757	1.428964
H	1.982255	1.233546	0.639377
H	1.261336	2.286804	1.463778
O	-1.220404	-0.462064	2.393362
H	-0.257591	-0.655497	2.504248
H	-1.199980	0.380752	1.883036
O	1.507025	-0.784763	2.269816
H	1.777353	0.154105	2.362703
H	1.430477	-0.829032	1.292258
O	0.825363	-1.929839	-2.321568
H	0.056898	-2.355496	-1.906785
H	1.198251	-1.405363	-1.582507
O	-2.297620	0.615037	-1.386317
H	-1.523561	0.734207	-1.987550
H	-2.069846	-0.235394	-0.939675
F	1.097740	-0.068708	-0.308051

25

O	2.245548	0.412928	1.956181
H	2.142693	1.194591	1.363256
H	1.338970	0.355926	2.345456
O	0.971376	0.306216	-1.741004
H	0.271403	0.668393	-1.151565
H	1.398259	-0.370004	-1.149564
O	1.482068	2.474289	0.230351
H	1.797576	2.076176	-0.600753
H	0.548860	2.163484	0.246402
O	-2.970544	0.281513	-1.244200
H	-3.341780	-0.344563	-0.602874
H	-2.237873	0.714745	-0.738971
O	-1.136233	-1.485562	-2.383739
H	-0.348701	-0.896372	-2.365532
H	-1.872536	-0.864563	-2.171210
O	-0.948027	-1.584337	0.349556
H	-0.931548	-0.602172	0.299120
H	-1.053677	-1.818126	-0.603698
O	1.790328	-1.501975	0.093820
H	2.048453	-0.845997	0.792725
H	0.841606	-1.682384	0.292983
O	-0.421999	0.433261	2.587822
H	-0.726334	-0.486673	2.543157
H	-0.659946	0.795454	1.699437
F	-0.845491	1.089135	0.072619

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O	1.544899	2.176694	1.472993
H	2.096543	2.718593	0.873846
H	0.795580	1.881602	0.875341
O	-1.685033	-0.460170	-1.801525
H	-1.195241	0.269571	-1.338415
H	-2.123198	-0.910636	-1.012423
O	2.061218	0.375471	-1.396730
H	1.222070	0.810979	-1.091517
H	2.463325	0.115008	-0.508922
O	-2.561207	1.248786	1.052183
H	-1.660068	1.323640	0.619023
H	-3.161227	1.615423	0.372531
O	0.607907	-1.904453	-1.699183
H	-0.272570	-1.454077	-1.892595
H	1.238218	-1.119439	-1.719770
O	-2.554957	-1.423991	0.574399
H	-2.691884	-0.463959	0.839469
H	-1.594408	-1.548115	0.816785
O	2.722645	-0.259220	1.157211
H	2.395910	0.655870	1.411337
H	1.870718	-0.779521	1.192606
O	0.183612	-1.269797	0.837199
H	0.374695	-1.687363	-0.073777
H	0.003263	-0.324928	0.550020
F	-0.236460	1.151698	-0.168175

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O	-0.397544	0.094985	2.498466
H	-0.479599	-0.721968	1.932386
H	-1.075307	0.707807	2.062895

O	0.762486	-0.959712	-2.550777
H	0.240542	-1.810720	-2.452431
H	0.175926	-0.314588	-2.057848
O	0.129089	3.548477	1.110578
H	0.710489	2.743887	0.943027
H	0.085212	3.971857	0.229736
O	1.265339	1.141777	0.667753
H	0.797739	0.753675	1.481465
H	0.556610	0.955949	-0.032304
O	-0.753309	-3.131148	-1.863062
H	-0.705610	-2.747539	-0.934379
H	-1.643296	-2.858297	-2.163102
O	-1.937317	1.759447	1.034793
H	-1.604151	1.308616	0.204535
H	-1.295771	2.527433	1.106055
O	2.151467	-1.317066	-0.260670
H	2.080385	-0.392465	0.105638
H	1.777483	-1.193843	-1.192317
O	-0.416727	-1.726223	0.415998
H	-0.656921	-0.887836	-0.099311
H	0.591051	-1.707425	0.293125
F	-0.697287	0.491297	-0.909218

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O	1.500295	2.239809	1.355840
H	0.793071	1.942566	0.710236
H	1.066975	2.133113	2.226208
O	-1.757290	-0.553726	-1.719455
H	-1.249157	0.214407	-1.345512
H	-2.120660	-0.957054	-0.869387
O	1.979948	0.361511	-1.663640
H	1.149505	0.793846	-1.332003
H	2.445684	0.175573	-0.787706
O	-2.417694	1.286980	1.151196
H	-3.093828	1.626777	0.531731
H	-1.572706	1.349351	0.615627
O	0.564966	-1.960745	-1.728229
H	-0.335221	-1.530878	-1.868523
H	1.178141	-1.170032	-1.841411
O	-2.422139	-1.401623	0.766807
H	-2.548556	-0.434554	1.010761
H	-1.444928	-1.510248	0.937219
O	2.842287	-0.067559	0.869568
H	2.469906	0.823080	1.150711
H	2.038964	-0.644892	0.999456
O	0.330872	-1.198862	0.798648
H	0.460956	-1.658475	-0.102203
H	0.109216	-0.275109	0.478044
F	-0.231566	1.165511	-0.300735

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O	0.116291	0.678715	-2.712278
H	0.178742	-0.303552	-2.874772
H	0.610910	0.697452	-1.850242
O	-1.132707	-1.500453	-0.151958
H	-1.308588	-1.321060	0.827483
H	-0.276040	-1.002263	-0.257557
O	-0.732259	1.583159	0.701373
H	0.001210	1.008852	0.348770
H	-1.420062	1.437448	-0.028616
O	2.029211	1.842947	1.479441
H	2.007107	1.300010	0.652488
H	1.131991	2.244929	1.462272
O	-1.227924	-0.529844	2.347320
H	-0.243433	-0.703366	2.459576
H	-1.190780	0.344118	1.855347
O	1.481098	-0.751876	2.236863
H	1.712990	0.213739	2.318838
H	1.425957	-0.785734	1.244351
O	0.762313	-1.957812	-2.299300
H	-0.011966	-2.320738	-1.815222
H	1.195186	-1.421498	-1.586537
O	-2.228064	0.696233	-1.322753
H	-1.452797	0.788661	-1.955890
H	-2.009570	-0.191192	-0.906038
F	1.142608	-0.072937	-0.336520

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O	2.179491	0.493024	1.883941
H	2.019931	1.260989	1.258369
H	1.273998	0.398022	2.307738
O	0.903089	0.254630	-1.695527
H	0.224204	0.581302	-1.043609
H	1.395438	-0.418952	-1.109379
O	1.423569	2.425060	0.099381
H	1.655114	1.940271	-0.728284
H	0.485484	2.110628	0.218993
O	-2.822931	0.468094	-1.395134
H	-3.444695	-0.021731	-0.820416
H	-2.124190	0.779762	-0.744477
O	-1.158281	-1.466516	-2.335658
H	-0.340301	-0.891618	-2.314417

H	-1.868189	-0.788078	-2.117011
O	-0.813802	-1.686764	0.329962
H	-0.859975	-0.694084	0.384107
H	-0.984568	-1.807277	-0.658176
O	1.873805	-1.460722	0.079975
H	2.061834	-0.754130	0.782194
H	0.912340	-1.690553	0.263193
O	-0.401735	0.352285	2.722336
H	-0.662003	-0.590794	2.705189
H	-0.695686	0.680589	1.822620
F	-0.849489	1.009940	0.223864

F -12 water molecules

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O	2.141975	-1.332828	-0.989967
H	2.586917	-1.351274	-0.103299
H	1.314645	-0.854929	-0.762692
O	2.862489	-1.094098	1.632878
H	2.733578	-0.122256	1.628591
H	2.006192	-1.435935	1.968561
O	-0.218043	3.363557	0.332186
H	-0.961193	2.847960	0.710785
H	0.577777	2.947015	0.724223
O	-1.959705	-1.560401	-1.023151
H	-2.378906	-1.640171	-0.127913
H	-1.186828	-0.996692	-0.801813
O	-0.128435	1.825493	-1.942846
H	-0.162378	2.560930	-1.278315
H	-0.073009	1.052479	-1.336900
O	0.128871	-1.822858	1.946360
H	0.081220	-1.049578	1.340769
H	0.166835	-2.559850	1.283637
O	-2.647912	-1.413603	1.627932
H	-2.650743	-0.433385	1.612352
H	-1.752078	-1.639816	1.958244
O	-2.857624	1.097445	-1.638370
H	-2.725517	0.125529	-1.632431
H	-1.998545	1.439516	-1.967695
O	0.211602	-3.364360	-0.323273
H	0.956205	-2.856147	-0.708439
H	-0.584475	-2.947727	-0.713991
O	-2.144275	1.329924	0.984110
H	-2.583211	1.347480	0.094037
H	-1.312353	0.856557	0.765651
O	2.651445	1.415188	-1.625228
H	1.757609	1.644665	-1.958571
H	2.652467	0.434885	-1.616297
O	1.947054	1.562736	1.021091
H	1.182024	0.988040	0.803476
H	2.369362	1.643120	0.127202
F	-0.003037	-0.006607	-0.010895

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O	1.559818	-1.277051	1.738902
H	1.037385	-0.727575	1.114887
H	0.840264	-1.629396	2.315501
O	-0.918488	-2.158357	2.599195
H	-1.419268	-1.320474	2.507188
H	-0.921681	-2.498224	1.675362
O	-1.625329	1.117115	-1.847485
H	-1.909588	1.806177	-1.190292
H	-0.984596	0.610396	-1.303786
O	-0.794806	-2.530556	-0.168884
H	-0.558324	-1.577338	-0.184133
H	0.066735	-2.916433	-0.457392
O	0.984775	2.323007	-2.450436
H	0.067928	1.982190	-2.508766
H	1.526611	1.508455	-2.368365
O	0.799245	2.545116	0.277912
H	0.935105	2.677386	-0.694940
H	0.496890	1.610424	0.291129
O	-2.025112	2.722069	0.289668
H	-1.066799	2.896338	0.408156
H	-2.200522	1.976343	0.904076
O	-3.120792	-0.968282	-0.660404
H	-2.493687	-1.716213	-0.720673
H	-2.742356	-0.298948	-1.271492
O	1.914788	-2.805254	-0.596638
H	1.928815	-2.429526	0.313351
H	2.122505	-2.017503	-1.140281
O	-2.125838	0.194215	1.560684
H	-1.247271	0.190062	1.124541
H	-2.671992	-0.249343	0.859303
O	2.228236	-0.082309	-1.549776
H	2.736987	0.281077	-0.780249
H	1.332694	-0.139217	-1.152618
O	3.093173	0.937136	0.844642
H	2.421971	1.652703	0.826594

H	2.719337	0.263655	1.445195
F	0.022376	0.004893	-0.031927

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O	1.849620	-1.557805	-0.825387
H	2.332912	-1.705369	0.031730
H	1.204695	-0.869085	-0.563189
O	2.827570	-1.600110	1.703445
H	2.913225	-0.618667	1.605555
H	1.930426	-1.703080	2.085643
O	-1.773600	1.745897	1.397659
H	-0.960798	1.290439	1.068494
H	-1.466411	2.338105	2.102257
O	-2.014575	-1.017211	-0.643794
H	-2.502175	-1.006487	0.220916
H	-1.202426	-0.519157	-0.402513
O	0.423688	1.632932	-1.987537
H	0.366815	1.183364	-1.115441
H	-0.345074	1.240446	-2.470729
O	0.034258	-1.631188	2.143864
H	0.108062	-0.827273	1.582793
H	-0.101066	-2.333736	1.454218
O	-2.710049	-0.812839	1.964262
H	-2.545848	0.156242	1.943808
H	-1.840588	-1.175839	2.237145
O	-2.094007	0.852044	-2.687687
H	-2.233384	0.111353	-2.057625
H	-2.266348	1.651605	-2.139841
O	-0.336546	-3.182193	-0.086948
H	0.472516	-2.824874	-0.513823
H	-1.041747	-2.584065	-0.422141
O	-1.887460	3.080765	-1.051256
H	-1.959142	2.675476	-0.158302
H	-0.958449	2.911095	-1.304782
O	3.112297	0.846794	-1.648186
H	2.878950	-0.103283	-1.590923
H	2.274221	1.247269	-1.966428
O	2.676833	1.065630	1.062667
H	1.711706	0.959062	0.945805
H	2.988128	1.077647	0.124074
F	0.151262	0.318681	0.306192

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O	2.308559	-0.920446	-1.163993
H	2.657156	-0.919332	-0.234933
H	1.419044	-0.520664	-1.047849
O	2.831908	-0.780561	1.525423
H	2.608306	0.175836	1.521263
H	1.960679	-1.188814	1.730541
O	-0.499074	3.443036	0.455522
H	-1.249600	2.855090	0.669304
H	0.285418	2.973523	0.813330
O	-3.628885	-1.197130	0.161598
H	-3.226943	-1.343428	1.047337
H	-2.935983	-1.496797	-0.466539
O	-0.041826	2.425803	-2.075121
H	-0.179728	1.514649	-1.748242
H	-0.234676	2.949504	-1.259394
O	0.174463	-1.616660	1.486759
H	0.050352	-0.891263	0.834869
H	0.330155	-2.386598	0.878827
O	-2.269175	-0.956448	2.609088
H	-2.229740	-0.056415	2.222362
H	-1.404061	-1.336638	2.335899
O	-1.455261	-1.818820	-1.511979
H	-0.970451	-0.990233	-1.285704
H	-1.688438	-1.734130	-2.449767
O	0.737115	-3.252002	-0.627929
H	1.413049	-2.618569	-0.951068
H	-0.080899	-2.937283	-1.075568
O	-2.233313	1.149551	0.721120
H	-2.940555	0.553480	0.381931
H	-1.439139	0.815971	0.247076
O	2.634093	1.944104	-1.588923
H	1.722971	2.170224	-1.899984
H	2.686154	0.970783	-1.674600
O	1.659045	1.711039	0.919898
H	0.976176	1.138782	0.506120
H	2.189390	1.948320	0.113372
F	-0.065189	0.179346	-0.487127

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O	2.230232	-1.270748	-0.755074
H	2.532312	-1.206958	0.189905
H	1.328982	-0.882602	-0.710170
O	2.650598	-0.941923	1.915208
H	2.391497	0.002953	1.834971
H	1.788994	-1.367956	2.125196
O	0.180232	3.662408	-0.126169
H	-0.789911	3.558112	0.038915
H	0.615571	3.042439	0.496198
O	-1.515958	-2.451491	-1.037862

H	-2.068383	-2.437097	-0.220453
H	-1.039548	-1.599217	-0.987508
O	0.120426	1.831092	-2.109394
H	0.121804	2.585163	-1.463440
H	-0.109055	1.064537	-1.545860
O	0.044968	-1.911990	1.813039
H	-0.089834	-1.208044	1.140006
H	0.307336	-2.681629	1.242725
O	-2.783770	-1.983161	1.389137
H	-2.908992	-1.055533	1.098957
H	-1.891623	-1.986349	1.794553
O	-2.494334	3.232496	-0.117356
H	-2.631911	2.259933	-0.016127
H	-2.609480	3.379969	-1.069077
O	0.813353	-3.647816	-0.169976
H	1.445769	-2.981474	-0.515596
H	-0.038045	-3.391201	-0.600225
O	-2.693292	0.515887	0.000466
H	-3.071028	0.239582	-0.850245
H	-1.729504	0.294239	-0.071563
O	2.742499	1.427352	-1.387295
H	1.865305	1.591263	-1.813323
H	2.791789	0.448496	-1.348946
O	1.507647	1.480020	1.035203
H	0.780376	0.922201	0.678407
H	2.099498	1.558849	0.240209
F	-0.189806	-0.158971	-0.258356

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O	2.083197	-1.337818	-0.984714
H	2.520705	-1.316875	-0.070754
H	1.247510	-0.844100	-0.772023
O	2.804850	-1.026372	1.593622
H	2.638502	-0.045630	1.566605
H	1.940471	-1.391631	1.923154
O	-0.210175	3.362736	0.328661
H	-0.954961	2.823066	0.707394
H	0.598676	2.927444	0.711823
O	-1.912879	-1.587027	-0.981123
H	-2.345148	-1.633697	-0.065925
H	-1.141895	-1.002114	-0.759577
O	-0.110025	1.871053	-1.902684
H	-0.154445	2.594317	-1.193641
H	-0.060060	1.074783	-1.311913
O	0.106432	-1.879175	1.903202
H	0.064354	-1.077404	1.319563
H	0.158626	-2.594838	1.186682
O	-2.658436	-1.381244	1.599712
H	-2.615724	-0.387609	1.568542
H	-1.751817	-1.634095	1.924106
O	-2.797525	1.035209	-1.598499
H	-2.632782	0.054407	-1.566382
H	-1.928576	1.399416	-1.919573
O	0.213513	-3.356686	-0.335338
H	0.958797	-2.814725	-0.712262
H	-0.596993	-2.921574	-0.713532
O	-2.095162	1.334068	0.986574
H	-2.521891	1.314317	0.067513
H	-1.252782	0.850481	0.777846
O	2.657162	1.367483	-1.598757
H	1.751405	1.622362	-1.922907
H	2.612675	0.373721	-1.567479
O	1.907834	1.595274	0.978249
H	1.140279	1.001493	0.766985
H	2.337759	1.630451	0.061438
F	-0.001471	0.000534	0.005414

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O	1.554792	-1.164096	1.786186
H	1.036099	-0.609947	1.145703
H	0.779409	-1.581670	2.281538
O	-0.835531	-2.193845	2.452786
H	-1.388646	-1.370463	2.400191
H	-0.845366	-2.490253	1.493862
O	-1.618956	1.128196	-1.828504
H	-1.881657	1.827560	-1.142582
H	-0.981080	0.604996	-1.274853
O	-0.773830	-2.517472	-0.265019
H	-0.584378	-1.542472	-0.250796
H	0.161928	-2.847551	-0.457677
O	0.933058	2.249658	-2.341988
H	-0.002142	1.915459	-2.401738
H	1.462297	1.406856	-2.287728
O	0.844895	2.537281	0.323642
H	0.942334	2.618085	-0.683221
H	0.517911	1.600797	0.369893
O	-1.978768	2.715749	0.309051
H	-1.002039	2.859710	0.437980
H	-2.173857	1.952942	0.919304
O	-3.147695	-0.964599	-0.706098
H	-2.512597	-1.716588	-0.784728
H	-2.750074	-0.265415	-1.294200

O	1.891393	-2.777359	-0.407063
H	1.866108	-2.309272	0.480186
H	2.107963	-2.022146	-1.014312
O	-2.167552	0.181043	1.553032
H	-1.270195	0.191584	1.128018
H	-2.691510	-0.259551	0.810394
O	2.152520	-0.171215	-1.561130
H	2.693083	0.227436	-0.806498
H	1.260648	-0.189865	-1.124583
O	3.150481	0.946425	0.699179
H	2.462519	1.666557	0.713869
H	2.805751	0.291881	1.353521
F	-0.008127	0.028325	-0.007872

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O	1.773711	-1.580190	-0.777102
H	2.295804	-1.707281	0.092208
H	1.155136	-0.860638	-0.484996
O	2.796099	-1.558508	1.660276
H	2.894482	-0.562608	1.526489
H	1.889017	-1.640340	2.059241
O	-1.812479	1.706119	1.359503
H	-0.948235	1.292007	1.073307
H	-1.567989	2.295437	2.101898
O	-1.876017	-1.036367	-0.657112
H	-2.401830	-1.012847	0.211659
H	-1.079491	-0.508098	-0.384427
O	0.439651	1.787875	-1.885293
H	0.403861	1.298780	-1.019328
H	-0.324583	1.351838	-2.381266
O	-0.011118	-1.645860	2.147639
H	0.095372	-0.822772	1.602268
H	-0.129531	-2.344191	1.418079
O	-2.733578	-0.830987	1.854086
H	-2.558349	0.151716	1.834327
H	-1.860326	-1.187747	2.171064
O	-1.978776	0.863923	-2.657063
H	-2.096800	0.105475	-2.021480
H	-2.209339	1.658838	-2.091168
O	-0.311267	-3.196022	-0.024610
H	0.510616	-2.813779	-0.444179
H	-1.007530	-2.574894	-0.384949
O	-1.942614	3.058888	-1.040699
H	-2.005442	2.629842	-0.142172
H	-0.985150	2.930877	-1.264395
O	3.004078	0.699476	-1.738142
H	2.679492	-0.231016	-1.589631
H	2.162642	1.167993	-1.994552
O	2.769220	1.058409	0.964786
H	1.783094	1.006919	0.918776
H	3.004405	1.001183	-0.013029
F	0.201253	0.361137	0.343984

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O	2.273140	-0.927246	-1.154504
H	2.597413	-0.870133	-0.192198
H	1.363554	-0.540568	-1.057889
O	2.797572	-0.638103	1.457577
H	2.489409	0.311028	1.461244
H	1.955382	-1.121614	1.691376
O	-0.604944	3.453781	0.294301
H	-1.327631	2.824146	0.556999
H	0.199288	3.050575	0.718785
O	-3.606495	-0.931492	0.130676
H	-3.210253	-1.207497	1.009419
H	-2.961316	-1.329231	-0.515249
O	0.068437	2.299365	-2.061076
H	-0.116286	1.401549	-1.692352
H	-0.202056	2.867228	-1.272726
O	0.268550	-1.733901	1.486363
H	0.098536	-0.987992	0.849488
H	0.427317	-2.483600	0.819485
O	-2.217590	-1.102292	2.474417
H	-2.103120	-0.158106	2.181746
H	-1.333148	-1.495899	2.231812
O	-1.509586	-1.827585	-1.473776
H	-1.004544	-1.001439	-1.224081
H	-1.688195	-1.730923	-2.430554
O	0.712876	-3.248666	-0.658638
H	1.378111	-2.576059	-0.969433
H	-0.136545	-2.914223	-1.061779
O	-2.135723	1.185057	0.891021
H	-2.867843	0.613475	0.495888
H	-1.354790	0.812475	0.398189
O	2.673079	1.899290	-1.483252
H	1.750017	2.117509	-1.833094
H	2.707968	0.910637	-1.562075
O	1.569823	1.788030	0.926841
H	0.897267	1.170475	0.537373
H	2.121258	1.967119	0.087602
F	-0.097835	0.111641	-0.425007

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O	2.160602	-1.258966	-0.747961
H	2.443196	-1.155503	0.224800
H	1.250800	-0.859847	-0.720532
O	2.568432	-0.837037	1.864232
H	2.287423	0.116750	1.770271
H	1.701100	-1.280276	2.082632
O	0.219203	3.774404	-0.003176
H	-0.762486	3.578648	0.045733
H	0.640476	3.091112	0.586793
O	-1.568749	-2.370023	-1.130297
H	-2.057063	-2.404059	-0.248701
H	-1.105125	-1.500588	-1.064955
O	0.085627	1.979029	-2.021936
H	0.220417	2.704872	-1.331705
H	-0.091768	1.177427	-1.465329
O	0.032730	-1.912499	1.770189
H	-0.103330	-1.173881	1.118902
H	0.300830	-2.665214	1.134540
O	-2.670333	-2.166577	1.351088
H	-2.865874	-1.204016	1.210618
H	-1.750800	-2.139775	1.738919
O	-2.324832	3.026237	-0.547032
H	-2.556303	2.157691	-0.110541
H	-1.891363	2.728652	-1.378472
O	0.677663	-3.562811	-0.205041
H	1.348381	-2.908913	-0.542289
H	-0.163062	-3.258511	-0.669502
O	-2.723591	0.461343	0.327507
H	-3.200715	0.152311	-0.470765
H	-1.760700	0.256386	0.120440
O	2.725476	1.377024	-1.355499
H	1.876228	1.598267	-1.831240
H	2.700507	0.379975	-1.316349
O	1.493071	1.558779	1.022723
H	0.741131	0.989472	0.706382
H	2.070694	1.573777	0.185086
F	-0.243181	-0.090833	-0.240454

F -16 water molecules

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O	-0.065556	1.922417	-1.692749
H	0.099535	2.580805	-0.971041
H	-0.029629	1.087266	-1.174983
O	2.295159	1.983609	2.194633
H	1.587738	1.423161	2.582211
H	2.697930	1.377812	1.528643
O	0.609251	3.294080	0.544236
H	1.306380	2.849465	1.107341
H	0.930478	4.202405	0.428317
O	2.592619	1.296516	-2.249320
H	1.698470	1.703892	-2.179445
H	2.381191	0.406656	-2.602391
O	1.492301	-1.316229	-2.353326
H	2.166079	-1.805581	-1.806778
H	0.932647	-0.910538	-1.664883
O	-2.498570	1.138146	0.533680
H	-2.776611	1.336425	-0.401847
H	-1.618215	0.740231	0.406600
O	-0.042292	0.481033	2.577011
H	0.012335	0.281843	1.621076
H	-0.587922	1.313230	2.631396
O	-0.381954	-3.414080	-2.090027
H	-1.174345	-2.836139	-2.007347
H	0.291241	-2.796056	-2.444641
O	0.442263	-2.809340	0.480881
H	0.091293	-3.206771	-0.357845
H	0.295735	-1.849230	0.340633
O	-2.151223	-1.379600	-1.426817
H	-2.641676	-1.587616	-0.581313
H	-1.339250	-0.976860	-1.056795
O	2.767767	0.229009	0.192435
H	1.808139	0.039309	0.220764
H	2.855279	0.701527	-0.682596
O	-1.388089	2.829768	2.379076
H	-0.711621	3.180657	1.753939
H	-2.019408	2.396252	1.762943
O	-3.131535	-1.523001	1.054938
H	-2.409213	-1.782989	1.682513
H	-3.109070	-0.542911	1.045763
O	-2.781550	1.287771	-2.120694
H	-2.680824	0.310653	-2.101523
H	-1.858031	1.619659	-2.175106
O	-1.097220	-2.170473	2.742539
H	-0.515401	-2.580297	2.066833
H	-0.722598	-1.272506	2.873421
O	3.064664	-2.469508	-0.460409
H	3.209719	-1.566056	-0.102326

H	2.251079	-2.759240	0.011209
F	0.016602	-0.210246	-0.131615
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O	0.209240	1.846458	-1.807382
H	0.243031	2.666096	-1.246761
H	0.209635	1.148417	-1.117011
O	2.255456	2.420292	1.603650
H	1.628142	1.927999	2.178003
H	2.696454	1.707221	1.087511
O	0.424361	3.663361	0.121464
H	1.179715	3.257263	0.640207
H	0.681490	4.584901	-0.037533
O	2.716705	0.981686	-2.543484
H	1.893058	1.506271	-2.408114
H	2.333792	0.102072	-2.741787
O	1.035188	-1.323986	-2.200547
H	1.686237	-1.934864	-1.760064
H	0.732242	-0.796772	-1.432356
O	-2.377222	0.816840	0.184937
H	-2.537135	0.990640	-0.784272
H	-1.450961	0.492453	0.195706
O	0.090495	0.926341	2.603772
H	0.176394	0.547945	1.701266
H	-0.565258	1.664412	2.472091
O	-1.526945	-3.878305	0.053916
H	-2.137353	-3.172298	0.387774
H	-1.560581	-3.758257	-0.909658
O	0.575475	-2.586700	1.118775
H	-0.125249	-3.160425	0.703110
H	0.387769	-1.693171	0.755978
O	-1.692264	-1.682605	-2.001969
H	-0.725343	-1.731415	-2.185448
H	-1.757242	-1.578739	-1.039042
O	2.933280	0.233970	0.054923
H	1.969988	0.082575	0.163551
H	2.996609	0.576063	-0.878153
O	-1.611442	2.907918	1.811571
H	-0.952422	3.328202	1.211260
H	-2.072431	2.268966	1.221826
O	-2.774497	-1.757404	1.070954
H	-2.209303	-1.669414	1.882495
H	-2.869512	-0.834651	0.746665
O	-2.366296	1.019631	-2.478474
H	-2.182533	0.053720	-2.515995
H	-1.467511	1.419513	-2.440769

O	-1.032844	-1.598763	3.152617
H	-0.350947	-2.081207	2.634676
H	-0.699335	-0.673358	3.139551
O	2.788225	-2.520733	-0.553927
H	3.104209	-1.633122	-0.279626
H	2.107800	-2.724669	0.128861
F	0.206906	-0.091737	0.089123
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O	0.765481	1.857358	-1.717994
H	0.754854	2.601991	-1.059929
H	0.530571	1.095086	-1.147044
O	1.996771	2.116379	2.294701
H	1.162832	1.689098	2.592428
H	2.456941	1.379686	1.828727
O	0.678500	3.478062	0.418526
H	1.259617	3.038742	1.105838
H	1.011916	4.385583	0.337487
O	3.332945	0.787732	-1.702442
H	2.515759	1.320614	-1.841770
H	3.067007	-0.100193	-2.026017
O	-1.012931	-1.418143	-2.364585
H	-0.216796	-1.854065	-2.719026
H	-0.682651	-0.983518	-1.552323
O	-2.338385	0.909134	-0.472460
H	-1.481215	0.487945	-0.263781
H	-2.254210	1.116993	-1.442342
O	-0.470782	0.833087	2.393472
H	-0.219025	0.464152	1.523316
H	-1.064662	1.600806	2.152930
O	-0.028180	-2.690932	0.944364
H	-0.540201	-2.432378	1.765873
H	0.057524	-1.819558	0.502408
O	2.696524	-2.822211	0.405668
H	1.782353	-2.958502	0.740789
H	2.907062	-1.912097	0.707278
O	-2.290591	-3.131453	-0.522262
H	-2.005534	-2.659884	-1.332677
H	-1.459603	-3.153645	0.009262
O	2.739819	-0.046271	0.787470
H	1.787544	-0.120258	0.572257
H	3.112848	0.313882	-0.065456
O	-1.846204	2.878798	1.363366
H	-2.184838	2.309881	0.634501
H	-1.011267	3.249181	0.991322
O	-3.546973	-1.224764	0.925285

H	-3.190175	-1.955838	0.357775
H	-3.299094	-0.420516	0.422195
O	-1.608913	1.255053	-3.056750
H	-1.431644	0.294315	-3.130181
H	-0.741550	1.620502	-2.768471
O	-1.604029	-1.648863	2.812585
H	-1.219118	-0.746303	2.881745
H	-2.372937	-1.500247	2.202578
O	1.958117	-1.674963	-1.938036
H	2.324980	-2.257011	-1.221839
H	1.368723	-1.102787	-1.417980
F	0.148417	-0.233279	-0.153482

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O	0.763475	2.153244	-1.590959
H	0.657020	1.400770	-0.970084
H	0.837057	2.928147	-0.959191
O	2.379311	2.298823	1.865819
H	1.666764	1.805903	2.328827
H	2.799903	1.620331	1.295444
O	0.705542	3.898663	0.385047
H	1.361901	3.402483	0.939404
H	-0.157033	3.528173	0.671161
O	2.954940	0.690243	-2.483364
H	2.300661	1.410220	-2.340241
H	2.365795	-0.079451	-2.641135
O	1.011974	-1.339349	-2.215145
H	1.612645	-1.971357	-1.733580
H	0.728216	-0.773613	-1.464844
O	-2.154751	0.128121	-0.561923
H	-2.161928	0.848710	-1.257023
H	-1.207306	0.047602	-0.301587
O	0.083486	0.872203	2.570486
H	0.264637	0.460383	1.696155
H	-0.589507	1.546100	2.311611
O	-1.756469	-3.729930	0.194079
H	-2.420426	-3.108052	0.591709
H	-1.685812	-3.364988	-0.723333
O	0.361091	-2.536089	1.211524
H	-0.396536	-3.062602	0.811320
H	0.296505	-1.658974	0.780931
O	-1.606176	-2.254523	-2.094352
H	-0.665681	-2.029035	-2.276247
H	-1.961433	-1.445720	-1.671642
O	3.096710	0.105003	0.173478
H	2.122382	0.016920	0.242434
H	3.211059	0.382524	-0.773932
O	-1.634256	2.450897	1.173758
H	-2.383038	2.912276	1.583885
H	-2.041909	1.757531	0.616458
O	-3.290949	-1.721070	1.176153
H	-2.672292	-1.540571	1.928799
H	-3.077326	-1.023083	0.523678
O	-1.871320	2.146791	-2.259919
H	-1.940194	1.866173	-3.185716
H	-0.898111	2.259466	-2.110790
O	-1.378273	-1.451678	3.117720
H	-0.712140	-1.989747	2.635572
H	-0.951824	-0.565852	3.116940
O	2.611843	-2.622618	-0.463532
H	3.013916	-1.780014	-0.161329
H	1.913985	-2.787259	0.211365
F	0.399512	-0.022647	0.050816

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O	0.448489	1.719621	-1.762285
H	0.362877	1.037819	-1.062213
H	0.455459	2.555446	-1.223217
O	2.169812	2.200154	1.698335
H	1.481144	1.748311	2.232226
H	2.619730	1.469574	1.216957
O	0.548742	3.586804	0.106997
H	1.237396	3.139272	0.679960
H	0.883340	4.482881	-0.055035
O	2.914202	0.753283	-2.449232
H	2.114312	1.316351	-2.325576
H	2.489433	-0.108651	-2.646580
O	1.130378	-1.459413	-2.240473
H	1.660122	-2.111342	-1.708245
H	0.716332	-0.938638	-1.527307
O	-2.385093	0.771515	0.082380
H	-2.454175	0.868522	-0.913748
H	-1.482175	0.407595	0.176523
O	-0.166976	0.882901	2.580438
H	-0.017344	0.486542	1.695444
H	-0.759560	1.659462	2.377820
O	-1.317277	-2.493165	-0.187774
H	-2.163926	-2.278836	0.301146
H	-0.825118	-1.646814	-0.149151
O	0.687104	-2.664707	1.674572
H	-0.043980	-2.927546	1.066627
H	0.784222	-1.722828	1.449808

O	-1.561866	-1.787244	-2.854062
H	-1.683719	-2.178824	-1.960466
H	-0.583038	-1.795120	-2.923402
O	2.907608	0.006128	0.157492
H	1.931170	-0.085683	0.182684
H	3.070808	0.341182	-0.766250
O	-1.660949	2.934033	1.599512
H	-0.937833	3.320404	1.052952
H	-2.089442	2.288395	0.991371
O	-3.371847	-1.563062	1.213592
H	-2.786917	-1.549625	2.013861
H	-3.228833	-0.675519	0.812893
O	-2.110343	0.886711	-2.539112
H	-1.938524	-0.076271	-2.705798
H	-1.214782	1.283541	-2.457256
O	-1.523623	-1.498170	3.198887
H	-0.791507	-2.079975	2.918396
H	-1.120899	-0.601243	3.143528
O	2.639476	-2.746591	-0.417489
H	3.002120	-1.874424	-0.149545
H	2.057559	-2.976163	0.336451
F	0.186601	-0.244328	0.117356

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O	0.068121	1.991204	-1.563215
H	0.207879	2.661378	-0.815898
H	0.062720	1.145347	-1.040134
O	2.263497	2.051389	2.041418
H	1.594664	1.436794	2.453670
H	2.663593	1.465642	1.331209
O	0.523263	3.397603	0.649051
H	1.285093	2.931583	1.163631
H	0.790059	4.336758	0.588833
O	2.524920	1.136328	-2.428680
H	1.655039	1.602129	-2.257101
H	2.222265	0.221530	-2.679634
O	1.432193	-1.431131	-2.371696
H	2.138883	-1.850500	-1.762214
H	0.865145	-0.982362	-1.702906
O	-2.569013	1.066261	0.616235
H	-2.700534	1.293755	-0.374889
H	-1.691601	0.625053	0.590955
O	0.061771	0.423525	2.556715
H	0.112919	0.247179	1.583554
H	-0.531867	1.257006	2.616794
O	-0.410103	-3.477307	-1.836382
H	-1.162834	-2.815643	-1.800512
H	0.294088	-2.925448	-2.270591
O	0.523395	-2.808734	0.571782
H	0.131571	-3.219302	-0.274411
H	0.366679	-1.843534	0.402718
O	-2.010055	-1.328471	-1.440584
H	-2.596153	-1.527531	-0.618943
H	-1.218417	-0.934504	-0.992128
O	2.781155	0.314270	0.063612
H	1.815382	0.100588	0.118636
H	2.836442	0.708832	-0.878356
O	-1.365300	2.644949	2.434010
H	-0.715927	3.078546	1.804387
H	-2.015630	2.235975	1.796908
O	-3.294537	-1.564175	0.831250
H	-2.556668	-1.791404	1.488616
H	-3.298997	-0.569521	0.869975
O	-2.583719	1.344957	-1.984764
H	-2.465744	0.355425	-2.036827
H	-1.646274	1.690188	-2.010903
O	-1.271709	-2.059055	2.535047
H	-0.621871	-2.521198	1.938331
H	-0.832725	-1.181544	2.708378
O	3.028847	-2.363798	-0.479108
H	3.159460	-1.429039	-0.154398
H	2.232398	-2.665246	0.046074
F	0.082329	-0.226420	-0.100303

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O	0.166528	1.852034	-1.808806
H	0.224494	2.644962	-1.176253
H	0.149078	1.101035	-1.159527
O	2.233612	2.453337	1.583504
H	1.591210	1.936136	2.147466
H	2.645271	1.722882	1.034974
O	0.362732	3.573184	0.160552
H	1.165994	3.198502	0.686760
H	0.559325	4.520304	0.016862
O	2.658852	0.961851	-2.502198
H	1.791405	1.449858	-2.389003
H	2.326925	0.043686	-2.702544
O	1.329881	-1.443971	-2.301841
H	1.946137	-2.023521	-1.733731
H	0.932045	-0.900612	-1.581404
O	-2.442902	0.628811	0.225276
H	-2.570753	0.819580	-0.771777

H	-1.504142	0.314671	0.244985
O	0.140372	0.912877	2.479814
H	0.208429	0.522026	1.574496
H	-0.587819	1.627248	2.341075
O	-1.726943	-3.513859	-0.042682
H	-2.285544	-2.886889	0.534572
H	-1.692947	-3.027530	-0.907664
O	0.496335	-2.633388	1.047039
H	-0.301473	-3.111955	0.612977
H	0.374157	-1.717884	0.686522
O	-1.396091	-1.603645	-2.051422
H	-0.512928	-1.801636	-2.467526
H	-1.099230	-1.135384	-1.237001
O	2.833686	0.265612	0.050792
H	1.863469	0.084923	0.120761
H	2.903265	0.593191	-0.914068
O	-1.632303	2.708549	1.785859
H	-0.986842	3.172975	1.175538
H	-2.104110	2.070162	1.176532
O	-2.984208	-1.758468	1.505384
H	-2.254616	-1.643076	2.196077
H	-2.963091	-0.895082	1.010713
O	-2.377218	1.005866	-2.383383
H	-2.134996	0.060490	-2.564097
H	-1.481101	1.450419	-2.335485
O	-0.883492	-1.552613	3.173359
H	-0.284693	-2.063168	2.558976
H	-0.536248	-0.621036	3.081496
O	2.821780	-2.538192	-0.407786
H	3.065115	-1.614640	-0.132564
H	2.043592	-2.743346	0.189814
F	0.127269	-0.206643	-0.077553

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O	0.821116	1.865363	-1.679226
H	0.814766	2.631191	-1.012350
H	0.557782	1.111682	-1.089360
O	1.989608	2.199780	2.214747
H	1.170323	1.730362	2.543086
H	2.461695	1.456042	1.738129
O	0.688738	3.500573	0.373968
H	1.283601	3.054107	1.088428
H	0.976145	4.434605	0.337984
O	3.272408	0.642840	-1.763281
H	2.464543	1.224352	-1.871469
H	2.916371	-0.242479	-2.050737
O	-0.978361	-1.450443	-2.388287
H	-0.053534	-1.771211	-2.566274
H	-0.836274	-0.976514	-1.535622
O	-2.357360	0.885809	-0.382179
H	-1.491884	0.475543	-0.135023
H	-2.205072	1.092775	-1.370667
O	-0.382537	0.829997	2.437225
H	-0.134179	0.438358	1.564611
H	-0.977533	1.619053	2.154531
O	-0.089756	-2.638716	1.007111
H	-0.637737	-2.340970	1.824946
H	-0.004482	-1.767069	0.542808
O	2.569085	-2.750809	0.359816
H	1.665391	-2.872416	0.767817
H	2.813345	-1.831481	0.653526
O	-2.153693	-3.278790	-0.654174
H	-1.843734	-2.756810	-1.440541
H	-1.363913	-3.214630	-0.039296
O	2.742468	0.021015	0.750211
H	1.772018	-0.066772	0.581032
H	3.078823	0.311620	-0.171669
O	-1.731441	2.829460	1.411292
H	-2.110957	2.265500	0.677504
H	-0.904235	3.215371	0.997941
O	-3.435633	-1.374970	0.763791
H	-3.044246	-2.100257	0.182289
H	-3.208610	-0.538128	0.276328
O	-1.571855	1.266035	-2.878812
H	-1.383326	0.305855	-3.038667
H	-0.678062	1.622440	-2.602006
O	-1.688698	-1.583294	2.779393
H	-1.284514	-0.673267	2.831458
H	-2.410466	-1.471730	2.073720
O	1.732968	-1.644774	-1.900190
H	2.111567	-2.250976	-1.175006
H	1.232269	-1.019722	-1.325708
F	0.122654	-0.197121	-0.105851

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O	0.455303	1.945372	-1.672324
H	0.347044	1.184054	-1.047155
H	0.547760	2.730620	-1.002523
O	2.327352	2.264335	1.801062
H	1.587157	1.790743	2.269806
H	2.723581	1.522208	1.262550
O	0.689737	3.694975	0.214441

H	1.359326	3.212567	0.799953
H	-0.173700	3.528135	0.684671
O	2.891524	0.896135	-2.283384
H	2.040639	1.420589	-2.184644
H	2.533001	0.008122	-2.554051
O	1.423535	-1.443099	-2.250485
H	1.955052	-2.082899	-1.660413
H	1.026570	-0.878715	-1.545320
O	-2.378650	0.759261	0.026471
H	-2.401969	0.984773	-0.974687
H	-1.469061	0.376835	0.117421
O	0.034203	0.869404	2.462839
H	0.153599	0.486980	1.556822
H	-0.606956	1.629679	2.281421
O	-1.886274	-3.404465	-0.284542
H	-2.456454	-2.763099	0.263980
H	-1.767245	-2.906091	-1.134469
O	0.295396	-2.676844	0.987692
H	-0.495337	-3.094846	0.484537
H	0.262199	-1.747361	0.643046
O	-1.287923	-1.470830	-2.217360
H	-0.368490	-1.696948	-2.536140
H	-1.066327	-1.048553	-1.356959
O	2.892535	0.064247	0.238770
H	1.909989	-0.049881	0.254923
H	3.032878	0.430516	-0.703639
O	-1.538691	2.786354	1.500354
H	-2.205240	3.259668	2.036722
H	-2.053413	2.136794	0.922149
O	-3.163816	-1.621544	1.214853
H	-2.479204	-1.552729	1.955822
H	-3.068216	-0.755346	0.737862
O	-2.035210	1.222250	-2.533704
H	-1.826940	0.273939	-2.740460
H	-1.127156	1.619621	-2.377957
O	-1.176924	-1.548182	3.025746
H	-0.561461	-2.077184	2.444098
H	-0.781169	-0.633819	2.982006
O	2.720392	-2.696831	-0.315606
H	3.001940	-1.796199	0.000304
H	1.900787	-2.872096	0.232016
F	0.169972	-0.201145	-0.061809

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O	0.359339	1.736213	-1.732096
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H	0.416980	2.550629	-1.128922
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H	2.652774	1.543033	1.206033
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H	1.305270	3.112343	0.759012
H	0.837308	4.456403	0.020219
O	2.783834	0.690188	-2.367014
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H	2.347487	-0.193709	-2.524005
O	1.205690	-1.546259	-2.132347
H	1.795328	-2.148298	-1.563827
H	0.755372	-1.037505	-1.414014
O	-2.412172	0.736511	0.085569
H	-2.434531	0.773199	-0.946179
H	-1.499325	0.387807	0.229114
O	-0.030253	0.943753	2.531939
H	0.105099	0.515021	1.649579
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O	-1.566006	-2.488725	-0.346532
H	-2.343456	-2.233870	0.282131
H	-1.054942	-1.645877	-0.345646
O	0.492068	-2.648126	1.420571
H	-0.250937	-2.970928	0.832621
H	0.536692	-1.713248	1.100213
O	-1.406750	-1.787460	-2.981867
H	-1.675663	-2.210644	-2.120796
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O	2.856269	0.093297	0.209648
H	1.874821	-0.038330	0.242864
H	2.973519	0.379371	-0.765566
O	-1.606867	2.826528	1.620446
H	-0.881670	3.229589	1.058015
H	-2.068316	2.205460	0.985043
O	-3.293694	-1.516330	1.336094
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H	-3.181105	-0.623713	0.900773
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O	-1.334328	-1.394835	3.180028
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H	-0.904997	-0.495403	3.100406
O	2.734546	-2.678323	-0.274605
H	3.015209	-1.764115	0.004089
H	2.032039	-2.893903	0.396821

F 0.158343 -0.269041 0.084470

F -20 water molecules

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O -1.576487 -1.464638 3.464004
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61

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H	-1.308281	-1.910709	-2.186901
O	0.181909	-2.533900	-2.874295
H	0.421061	-1.644816	-3.263250
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O	1.953618	-3.334954	-0.928205
H	1.391997	-3.331168	-0.120919
H	1.312359	-3.187770	-1.663597
O	2.495630	-1.830244	2.901113
H	2.946174	-1.072998	2.467502
H	1.885366	-1.407076	3.548244
O	-4.256180	1.856411	-1.342048
H	-3.612911	1.729775	-2.070832
H	-3.694427	2.199951	-0.604703
O	1.022737	3.435254	0.763047
H	1.970642	3.305348	0.491092
H	0.890021	2.781373	1.483630
F	-0.188991	-0.368048	0.185300
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H	0.212328	2.615996	-0.436602
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O	0.806155	1.348378	2.222294
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O	0.501611	-0.293768	4.310086
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H	0.436990	-0.018462	5.237248
O	3.274530	0.492916	1.350263
H	2.427962	0.868495	1.702807
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O	-2.670620	2.412856	0.467130
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O	-1.653562	-1.362794	-1.603457
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H	-0.918719	-1.814487	-2.103495
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H	1.186242	-1.714099	-2.218174
H	0.527355	-1.527453	-3.587370
O	0.328921	-2.698005	1.645107
H	1.134634	-2.374341	2.141425
H	0.014878	-1.888553	1.190417
O	2.038805	1.172657	-2.504459
H	2.217988	0.354350	-1.993096
H	1.210541	1.513915	-2.094567
O	-4.192236	-0.875675	-0.627058
H	-4.298134	0.019378	-1.043153
H	-3.434144	-1.261742	-1.113004
O	2.073315	-0.932280	-0.687656
H	2.196787	-1.921695	-0.584946
H	1.207543	-0.750986	-0.253176
O	1.887439	-3.565409	-0.449004
H	1.236908	-3.483948	0.290413

H	1.349082	-3.768129	-1.232216
O	2.427549	-1.672683	2.984756
H	2.900354	-0.971382	2.488683
H	1.858876	-1.177134	3.619761
O	-4.178999	1.651359	-1.680179
H	-3.463811	1.494655	-2.333319
H	-3.699421	2.029893	-0.902032
O	0.999767	3.543544	0.603895
H	1.910349	3.340058	0.259742
H	0.917319	2.956238	1.386356
F	-0.257661	-0.350488	0.443810

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O	-1.439427	-2.080052	3.378627
H	-2.061516	-1.478429	2.919029
H	-1.113690	-2.640542	2.641049
O	0.605407	0.895607	-4.404723
H	1.219435	1.285494	-3.744926
H	-0.284949	1.146733	-4.071223
O	3.150830	3.064624	0.119216
H	2.927538	2.711923	-0.769419
H	3.365003	2.254804	0.626914
O	-2.817532	-0.432337	1.430094
H	-1.918403	-0.457574	1.040686
H	-3.371812	-0.807649	0.688441
O	-0.345716	1.982650	-0.784987
H	-0.339202	1.109326	-0.334591
H	0.009896	2.647157	-0.102186
O	-1.804623	1.316982	-3.009120
H	-1.768675	0.365678	-2.730395
H	-1.340648	1.775074	-2.274558
O	0.645934	1.002476	2.317227
H	1.567719	0.888651	1.954532
H	0.129841	0.414922	1.727893
O	0.887944	-0.937306	4.229761
H	0.036982	-1.384701	3.985158
H	0.809230	-0.084478	3.745974
O	3.054030	0.496827	1.248485
H	3.236677	-0.257555	1.866574
H	2.815266	0.049421	0.405318
O	-2.918165	2.209957	0.596926
H	-2.066153	2.253944	0.123186
H	-2.920021	1.322020	1.027083
O	-1.525395	-1.242050	-2.074492
H	-1.114947	-1.000208	-1.218604
H	-0.756043	-1.539079	-2.640025
O	0.725124	-1.650212	-3.439262
H	1.322497	-1.496062	-2.679262
H	0.708575	-0.768176	-3.896483
O	2.269562	-3.056503	0.522535
H	1.324636	-3.264994	0.692396
H	2.579368	-2.674411	1.379646
O	2.047735	1.657985	-2.138649
H	2.264985	0.748209	-1.847179
H	1.172887	1.831521	-1.715889
O	-4.037970	-1.210465	-0.841575
H	-4.223226	-0.289204	-1.167374
H	-3.266771	-1.473900	-1.383011
O	1.952424	-0.875401	-0.928439
H	2.203663	-1.748927	-0.493577
H	1.075535	-0.701611	-0.516884
O	-0.457203	-3.071670	1.016475
H	-0.485275	-2.142250	0.696078
H	-1.052256	-3.568061	0.432206
O	2.959782	-1.708729	2.793715
H	3.666293	-1.999171	3.390841
H	2.169818	-1.506769	3.383085
O	-4.271708	1.363430	-1.629756
H	-3.538594	1.443255	-2.277842
H	-3.886512	1.767170	-0.813561
O	0.650500	3.458869	1.077920
H	0.588199	2.721217	1.725988
H	1.598609	3.429850	0.780743
F	-0.397062	-0.485856	0.277698

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O	-1.517013	-2.050270	3.108787
H	-0.963002	-2.516296	2.446432
H	-2.012396	-1.375876	2.586665
O	0.331919	0.174990	-3.791824
H	1.043116	0.756364	-3.458266
H	-0.493264	0.678375	-3.644361
O	3.653401	2.713446	0.013104
H	3.315680	2.446543	-0.868708
H	3.814224	1.857648	0.469093
O	-2.538638	-0.070099	1.452365
H	-3.289519	-0.346235	0.848454
H	-1.729114	-0.186475	0.914351
O	-0.263223	2.186427	-0.862034
H	-0.251031	1.260648	-0.534376
H	0.269247	2.701847	-0.172921
O	-2.145579	1.368304	-2.820755

H	-2.182114	0.448374	-2.451668
H	-1.552138	1.849953	-2.209023
O	1.028758	0.779503	2.071411
H	0.811553	0.299601	2.915492
H	0.497313	0.343699	1.371651
O	0.580783	-0.821196	4.148557
H	-0.276154	-1.268024	3.884643
H	0.429593	-0.429719	5.022354
O	3.541673	0.170925	1.278873
H	2.677449	0.482569	1.651546
H	3.241117	-0.238014	0.431639
O	-2.614218	2.612001	0.794515
H	-1.823500	2.605479	0.219430
H	-2.614905	1.714741	1.202587
O	-2.058434	-1.142748	-1.711870
H	-1.374182	-0.904846	-1.049026
H	-1.538591	-1.753494	-2.306554
O	-0.210377	-2.437387	-3.104852
H	0.437770	-2.817368	-2.471772
H	0.141838	-1.543584	-3.332920
O	0.439162	-2.757699	1.191239
H	1.249456	-2.536266	1.733550
H	0.173777	-1.903678	0.789734
O	2.214407	1.690069	-2.264616
H	2.341619	0.782858	-1.891241
H	1.363677	1.981378	-1.871169
O	-4.395564	-0.663703	-0.375673
H	-4.514331	0.264096	-0.704489
H	-3.697111	-1.024862	-0.965187
O	2.227392	-0.662587	-0.962519
H	2.271289	-1.623420	-1.196818
H	1.302151	-0.560363	-0.646716
O	1.679178	-3.269556	-1.200261
H	2.241321	-4.055941	-1.274674
H	1.235304	-3.327990	-0.318312
O	2.557704	-2.086584	2.728738
H	3.060531	-1.357875	2.305846
H	2.005820	-1.642827	3.410839
O	-4.408816	1.986606	-1.184117
H	-3.773211	1.892863	-1.925007
H	-3.832266	2.303123	-0.444977
O	1.179318	3.255705	1.048452
H	2.109309	3.170077	0.715643
H	1.081124	2.476946	1.642601
F	-0.231704	-0.358016	0.062271

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O	-1.729863	-1.743912	3.296862
H	-1.384686	-2.378004	2.611827
H	-2.248546	-1.095538	2.739446
O	0.732866	0.288511	-4.366818
H	1.328386	0.767734	-3.726507
H	-0.172838	0.600910	-4.083738
O	3.306671	2.829042	-0.183838
H	2.994009	2.397884	-1.027068
H	3.455894	2.035897	0.408191
O	-2.793495	-0.025929	1.392809
H	-3.324459	-0.494086	0.645254
H	-1.871012	-0.090594	1.040687
O	-0.318199	2.005830	-0.944602
H	-0.351388	1.152271	-0.437738
H	0.154883	2.680402	-0.281342
O	-1.650462	0.965053	-3.123210
H	-1.636403	0.050976	-2.687610
H	-1.209083	1.536962	-2.439523
O	0.760055	1.168746	2.221871
H	0.686214	0.586332	3.054389
H	0.278962	0.614579	1.554771
O	0.572184	-0.723046	3.991624
H	-0.351133	-1.119540	3.771015
H	0.544545	-0.511951	4.946153
O	3.192167	0.538666	1.315624
H	2.299529	0.826055	1.697893
H	2.918743	-0.020477	0.534855
O	-2.936405	2.428691	0.156736
H	-2.023562	2.423106	-0.227945
H	-2.943421	1.617849	0.743795
O	-1.487655	-1.404242	-1.870284
H	-1.091771	-1.031861	-1.042850
H	-0.656035	-1.773291	-2.362241
O	0.754925	-2.011591	-3.010075
H	0.784524	-1.194621	-3.614486
H	1.357290	-1.747944	-2.263865
O	2.265795	-3.035081	0.808522
H	2.542586	-2.579422	1.679309
H	1.294015	-3.200391	0.948453
O	2.057924	1.346523	-2.175981
H	2.243277	0.466773	-1.751559
H	1.173606	1.613612	-1.786543
O	-3.961675	-1.077188	-0.714706
H	-4.115219	-0.210099	-1.223486
H	-3.180148	-1.454787	-1.193797

O	2.036108	-1.000713	-0.704894
H	2.231783	-1.880336	-0.157034
H	1.145343	-0.749042	-0.345098
O	-0.467383	-2.896805	1.144951
H	-0.458399	-1.962409	0.806954
H	-1.013677	-3.391626	0.499889
O	2.938016	-1.671778	2.966975
H	3.214430	-0.843053	2.487324
H	2.082971	-1.401706	3.408512
O	-4.153305	1.279741	-1.954586
H	-3.360023	1.218177	-2.554703
H	-3.775280	1.794369	-1.173521
O	0.897690	3.448910	0.756754
H	1.854414	3.316015	0.431540
H	0.825504	2.805229	1.512340
F	-0.351428	-0.351312	0.319353

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O	-1.483847	-1.883546	3.278313
H	-0.943512	-2.381288	2.603224
H	-2.014968	-1.234369	2.729304
O	0.541376	0.013412	-4.114510
H	1.198728	0.560424	-3.594962
H	-0.330712	0.434476	-3.867652
O	3.445595	2.620200	-0.156013
H	3.108108	2.233655	-1.009596
H	3.585352	1.824051	0.429016
O	-2.595843	-0.019923	1.584089
H	-3.249413	-0.408320	0.887355
H	-1.723234	-0.078115	1.118025
O	-0.273354	2.124431	-0.877685
H	-0.258343	1.249596	-0.405547
H	0.259337	2.757705	-0.226307
O	-1.755003	1.012558	-2.921526
H	-1.782488	0.125768	-2.434049
H	-1.260397	1.599071	-2.288764
O	0.901175	1.222526	2.316061
H	0.740088	0.700934	3.171703
H	0.410913	0.685286	1.642411
O	0.532237	-0.530335	4.214951
H	-0.319911	-1.036926	3.940605
H	0.443001	-0.338790	5.169251
O	3.317362	0.336639	1.473018
H	2.463655	0.723819	1.841265
H	2.998950	-0.126784	0.636469
O	-2.764659	2.497182	0.468704
H	-1.884413	2.490762	0.011780
H	-2.742868	1.669859	1.030291
O	-1.710532	-1.311483	-1.584798
H	-1.126190	-1.017867	-0.839613
H	-1.082703	-1.841943	-2.183783
O	0.195483	-2.327753	-3.043164
H	0.422303	-1.424596	-3.492714
H	-0.063633	-2.923056	-3.774951
O	0.355812	-2.693113	1.334514
H	1.189528	-2.473250	1.887584
H	0.101699	-1.797495	0.997843
O	2.053834	1.416609	-2.291756
H	2.185035	0.546263	-1.796514
H	1.216411	1.769858	-1.880228
O	-4.095783	-0.898449	-0.375411
H	-4.223048	-0.017666	-0.863737
H	-3.338170	-1.292327	-0.885280
O	2.172935	-0.684719	-0.703192
H	2.170306	-1.703802	-0.879716
H	1.260418	-0.536059	-0.340465
O	1.756991	-3.205095	-1.023207
H	1.163344	-3.217952	-0.220655
H	1.147724	-3.019091	-1.796755
O	2.396568	-1.934941	2.841854
H	2.877296	-1.182594	2.398488
H	1.822169	-1.466575	3.513000
O	-4.177186	1.487154	-1.591169
H	-3.433971	1.376188	-2.243726
H	-3.710569	1.947209	-0.823412
O	1.102688	3.454854	0.806733
H	2.035622	3.233538	0.471835
H	0.995296	2.821098	1.568034
F	-0.222734	-0.239481	0.359678

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O	-1.546210	-1.558523	3.503734
H	-1.004633	-2.154071	2.917627
H	-2.094545	-1.027545	2.854763
O	0.420251	0.286416	-4.467597
H	1.086842	0.736801	-3.879555
H	-0.448073	0.610271	-4.089123
O	3.427915	2.506100	-0.345360
H	3.056804	2.111524	-1.182241
H	3.536701	1.712598	0.250486
O	-2.653016	-0.044757	1.495546
H	-3.255120	-0.496665	0.792268

H	-1.756775	-0.142225	1.085189
O	-0.291328	1.987254	-0.960325
H	-0.282803	1.137131	-0.446286
H	0.254011	2.663409	-0.357133
O	-1.806395	0.979219	-3.005776
H	-1.775503	0.069053	-2.560809
H	-1.304504	1.546187	-2.359385
O	0.869718	1.261465	2.156457
H	0.715418	0.867482	3.082537
H	0.341693	0.669492	1.562670
O	0.493831	-0.150513	4.305285
H	-0.367783	-0.665716	4.082351
H	0.368523	0.225798	5.198373
O	3.194727	0.239935	1.264735
H	2.359983	0.679148	1.624178
H	2.869232	-0.271443	0.469623
O	-2.814665	2.435891	0.339289
H	-1.935500	2.423272	-0.116835
H	-2.793500	1.606488	0.901145
O	-1.598125	-1.384486	-1.762179
H	-1.140555	-1.066950	-0.942727
H	-0.830779	-1.760912	-2.334152
O	0.509401	-2.020128	-3.156729
H	1.180263	-1.750676	-2.482636
H	0.487825	-1.200310	-3.762470
O	0.332045	-2.615247	1.734726
H	1.142452	-2.281401	2.275546
H	0.073766	-1.815737	1.210559
O	1.979185	1.253716	-2.374809
H	2.126820	0.358017	-1.965447
H	1.143097	1.574966	-1.927340
O	-4.018475	-1.042632	-0.510672
H	-4.178557	-0.159938	-0.989198
H	-3.267655	-1.423074	-1.035485
O	1.997004	-1.037355	-0.877635
H	2.093198	-2.046731	-0.675252
H	1.125747	-0.808702	-0.453210
O	1.925388	-3.530656	-0.214378
H	1.261235	-3.383256	0.530305
H	1.425637	-4.029176	-0.892074
O	2.363683	-1.692384	3.106333
H	2.831617	-1.036207	2.518294
H	1.823285	-1.119686	3.721404
O	-4.220045	1.346970	-1.687625
H	-3.472362	1.268877	-2.341894
H	-3.771851	1.839480	-0.929613
O	1.106160	3.433565	0.591297
H	2.034413	3.185826	0.261961
H	0.995343	2.826000	1.374524
F	-0.256384	-0.359710	0.340976

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O	-1.572508	-2.172761	3.112301
H	-2.147251	-1.494004	2.660036
H	-1.244338	-2.713120	2.347533
O	0.539444	0.723254	-4.291928
H	1.136806	1.177951	-3.636175
H	-0.369509	0.961986	-3.949970
O	3.165591	2.975572	0.035551
H	2.868991	2.572149	-0.827393
H	3.390797	2.181351	0.584090
O	-2.764318	-0.260283	1.474301
H	-1.846759	-0.249973	1.101254
H	-3.294178	-0.687249	0.700077
O	-0.465114	2.088762	-0.720880
H	-0.409621	1.214088	-0.253600
H	-0.004906	2.765394	-0.049823
O	-1.817437	1.139245	-2.913069
H	-1.748757	0.196480	-2.556784
H	-1.378291	1.670937	-2.194446
O	0.791575	1.147395	2.361959
H	1.730452	0.973659	2.008074
H	0.261784	0.592161	1.735359
O	0.734941	-1.073604	3.948600
H	-0.134657	-1.484811	3.634179
H	0.710168	-0.153855	3.565271
O	3.144728	0.505840	1.307007
H	3.268201	-0.288354	1.920039
H	2.863735	0.057270	0.457788
O	-3.069559	2.278492	0.474987
H	-2.173007	2.356009	0.060697
H	-3.014874	1.415945	0.981469
O	-1.469181	-1.313409	-1.838446
H	-1.052922	-0.959388	-1.012895
H	-0.648412	-1.581543	-2.413088
O	0.713644	-1.680921	-3.165091
H	1.331091	-1.448921	-2.421744
H	0.675123	-0.810111	-3.691324
O	2.375627	-3.038401	0.385929
H	1.409465	-3.253267	0.502302
H	2.623428	-2.670307	1.293085
O	1.916494	1.639055	-2.062471

H	2.127019	0.725830	-1.730519
H	1.041529	1.852653	-1.623346
O	-3.946802	-1.199242	-0.669640
H	-4.171966	-0.302487	-1.093927
H	-3.150739	-1.477200	-1.192668
O	2.013147	-0.815773	-0.817878
H	2.260724	-1.749921	-0.407129
H	1.142076	-0.625705	-0.376408
O	-0.347405	-2.988461	0.777235
H	-0.325277	-1.999028	0.677807
H	-0.901640	-3.289818	0.026751
O	2.877306	-1.748430	2.664191
H	3.517686	-2.117568	3.304298
H	2.012942	-1.568045	3.205974
O	-4.307473	1.242143	-1.682433
H	-3.528746	1.269831	-2.303093
H	-3.931543	1.710763	-0.872183
O	0.737238	3.506123	1.006210
H	0.693644	2.787706	1.701249
H	1.691965	3.413438	0.669827
F	-0.311735	-0.344074	0.396432

61

O	-1.437968	-2.021840	3.188603
H	-0.943723	-2.500270	2.469296
H	-1.960921	-1.321094	2.696895
O	0.382043	0.268859	-4.144464
H	1.066905	0.770879	-3.623028
H	-0.464878	0.699591	-3.842691
O	3.502050	2.554730	-0.138997
H	3.110510	2.243041	-1.001089
H	3.640389	1.713456	0.377016
O	-2.537464	-0.035772	1.643965
H	-3.227688	-0.364614	0.948461
H	-1.687166	-0.096302	1.138892
O	-0.261421	2.205009	-0.747025
H	-0.260544	1.298702	-0.339697
H	0.311614	2.777100	-0.073739
O	-1.861546	1.275954	-2.803685
H	-1.880874	0.350092	-2.388921
H	-1.323718	1.803119	-2.155240
O	1.013015	1.045312	2.311116
H	0.860895	0.480060	3.141591
H	0.475576	0.574068	1.624230
O	0.654669	-0.790345	4.130235
H	-0.216169	-1.267027	3.864268
H	0.604124	-0.637065	5.094298
O	3.355089	0.142408	1.306728
H	2.529105	0.535125	1.731203
H	2.996812	-0.252344	0.455176
O	-2.687970	2.554790	0.716426
H	-1.831947	2.562343	0.215733
H	-2.660182	1.686028	1.212318
O	-1.825526	-1.138331	-1.666944
H	-1.189409	-0.919816	-0.941544
H	-1.253331	-1.668128	-2.351799
O	-0.197094	-2.221341	-3.325607
H	0.457280	-2.609047	-2.683820
H	0.174293	-1.326271	-3.614052
O	0.338804	-2.753591	1.143010
H	1.196012	-2.583253	1.688033
H	0.086672	-1.833496	0.872987
O	1.995692	1.559873	-2.285629
H	2.110402	0.644479	-1.882151
H	1.173234	1.892722	-1.827549
O	-4.120384	-0.753281	-0.305229
H	-4.255133	0.162756	-0.721594
H	-3.389299	-1.117083	-0.877245
O	2.082334	-0.695323	-0.901509
H	2.020688	-1.675337	-1.151296
H	1.197267	-0.532513	-0.477371
O	1.367661	-3.179212	-1.285945
H	1.985494	-3.935507	-1.336213
H	0.943355	-3.224515	-0.367733
O	2.427816	-2.155118	2.614101
H	2.912336	-1.396155	2.185516
H	1.900300	-1.705751	3.335967
O	-4.205479	1.711965	-1.344905
H	-3.487011	1.624726	-2.029020
H	-3.702481	2.112008	-0.567039
O	1.219008	3.379789	0.965564
H	2.132432	3.154227	0.582018
H	1.116894	2.697307	1.684143
F	-0.223865	-0.248614	0.309143

Cl – 1 water molecule

4

O	-0.528158	-0.208956	-0.629380
H	-1.188500	0.105091	0.006158

H 0.308373 -0.077129 -0.122738
Cl 1.908097 0.328781 1.216916
4

O 0.582974 -0.499366 0.359568
H 1.077970 -0.307811 -0.450454
H -0.249900 0.009316 0.210790
Cl -1.943328 1.199286 -0.348715
4

O -0.141606 -0.812735 0.171172
H 0.313016 0.037146 -0.039466
H -1.062323 -0.523681 0.266141
Cl 1.099592 1.962549 -0.542549
4

O -0.454012 0.435312 0.561852
H -0.014722 -0.148252 1.199131
H -0.086226 0.102101 -0.291657
Cl 0.891850 -0.709882 -2.008432
4

O 0.360601 0.092328 0.746683
H 0.187351 -0.171292 -0.187867
H -0.429225 0.609371 0.962595
Cl -0.352459 -0.661363 -2.199658
4

O -0.514414 -0.210865 -0.629514
H -1.217367 0.095395 -0.024306
H 0.302429 -0.055401 -0.072232
Cl 1.929164 0.318658 1.197007
4

O 0.571110 -0.496929 0.364331
H 1.088295 -0.316286 -0.444662
H -0.260064 0.031265 0.183367
Cl -1.931626 1.183376 -0.331848
4

O -0.134866 -0.810245 0.170764
H 0.310951 0.059810 -0.046201
H -1.064115 -0.524527 0.266739
Cl 1.096709 1.938241 -0.536004
4

O -0.456398 0.432574 0.550823
H -0.024186 -0.139919 1.213733
H -0.057151 0.082523 -0.297931
Cl 0.874626 -0.695899 -2.005731
4

O 0.364333 0.089169 0.745861
H 0.185123 -0.175624 -0.203280
H -0.437373 0.609060 0.949673
Cl -0.345815 -0.653562 -2.170501

Cl – 2 water molecules

7

O -1.467433 -0.614005 -0.184897
H -1.307212 0.273768 -0.567124
H -0.557188 -0.827351 0.101423
O 1.265609 -0.395745 0.420114
H 1.045423 0.378590 -0.153625
H 1.074416 -0.047429 1.306381
Cl 0.064163 1.982377 -1.182623
7

O 1.383669 0.647217 -0.553130
H 0.921640 -0.207234 -0.447329
H 0.655892 1.252458 -0.299969
O -0.658256 -1.254672 0.120722
H -0.335216 -1.328683 1.032835
H -1.061107 -0.352319 0.116809
Cl -1.469922 1.750805 0.252436
7

O 0.247651 -0.116571 1.353271
H 1.071489 0.395381 1.326530
H 0.409549 -0.793629 0.651659
O -0.967717 0.851333 -0.988858
H -0.458975 0.106230 -1.370497
H -0.709931 0.749937 -0.050045
Cl 0.814390 -1.743483 -1.247606
7

O 0.377313 -1.252401 -0.589618
H 0.813998 -1.470929 0.248655

H 0.743720 -0.357002 -0.788335
O -1.193146 0.691166 0.819027
H -0.955285 -0.150373 0.384191
H -0.472561 1.257862 0.472029
Cl 1.313662 1.720919 -0.773629
7

O -0.195348 -1.560291 0.345496
H -0.233419 -1.290626 -0.595916
H -0.188926 -0.672644 0.755196
O 0.108230 1.232827 0.658580
H -0.141916 1.094759 -0.287821
H 1.068073 1.095084 0.637867
Cl -0.404435 0.288548 -2.247833
7

O -1.467223 -0.609582 -0.171651
H -1.285270 0.283755 -0.561268
H -0.537248 -0.830491 0.092107
O 1.256378 -0.397096 0.412994
H 1.024587 0.393104 -0.163028
H 1.055703 -0.044450 1.303526
Cl 0.070853 1.954964 -1.173031
7

O 1.374618 0.613475 -0.530939
H 0.861367 -0.230965 -0.457441
H 0.650636 1.232931 -0.255279
O -0.635726 -1.235026 0.106590
H -0.287255 -1.273161 1.020126
H -1.052059 -0.320740 0.096778
Cl -1.474881 1.721058 0.242538
7

O 0.254963 -0.157306 1.359041
H 0.995929 0.468609 1.230118
H 0.429750 -0.814435 0.619644
O -0.921435 0.883563 -0.962516
H -0.410380 0.125593 -1.347574
H -0.726296 0.702378 -0.008045
Cl 0.783924 -1.759204 -1.216215
7

O 0.341396 -1.224431 -0.574472
H 0.824393 -1.433433 0.249810
H 0.712692 -0.317076 -0.789567
O -1.203322 0.675024 0.802974
H -0.918996 -0.182848 0.398421
H -0.467237 1.240211 0.452305
Cl 1.338775 1.681794 -0.767151
7

O -0.180286 -1.543384 0.341671
H -0.245309 -1.260477 -0.606967
H -0.174186 -0.639729 0.747720
O 0.093349 1.227451 0.657841
H -0.130716 1.062267 -0.307430
H 1.059308 1.069359 0.658626
Cl -0.409898 0.272169 -2.225892

Cl – 4 water molecules

13

O 1.301585 1.453533 0.421205
H 0.432438 1.628070 0.835990
H 1.409593 0.501860 0.661471
O -0.421168 0.929055 -1.651512
H -1.120802 1.029206 -0.972100
H 0.372204 1.132576 -1.100231
O -0.753701 -1.657317 -0.839462
H -0.518359 -0.823166 -1.314664
H -1.366127 -1.296823 -0.168214
O 0.952759 -1.139573 1.274898
H 0.184924 -0.681812 1.675053
H 0.534471 -1.477480 0.447358
Cl -1.709365 0.661348 1.240915
13

O 1.430468 1.263518 0.506804
H 0.584818 1.538949 0.913052
H 1.421000 0.303765 0.742494
O -0.235137 1.025485 -1.638969
H -0.967803 1.192354 -1.011467
H 0.534925 1.143513 -1.030007
O -0.860414 -1.521756 -0.934098
H -0.501669 -0.718140 -1.384699
H -1.457164 -1.089798 -0.289826
O 0.749017 -1.276707 1.287171
H 0.330409 -1.556852 0.437867

H	0.013903	-0.746382	1.660490
Cl	-1.683805	0.765389	1.209871

13

O	1.312987	-0.215464	-1.072310
H	0.665908	-0.948461	-0.976114
H	1.510050	0.031636	-0.135587
O	-1.042140	-1.715422	-0.708792
H	-1.119262	-1.489663	0.245032
H	-1.363200	-0.880389	-1.103811
O	1.530337	0.591353	1.524881
H	0.604049	0.328779	1.750455
H	1.471348	1.554821	1.428386
O	-1.136380	1.130666	-0.964174
H	-1.290595	0.932997	-0.015238
H	-0.206837	0.836046	-1.096699
Cl	-1.438863	-0.104229	1.965765

13

O	1.127491	1.582171	0.410646
H	0.199017	1.733712	0.679390
H	1.262322	0.677200	0.782118
O	-0.226066	0.720049	-1.809834
H	-1.027556	0.816992	-1.255139
H	0.454645	1.042738	-1.172608
O	-0.508784	-1.794885	-0.714079
H	-0.243071	-1.016829	-1.259815
H	-1.227530	-1.392254	-0.184990
O	0.844260	-0.911614	1.528067
H	-0.005126	-0.486173	1.766522
H	0.564071	-1.389709	0.711543
Cl	-1.921882	0.617593	0.896988

13

O	-0.722489	1.745520	-0.637876
H	0.149635	1.759505	-1.082768
H	-1.021906	0.840363	-0.896862
O	-0.867903	-0.915540	-1.330116
H	-0.851756	-1.237350	-0.394751
H	0.076759	-0.701538	-1.498927
O	0.877901	0.740428	1.358528
H	1.476489	0.514298	0.609759
H	0.187613	1.240576	0.860326
O	-0.570180	-1.527957	1.311264
H	0.104914	-2.224586	1.323255
H	-0.040893	-0.694480	1.430590
Cl	2.010182	0.388614	-1.537403

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O	1.268634	1.420729	0.393720
H	0.380072	1.570564	0.807457
H	1.384413	0.454831	0.650432
O	-0.404870	0.911084	-1.661072
H	-1.130540	1.030097	-0.996860
H	0.379350	1.112979	-1.062599
O	-0.719055	-1.618721	-0.794907
H	-0.491433	-0.771060	-1.290116
H	-1.331268	-1.226116	-0.121691
O	0.962672	-1.125796	1.259284
H	0.179843	-0.674931	1.667881
H	0.512732	-1.450046	0.418866
Cl	-1.692098	0.625863	1.240312

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O	1.360437	1.249410	0.506795
H	0.470681	1.459331	0.894074
H	1.387199	0.270069	0.736082
O	-0.189255	1.003237	-1.680745
H	-0.957687	1.218741	-1.097649
H	0.545852	1.104013	-0.996750
O	-0.855764	-1.475057	-0.859595
H	-0.498728	-0.663798	-1.338139
H	-1.415604	-1.000694	-0.189413
O	0.799762	-1.290335	1.244694
H	0.325387	-1.532306	0.387748
H	0.067101	-0.779520	1.671040
Cl	-1.680833	0.760248	1.190541

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O	1.255290	-0.162300	-1.046490
H	0.611507	-0.917824	-0.937042
H	1.472695	0.064981	-0.091261
O	-1.021013	-1.698211	-0.725825
H	-1.106821	-1.493988	0.244475
H	-1.320283	-0.815175	-1.080735
O	1.575891	0.556990	1.544570
H	0.622216	0.312889	1.744327
H	1.527566	1.530037	1.453198
O	-1.184853	1.043361	-1.022401
H	-1.322319	0.906527	-0.046267
H	-0.216937	0.790528	-1.118637
Cl	-1.395539	-0.065146	1.923882

13

O	1.112710	1.553667	0.386072
H	0.173988	1.697065	0.666637
H	1.234594	0.630773	0.771990
O	-0.216785	0.677414	-1.791828
H	-1.027371	0.796788	-1.232980
H	0.460176	1.022333	-1.130859
O	-0.473566	-1.762887	-0.678800
H	-0.226246	-0.963334	-1.240052
H	-1.210701	-1.351483	-0.160176
O	0.845992	-0.886104	1.499270
H	-0.021340	-0.466031	1.733280
H	0.544768	-1.357728	0.660711
Cl	-1.904428	0.608516	0.895542

13

O	-0.625576	1.767829	-0.711632
H	0.276293	1.633769	-1.099124
H	-0.998625	0.849721	-0.900413
O	-1.044716	-0.835985	-1.264908
H	-0.969358	-1.190992	-0.326735
H	-0.075830	-0.708345	-1.469093
O	0.701353	0.841629	1.448293
H	1.391972	0.560245	0.785819
H	0.083225	1.306555	0.802335
O	-0.344612	-1.603559	1.235700
H	0.453669	-2.021710	0.852299
H	-0.005050	-0.664282	1.416495
Cl	1.965617	-0.007023	-1.254016

Cl – 8 water molecules

25

O	1.713139	-1.622482	-0.875041
H	1.046345	-1.661775	-1.606718
H	1.185085	-1.806117	-0.068194
O	0.030034	-1.454724	1.375838
H	0.595379	-0.703422	1.707132
H	-0.544078	-1.003475	0.715286
O	-0.184814	-1.278572	-2.814375
H	-0.835058	-0.937054	-2.165857
H	0.189483	-0.443171	-3.182878
O	-2.355624	-0.805026	2.749810
H	-2.824306	-0.689422	1.905775
H	-1.516483	-1.227468	2.462349
O	1.388676	0.789812	2.023781
H	1.559431	1.047934	1.092446
H	0.519539	1.224932	2.218077
O	-1.172775	1.653734	2.295683
H	-1.612574	0.850296	2.660285
H	-1.367674	1.554151	1.341530
O	1.326759	1.047494	-0.767307
H	0.350417	0.967191	-0.663426
H	1.605725	0.090348	-0.814704
O	0.780154	1.265513	-3.447365
H	-0.077406	1.714143	-3.381043
H	1.135797	1.321824	-2.529471
Cl	-1.736250	0.333090	-0.535125

25

O	-1.204331	0.811039	-2.009143
H	-1.465773	1.335385	-1.211251
H	-0.240261	0.997563	-2.103052
O	-2.780730	-0.471088	1.281183
H	-2.283237	-0.382043	2.130253
H	-2.167413	-0.972880	0.701442
O	1.592009	-1.810989	-1.945009
H	2.302369	-1.675636	-1.275788
H	0.768473	-1.845493	-1.410946
O	-0.726283	-1.317865	-0.427825
H	-0.974864	-0.604161	-1.081483
H	-0.134311	-0.834428	0.191929
O	1.540303	0.945399	-1.870462
H	1.476739	1.002005	-0.896047
H	1.585973	-0.027655	-2.040835
O	-1.750917	1.884084	0.434244
H	-2.247898	1.078787	0.732602
H	-0.842698	1.704488	0.749838
O	3.498914	-0.820337	-0.201999
H	2.874868	-0.425320	0.442475
H	3.710374	-0.072722	-0.783744
O	-1.188938	0.084044	3.440022
H	-0.378437	0.180727	2.895040
H	-1.437368	1.001856	3.634006
Cl	1.094938	0.619485	1.314503

25

O	0.832956	3.344038	0.130723

H	0.136425	3.842220	0.586272
H	0.916535	2.528319	0.668924
O	-2.150501	1.635604	0.248882
H	-1.680297	1.905223	-0.580343
H	-1.414938	1.407726	0.850979
O	2.818022	-1.545516	1.267857
H	3.453276	-1.061154	0.717101
H	2.151600	-0.862760	1.499613
O	-2.294414	-1.007981	-0.626132
H	-2.406070	-0.098490	-0.258595
H	-1.939606	-1.531483	0.134922
O	-0.894374	-2.317745	1.325741
H	-0.178584	-2.631310	0.715016
H	-0.529438	-1.477939	1.667942
O	1.130343	-2.871564	-0.431971
H	0.893210	-2.070283	-0.949808
H	1.832264	-2.522195	0.170280
O	0.248719	-0.388986	-1.304847
H	-0.704853	-0.655355	-1.178655
H	0.485678	-0.052124	-0.411223
O	-0.566449	2.232704	-1.921599
H	-0.191769	1.324755	-1.919779
H	0.026010	2.715838	-1.295882
Cl	0.548052	0.597417	1.669525

25

O	1.360392	-0.872086	-1.093024
H	1.137856	-0.032077	-0.637033
H	1.281200	-1.525085	-0.344155
O	0.739350	-2.312956	1.072296
H	1.048190	-1.709472	1.792818
H	-0.180698	-1.976830	0.965099
O	-1.316878	-1.106003	-1.919174
H	-1.396707	-0.148104	-2.158821
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Cl – 12 water molecules

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H	0.388675	3.068370	-1.404896
H	-0.398936	2.906838	-0.117737
O	-3.082335	1.515973	1.049174
H	-3.066799	1.865876	0.097881
H	-2.121676	1.414323	1.243164

O	3.919489	0.094644	-0.128957
H	3.314991	-0.592737	-0.526602
H	3.500798	0.934149	-0.462257
O	1.807012	-1.536198	-0.757037
H	1.275081	-0.755324	-0.464972
H	1.867852	-2.067136	0.123580
O	-2.826894	2.257672	-1.527273
H	-1.954248	2.744596	-1.458864
H	-2.531039	1.338259	-1.773450
O	2.745493	-0.229309	2.284392
H	3.270567	-0.075391	1.432953
H	1.902229	0.241370	2.085816
O	-1.802015	-0.293183	-1.590017
H	-1.108972	0.096373	-0.999203
H	-2.487415	-0.623770	-0.898058
O	-0.971171	-2.213343	1.244753
H	-0.843370	-2.490522	0.272054
H	-0.674743	-1.268763	1.232401
O	-0.571126	-2.731519	-1.353360
H	-1.054918	-1.913692	-1.661588
H	0.373996	-2.408115	-1.328593
O	1.805398	-2.656401	1.608726
H	2.141131	-1.788937	2.007279
H	0.817392	-2.609772	1.706905
O	-3.386564	-1.061927	0.358780
H	-2.675621	-1.550065	0.854042
H	-3.361748	-0.128340	0.746291
O	2.235192	2.193051	-0.887152
H	1.621583	1.791929	-0.216762
H	2.569362	2.995226	-0.435372
Cl	0.062008	0.757091	0.807427

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O	-0.252844	3.036391	-1.187619
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H	0.629633	2.568535	-1.189454
O	-3.450270	1.476656	0.115000
H	-2.676533	1.734962	0.687670
H	-3.526056	0.478638	0.263259
O	3.703560	-0.567669	0.062806
H	3.270007	-1.374025	-0.368361
H	3.241848	0.199790	-0.370923
O	2.321662	-2.712498	-0.735912
H	1.450023	-2.248706	-0.750899
H	2.326849	-3.098572	0.196393
O	-0.939311	1.968131	1.163011
H	-0.700855	2.467104	0.305008
H	-0.762779	1.026939	0.899967
O	1.705815	2.005049	1.921960
H	1.832986	1.059688	2.214512
H	0.712517	2.089046	1.863504
O	-1.967169	1.044336	-2.025716
H	-1.353785	0.391589	-1.597035
H	-2.590046	1.286957	-1.245043
O	2.292644	-3.438669	1.859711
H	2.211757	-2.487265	2.160524
H	1.399108	-3.801285	2.023552
O	-3.607357	-1.071308	-2.543488
H	-3.035720	-0.248995	-2.553175
H	-3.009265	-1.762685	-2.891292
O	2.034168	-0.733142	2.096211
H	2.754969	-0.642587	1.368964
H	1.209990	-0.810656	1.549966
O	-3.415542	-1.201774	0.151222
H	-2.431764	-1.268791	0.211210
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H	1.271967	0.680093	-0.662707
H	1.920709	1.719711	0.304964
Cl	-0.227034	-0.837191	-0.156794

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O	-0.098388	2.980295	-0.610630
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H	0.804356	2.569175	-0.500076
O	-3.237072	0.401526	1.366891
H	-2.618217	1.166379	1.508899
H	-2.631389	-0.362055	1.496636
O	3.651032	-0.852470	0.319776
H	3.095274	-1.432630	-0.268341
H	3.280319	0.045744	0.098287
O	1.693690	-2.131715	-1.221555
H	1.050103	-1.990953	-0.476223
H	1.811175	-3.103953	-1.249658
O	-0.880899	1.930316	1.725667
H	-0.646812	2.408608	0.857030
H	-0.701594	0.982357	1.499006
O	1.802416	1.821108	2.540827
H	1.956493	0.842807	2.744537
H	0.811866	1.914756	2.497674
O	-1.054993	0.707299	-1.694371
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H	-0.695722	0.008000	-2.354827
O	-2.231556	-2.370565	-1.389047
H	-1.695495	-2.229825	-0.574397
H	-2.845825	-1.563162	-1.365525
O	-0.315836	-1.408989	-3.030501
H	-1.049428	-1.872975	-2.511594
H	0.498669	-1.655689	-2.514081
O	2.293776	-0.821724	2.666890
H	1.413491	-1.079196	2.303151
H	2.874834	-0.886710	1.842451
O	-3.626739	-0.076291	-1.288069
H	-3.592504	0.134171	-0.306779
H	-2.780032	0.352147	-1.599593
O	1.987798	1.303722	-0.013209
H	1.328917	0.570126	0.003305
H	1.999516	1.580049	0.979083
Cl	-0.307212	-1.036890	0.856164

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O	1.374904	2.525411	-1.266247
H	2.017136	2.372546	-0.488083
H	1.659258	1.820956	-1.934044
O	-3.139287	0.296644	-0.180697
H	-2.283092	0.758773	-0.375945
H	-3.115262	-0.511993	-0.794409
O	2.976058	1.893731	0.735450
H	2.384635	1.601477	1.500373
H	3.252637	1.025900	0.331402
O	-0.308912	-0.862094	-2.128719
H	0.113075	-1.389552	-1.402944
H	-0.543045	-0.032220	-1.618232
O	-1.153547	1.795441	2.355959
H	-1.044821	1.834042	1.368899
H	-1.607681	0.912919	2.463936
O	1.384401	0.932840	2.677590
H	0.456140	1.327964	2.642033
H	1.247406	0.046078	2.263859
O	-2.830751	-1.913837	-1.630740
H	-1.939737	-1.639579	-1.978266
H	-2.592087	-2.466645	-0.824553
O	-0.533568	1.177445	-0.300838
H	-0.020929	0.479422	0.185689
H	0.216951	1.808375	-0.707323
O	-2.135200	-3.223241	0.645771
H	-2.390217	-2.525088	1.304445
H	-1.158201	-3.094550	0.607604
O	3.252037	-0.488279	-0.564510
H	4.021889	-1.091813	-0.542309
H	2.518367	-0.989310	-0.116073
O	-2.192028	-0.766228	2.036322
H	-1.280191	-1.011314	1.736667
H	-2.612116	-0.364588	1.190887
O	2.056831	0.435747	-2.832968
H	1.205897	-0.078010	-2.773286
H	2.599846	0.018134	-2.106211
Cl	0.660947	-1.532323	0.791769

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O	0.467006	0.011550	3.746837
H	1.175078	-0.308518	3.147631
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O	0.233072	-2.898056	1.205262
H	-0.355855	-2.442142	0.554712
H	0.872582	-2.174788	1.425820
O	1.372421	-1.049494	-2.859734
H	1.479052	-1.841276	-2.259878
H	1.198394	-0.311578	-2.242215
O	1.793946	-3.104976	-1.161682
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H	2.638107	-2.787220	-0.764673
O	-1.404838	-1.134864	-3.038311
H	-1.649948	-0.185804	-2.945325
H	-0.439779	-1.123613	-3.229106
O	-2.171368	3.803502	0.853133
H	-1.646913	3.960421	0.030544
H	-1.599511	3.236133	1.408538
O	3.804493	0.084741	-1.940090
H	3.258349	0.782697	-1.533675
H	3.169141	-0.350325	-2.546914
O	3.854587	-1.743567	-0.008226
H	4.757234	-2.029713	0.199352

H	3.942054	-1.043371	-0.715231
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H	-0.306597	-0.561684	-0.469286
H	-1.258465	-1.350209	-1.415839
O	-0.854682	4.008647	-1.547446
H	-1.300569	3.245782	-1.977119
H	0.022936	3.643140	-1.341370
O	-0.511253	1.862507	2.064678
H	-0.116505	1.281405	2.776505
H	0.097049	1.778407	1.303733
O	1.938259	-0.797046	1.575441
H	1.683511	-0.092336	0.944260
H	2.770628	-1.158407	1.172568
O	-1.491727	-1.829204	3.166007
H	-1.996031	-1.220229	2.580054
H	-0.960782	-2.372974	2.543437
O	-3.751884	1.884512	-0.256524
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H	-3.300412	2.660629	0.166407
Cl	0.986369	1.251738	-0.659169

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O	0.850416	0.172921	3.468602
H	1.526939	-0.126095	2.823452
H	0.193669	-0.569315	3.499039
O	-2.145307	1.338815	-1.868173
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O	-2.569169	-0.169938	1.556896
H	-2.163983	-0.667497	0.806528
H	-1.896395	0.541383	1.722707
O	0.609617	-2.767912	1.243599
H	-0.061916	-2.393403	0.621377
H	1.239896	-2.007252	1.332874
O	1.256353	-1.282097	-2.634124
H	1.034584	-0.531522	-2.044589
H	2.114678	-0.977080	-2.993829
O	2.077217	-3.377740	-1.062321
H	1.561792	-3.336653	-0.227246
H	1.672169	-2.687173	-1.636713
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H	-1.847664	-0.297093	-2.736866
H	-0.647970	-1.212229	-3.143456
O	-2.359562	3.752350	1.360102
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H	3.077115	0.877239	-1.959663
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O	-1.310842	4.000235	-1.184338
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O	2.263953	-0.614955	1.248994
H	1.893903	0.050477	0.633104
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O	-1.037115	-1.804525	3.286058
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H	-3.439606	2.563284	0.615966
Cl	0.859337	1.278694	-0.838897

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O	1.142631	0.321848	3.471527
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O	-1.996216	-0.133260	1.227912
H	-1.608834	-0.592185	0.451962
H	-1.359281	0.600985	1.444693
O	0.665513	-2.544485	1.063617
H	0.056811	-2.385638	0.311054
H	1.209196	-1.712223	1.074399
O	1.608504	-2.632779	-2.423425
H	0.753358	-2.335625	-2.053759
H	2.126491	-1.797492	-2.493453
O	2.773075	-3.777787	-0.228000
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O	-2.734993	-0.839322	-2.677440

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O	-2.167481	3.850738	1.493252
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O	-0.679285	-1.369254	-1.046682
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H	-2.006799	3.535793	-1.573371
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O	-0.323957	1.863335	1.885199
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H	0.195002	1.922472	1.057468
O	2.150225	-0.304085	1.049655
H	1.818883	0.330934	0.382953
H	3.014102	-0.666157	0.693773
O	-0.769006	-1.656110	3.198446
H	-1.382896	-1.147785	2.622329
H	-0.258844	-2.165313	2.525810
O	-3.769891	1.868172	0.583223
H	-3.299430	1.071191	0.916573
H	-3.276502	2.626591	0.994910
Cl	0.606271	1.495464	-1.095295

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O	0.923071	0.840163	3.283486
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O	0.690431	-3.016432	0.485773
H	0.303450	-2.655726	-0.354444
H	1.128236	-2.214686	0.872541
O	1.877671	-2.372990	-3.193749
H	0.959542	-2.320831	-2.851968
H	2.206484	-1.456902	-3.052878
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H	2.256137	-3.471225	-0.362019
H	2.658402	-3.159074	-1.816130
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O	2.707443	0.158077	-2.433160
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H	1.324031	3.717620	1.598447
H	0.667335	2.551423	0.825770
O	1.887949	-0.692823	1.186128
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O	-1.820331	-2.471319	1.565945
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H	-2.895941	2.710602	1.548478
Cl	0.151310	1.142319	-0.746456

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O	1.711791	1.697193	2.946480
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H	1.959160	0.987466	2.304667
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H	-2.226196	0.579860	-1.243637
H	-3.311965	0.781862	-0.145050
O	-1.143787	1.031948	3.007449
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O	0.846868	-2.547842	0.891962
H	0.493144	-2.548729	-0.033811
H	1.343763	-1.690030	0.962884
O	2.181152	-2.913638	-2.651520
H	1.225841	-2.900537	-2.434338
H	2.401286	-1.956019	-2.700788
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H	2.487345	-3.297326	0.368244
H	2.918803	-3.320281	-1.104932
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O	-2.578749	3.821455	0.870679
H	-2.605244	3.714105	-0.112112
H	-1.641676	3.650976	1.100788
O	2.728909	-0.185360	-2.460595
H	1.905334	0.290333	-2.229156
H	3.036395	0.235777	-3.279197
O	4.277472	-0.850836	-0.235964
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H	-1.709798	3.002528	-1.967004
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H	0.765919	2.651097	1.854960
H	0.112388	2.393303	0.457193
O	2.050541	-0.157221	0.986387
H	1.554176	0.301177	0.278082
H	2.963335	-0.324384	0.596326
O	-1.301143	-0.949674	1.167637
H	-0.589533	-1.633374	1.262303
H	-0.953711	-0.362658	0.465638
O	-3.530539	1.363242	1.394852
H	-2.889169	1.099168	2.083606
H	-3.292739	2.319553	1.250884
Cl	-0.019609	0.917662	-1.191697

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O	0.458725	0.155055	3.649050
H	1.206961	-0.157815	3.075627
H	-0.206069	-0.606930	3.566552
O	-1.724533	1.615991	-2.226087
H	-0.903173	1.421279	-1.709919
H	-2.464347	1.613884	-1.506043
O	-2.695639	-0.106176	1.472860
H	-2.260426	-0.575277	0.698781
H	-1.999136	0.597312	1.688309
O	0.271783	-2.722790	1.098975
H	-0.330038	-2.244943	0.448830
H	0.939916	-1.998367	1.326287
O	1.293921	-1.199031	-2.658920
H	1.448053	-2.021944	-2.063294
H	1.124308	-0.476569	-2.004225
O	1.885026	-3.221102	-1.076187
H	1.274882	-3.229277	-0.283630
H	2.716481	-2.812355	-0.696331
O	-1.444234	-1.006310	-3.031851
H	-1.599734	-0.019387	-2.974685
H	-0.457082	-1.093470	-3.156350
O	-2.237779	3.758131	0.873604
H	-1.622376	3.932545	0.097242
H	-1.700511	3.159709	1.457978
O	3.724776	-0.052642	-2.089340
H	3.274631	0.725157	-1.691520
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H	3.924870	-1.032003	-0.819573
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O	-0.786081	1.706756	1.967420
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O	2.024466	-0.743728	1.576664
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H	2.862231	-1.095803	1.135349
O	-1.310974	-1.806283	3.189208
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O	-3.547130	1.781737	-0.359354
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Cl	0.977299	1.222009	-0.619145

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O	0.852638	0.204247	3.580715
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O	-2.078717	1.479644	-2.013065
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H	-2.750667	1.473730	-1.229031
O	-2.487971	-0.269730	1.726595
H	-2.114049	-0.724872	0.913584
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O	0.573368	-2.713375	1.115465
H	-0.115620	-2.315667	0.503323
H	1.212157	-1.934355	1.241985
O	1.111550	-1.266206	-2.659685
H	0.858079	-0.613302	-1.962271
H	1.984825	-0.864994	-2.927449
O	2.152336	-3.286814	-1.075774
H	1.575710	-3.272663	-0.259938
H	1.703204	-2.625280	-1.676110
O	-1.711550	-1.079843	-2.877113
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O	-1.101949	-1.226976	-0.343709
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H	-0.133162	1.637487	1.201830
O	2.222262	-0.633260	1.360908
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O	-0.857134	-1.850986	3.324100
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H	-1.410966	0.573163	1.575075
O	0.753797	-2.517876	1.163651
H	0.116764	-2.288929	0.435925
H	1.330663	-1.680090	1.192773
O	1.253363	-2.520648	-2.508476
H	0.502885	-2.185267	-1.952744
H	1.834530	-1.712161	-2.599738
O	2.662429	-3.615487	-0.482569
H	1.994268	-3.401002	0.227616
H	2.165335	-3.306683	-1.304228
O	-2.552997	-0.836391	-2.557345
H	-2.572367	0.168138	-2.439892
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O	-2.321153	3.702243	1.326188
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O	4.117559	-1.394512	-0.251834
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H	-3.262871	2.461019	0.762901
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H	-3.212787	1.198111	0.178243
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O	0.631863	-2.764322	0.417338
H	0.254875	-2.388133	-0.443426
H	1.107322	-1.969507	0.819348
O	1.815347	-2.352871	-3.201553
H	0.889699	-2.255356	-2.847222
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O	-2.042583	4.009139	1.132222
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H	-1.116966	3.741285	1.383197
O	2.752756	0.073869	-2.305844
H	1.986809	0.581257	-1.936720
H	3.189720	0.699850	-2.918245
O	4.008296	-1.179323	-0.225767
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H	3.716301	-0.622156	-0.999077
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H	-2.568915	1.170609	1.984129
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Cl	0.187894	1.162045	-0.763535

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O	1.482978	1.647832	3.002572
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O	0.961599	-2.597787	0.861598
H	0.561995	-2.538003	-0.062747
H	1.441388	-1.712719	0.978284
O	2.104687	-2.895005	-2.794585
H	1.158347	-2.864462	-2.493485
H	2.330706	-1.924078	-2.829936
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H	-0.113463	-1.277670	-1.643629
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O	-2.450646	3.065368	-1.872832
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O	-0.130568	2.892169	1.316556
H	0.620695	2.598190	1.933865
H	0.029500	2.376020	0.487151
O	2.090612	-0.191917	1.107469
H	1.538029	0.248000	0.411541
H	2.995056	-0.363938	0.621612
O	-1.186837	-1.093229	1.316839
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H	-2.954436	1.326099	2.069236
H	-3.317758	2.554690	1.174194
Cl	0.071559	0.850037	-1.048838

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O	-0.201768	3.086632	1.243503
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O	0.110668	1.664264	3.725460
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Cl	0.010978	0.056024	0.141214

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O	-2.487241	-2.122076	2.379275
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H	-1.645020	-2.562541	2.132424
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O	1.647756	-0.169721	-3.681106
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O	-3.838597	-1.410736	0.082872
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O	0.283210	2.227975	3.603770
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O	-1.529242	1.780880	-2.038670
H	-2.393693	1.638536	-1.567408
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O	1.804976	-2.045843	-1.681548
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O	-1.713668	0.571723	2.851603
H	-0.975854	1.090758	3.279110
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Cl	0.023938	0.009693	0.149209

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H	3.594934	-1.922565	0.669876
O	-3.596249	1.375337	-0.555232
H	-4.454396	1.660482	-0.906463
H	-3.726946	0.417135	-0.279919
O	2.155607	1.598998	-1.784107
H	1.596307	1.033099	-1.220903
H	1.673331	2.475180	-1.749077
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H	-2.365328	-1.259498	2.678402
H	-1.714852	-2.534718	2.089647
O	0.046218	-2.874242	1.496275
H	-0.037230	-3.375928	0.632395
H	0.021742	-1.946197	1.194409
O	1.522232	-0.294582	-3.769097
H	1.810341	0.492272	-3.258125
H	1.702839	-1.033074	-3.142092
O	-3.906046	-1.193966	0.022115
H	-3.460220	-1.542182	0.835807
H	-3.355549	-1.546477	-0.711176
O	2.668552	-2.249984	2.168744
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H	3.071435	-2.789475	2.866622
O	-2.705410	2.971648	1.462830
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H	-2.636712	2.264991	2.138139
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H	-0.237967	3.328054	-1.847016
O	0.331594	1.672582	3.619778
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H	1.141833	1.187562	3.345616
O	-1.435406	1.895478	-2.075160
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H	3.642999	1.068082	0.907746
H	3.538701	1.406277	-0.609774
O	2.419360	0.453273	2.222378
H	1.720318	0.388076	1.543311
H	2.613226	-0.503268	2.394186
O	1.762803	-2.034870	-1.658784
H	1.173831	-1.439009	-1.160757
H	2.636932	-1.931341	-1.167980
O	-0.172869	-3.885290	-0.980179
H	-0.880794	-3.292138	-1.325811
H	0.642350	-3.451513	-1.317144
O	-1.187982	-0.325760	-3.735603
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H	-1.611315	0.398517	1.816753
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H	-3.642641	0.208167	-0.455777
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H	1.599905	0.995634	-1.103408
H	1.724886	2.414207	-1.691565
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O	-0.026816	-2.967093	1.364081
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H	-0.003275	-2.052231	1.027540
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O	-3.825070	-1.402902	-0.160398
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O	1.808485	-2.139541	-1.461176
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H	2.628874	-2.016597	-0.888811
O	-0.135867	-4.055546	-1.097257
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H	-1.167181	0.417432	-3.462757
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O	-1.817897	0.540429	2.804757
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H	3.868113	-0.542224	0.378485
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H	-2.676687	-1.383732	2.463627
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O	-0.099890	-2.831177	1.592979
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O	2.007458	-0.242953	-3.520142
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H	2.076121	-0.993427	-2.886879
O	-2.939215	-1.043894	-0.407215
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H	-1.991242	-0.814670	-0.398685
O	2.458148	-2.107874	2.667597
H	1.609596	-2.516233	2.390291
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O	-2.909888	2.864389	1.573498
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H	3.421680	1.487517	-0.168127
O	2.018716	0.540345	2.544572
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O	1.768982	-2.099902	-1.483018
H	1.042361	-1.538490	-1.156557
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O	-0.153794	-3.948771	-0.815324
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H	0.713433	-3.591985	-1.101656
O	-0.650216	-0.442539	-3.908270
H	-0.979553	0.407996	-3.553556
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O	-2.084323	0.392377	2.573109
H	-1.385604	0.807061	3.155883
H	-1.610999	0.289090	1.728840
Cl	0.001338	0.054095	0.102228

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O	-0.237316	3.060551	1.228735
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H	3.937977	-0.681229	0.148161
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H	-2.404969	-1.281970	2.545473
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O	-0.043627	-2.837172	1.364109
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O	1.661880	-0.029150	-3.608006
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O	2.479842	-2.252959	2.371679
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H	2.993815	-2.187450	1.513309

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O	0.204708	1.761991	3.661139
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O	2.125963	0.334109	2.376446
H	1.452824	0.300744	1.655352
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H	1.184784	-1.372507	-1.224325
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O	1.532355	-0.135209	-3.652791
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O	-3.691629	-1.183668	0.021742
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O	0.327251	2.009397	3.529978
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O	-1.516862	1.712236	-2.140263
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H	-3.159812	-1.450155	-0.738152
O	2.533355	-2.225605	2.126123
H	1.607838	-2.591136	1.948351
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H	-0.355088	3.197566	-1.853584
O	0.420164	1.856007	3.538165
H	0.315203	2.508452	2.791022
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O	-1.469171	1.807644	-2.163948
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O	4.069209	0.839850	0.087378
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O	2.296127	0.418812	2.161238
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H	1.246140	-1.371831	-1.100782
H	2.712115	-1.953756	-1.103127
O	-0.051643	-3.819868	-0.929695
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H	0.760701	-3.342921	-1.270065
O	-1.191733	-0.394135	-3.787174
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H	-1.395627	0.345681	1.828754
Cl	-0.007159	0.078827	0.061610

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H	-0.103515	2.182644	0.704642
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O	2.136055	1.610865	-1.563307
H	1.503967	1.021248	-1.087736
H	1.584196	2.478223	-1.624020
O	-2.645724	-2.032115	2.142133
H	-2.411518	-1.181949	2.598884
H	-1.757332	-2.460975	1.991052
O	-0.055969	-2.832113	1.509092
H	-0.024943	-3.357037	0.622097
H	-0.022261	-1.903477	1.184690
O	1.733872	-0.325457	-3.544103
H	1.950058	0.490992	-3.020223
H	1.924927	-1.050614	-2.879472
O	-3.704746	-1.171558	-0.184801

H	-3.306284	-1.492132	0.687785
H	-3.105963	-1.571225	-0.875662
O	2.538524	-2.338534	2.403725
H	2.409215	-1.376491	2.629961
H	1.619529	-2.638638	2.153886
O	-2.832012	2.791620	1.392099
H	-3.177891	2.321082	0.572202
H	-2.656457	2.018154	2.000921
O	-1.625501	-1.972240	-1.749257
H	-1.375076	-1.478562	-2.627141
H	-1.205035	-1.382259	-1.081006
O	0.446781	3.616403	-1.610820
H	0.204518	3.665419	-0.641825
H	-0.316537	3.086984	-1.975822
O	0.164898	2.024119	3.498189
H	0.094698	2.619358	2.700607
H	0.980662	1.490504	3.280633
O	-1.407535	1.670344	-2.211773
H	-2.314506	1.617771	-1.748226
H	-0.863637	1.146752	-1.578509
O	3.763067	0.955797	0.456357
H	3.282131	1.357425	-0.333779
H	4.584429	1.476116	0.559180
O	2.076516	0.386375	2.435690
H	1.352093	0.178788	1.798351
H	2.788029	0.731390	1.805806
O	1.926714	-2.038858	-1.459799
H	1.294575	-1.443074	-0.996560
H	2.770632	-1.969079	-0.850071
O	0.053744	-3.919420	-0.871890
H	-0.653487	-3.356116	-1.305242
H	0.877215	-3.431093	-1.162058
O	-0.922080	-0.523150	-3.781394
H	-1.213234	0.345934	-3.388058
H	0.090142	-0.452992	-3.730679
O	-1.868497	0.563250	2.648148
H	-1.081787	1.039781	3.099994
H	-1.487714	0.335181	1.769027
Cl	-0.001985	0.014029	0.100768
61			
O	-0.331351	3.117667	1.127343
H	-1.361542	3.104925	1.186432
H	-0.150301	2.211397	0.786186
O	3.613076	-1.624492	0.305546
H	3.835172	-0.619265	0.400799
H	4.466853	-2.067352	0.127197
O	-3.544882	1.456280	-0.866511
H	-4.424780	1.566906	-1.279048
H	-3.466151	0.468657	-0.653622
O	2.268602	1.691150	-1.392532
H	1.642796	1.066472	-0.957843
H	1.699973	2.546049	-1.427091
O	-2.767438	-2.064203	2.030758
H	-2.580523	-1.204589	2.496980
H	-1.851924	-2.462864	1.935810
O	-0.171319	-2.728858	1.482388
H	-0.123509	-3.255168	0.587281
H	-0.093370	-1.804450	1.152172
O	1.995941	-0.074323	-3.534127
H	2.157479	0.687796	-2.913492
H	2.132031	-0.858226	-2.930645
O	-2.898091	-1.070886	-0.389263
H	-2.981001	-1.499579	0.544004
H	-1.942455	-0.825508	-0.401754
O	2.286976	-2.128708	2.612469
H	1.415000	-2.494560	2.289592
H	2.842455	-2.084700	1.778897
O	-2.908289	2.783495	1.398194
H	-3.233691	2.371965	0.543632
H	-2.757393	1.977150	1.969394
O	-1.713833	-2.567885	-2.400711
H	-1.281152	-1.776441	-2.862502
H	-2.355443	-2.149388	-1.771977
O	0.550518	3.688035	-1.419180
H	0.252576	3.712020	-0.465932
H	-0.196711	3.187754	-1.851460
O	-0.029474	1.915757	3.640441
H	-0.048544	2.551706	2.873178
H	0.778297	1.364872	3.421913
O	-1.300146	1.815438	-2.240876
H	-2.229196	1.788832	-1.839063
H	-0.804266	1.258718	-1.595370
O	3.935451	0.921100	0.651595
H	3.298611	0.923589	1.422671
H	3.427288	1.353486	-0.093450
O	1.956828	0.460175	2.501106
H	1.350917	0.400705	1.724370
H	2.096880	-0.541601	2.701183
O	1.842872	-1.963289	-1.591607
H	1.112430	-1.391365	-1.261658
H	2.554487	-1.863943	-0.866845

O 0.004000 -3.851666 -0.847249
H -0.690758 -3.399276 -1.440732
H 0.830881 -3.395872 -1.164170
O -0.675009 -0.465404 -3.691665
H -1.025258 0.387411 -3.322869
H 0.324383 -0.323740 -3.669433
O -1.975882 0.503419 2.597027
H -1.238702 0.974479 3.137146
H -1.516023 0.350769 1.740157
Cl -0.005813 0.086281 0.062823

Br -1 water molecule

4

O -0.355795 -0.774070 -0.215717
H 0.563297 -1.053383 -0.339605
H -0.255097 0.161096 0.060031
Br 0.268802 2.399173 0.704188
4

O 0.699266 0.506998 -0.061109
H 0.600968 0.374584 -1.016187
H -0.044544 -0.019480 0.300153
Br -1.892742 -1.319210 0.946982
4

O -0.815052 -0.249785 0.192609
H -1.032929 0.656522 -0.070482
H 0.156853 -0.274123 0.067434
Br 2.475759 -0.004424 -0.338003
4

O 0.063178 0.058926 -0.874068
H -0.202327 -0.231482 0.023896
H 0.665198 0.793639 -0.682046
Br -0.647336 -0.752233 2.298003
4

O 0.162286 0.057782 0.851812
H -0.266527 -0.121436 -0.011426
H 1.025790 0.407003 0.581657
Br -1.171579 -0.446621 -2.179751
4

O -0.359416 -0.766405 -0.212851
H 0.572616 -1.033923 -0.334357
H -0.253633 0.181784 0.065761
Br 0.261641 2.351359 0.690344
4

O 0.701338 0.507711 -0.056256
H 0.596967 0.371957 -1.018217
H -0.057045 -0.027456 0.298770
Br -1.878313 -1.309319 0.945543
4

O -0.808165 -0.255802 0.193511
H -1.031174 0.657951 -0.071152
H 0.176730 -0.259819 0.060138
Br 2.447240 -0.014139 -0.330940
4

O 0.054929 0.051824 -0.867787
H -0.194797 -0.225972 0.052860
H 0.664870 0.793019 -0.685182
Br -0.646288 -0.750022 2.265894
4

O 0.158419 0.058268 0.851391
H -0.281855 -0.129748 -0.019702
H 1.022530 0.406053 0.556686
Br -1.149123 -0.437844 -2.146083

Br -2 water molecules

7

O 0.384796 -0.832583 -1.351266
H 0.719912 -0.330983 -0.579419
H -0.539592 -0.972928 -1.075306
O 0.666679 0.702367 0.997489
H -0.254680 0.376025 1.104479
H 0.537749 1.545925 0.534840
Br -2.407565 -0.490498 0.637381
7

O 0.083595 1.629119 -0.198934
H -0.354161 1.394383 0.638963

H 0.222294 0.736645 -0.579947
O 0.260187 -1.103911 -0.764850
H 1.142015 -1.242914 -0.383076
H -0.322105 -1.134161 0.027388
Br -1.428862 -0.623062 2.022707
7

O -1.558306 0.490333 0.199826
H -1.341299 -0.245326 0.801346
H -0.756233 0.503016 -0.359615
O 1.089095 0.233192 -0.902005
H 1.406377 0.921758 -0.297027
H 1.027778 -0.552542 -0.314592
Br 0.364724 -2.043446 1.409343
7

O -0.407842 0.405385 -1.263843
H -1.313733 0.654863 -1.020498
H 0.129076 0.962979 -0.659427
O 0.242887 -1.422091 0.773633
H -0.031840 -0.986025 -0.060179
H 0.559669 -0.646938 1.273378
Br 1.065546 1.794895 1.424297
7

O -0.080737 1.225688 1.077993
H -0.436588 0.841556 0.249615
H 0.425284 0.463844 1.415130
O -0.610929 -0.361931 -1.214872
H 0.110860 -0.005605 -1.756580
H -0.141097 -1.001542 -0.634310
Br 1.287189 -1.909829 1.036521
7

O 0.386318 -0.849013 -1.330859
H 0.708281 -0.303976 -0.565067
H -0.552749 -0.960448 -1.052034
O 0.670357 0.687528 0.976913
H -0.264637 0.349391 1.064566
H 0.525793 1.556138 0.549533
Br -2.366064 -0.482295 0.625147
7

O 0.079893 1.613390 -0.165330
H -0.387381 1.319501 0.651375
H 0.229807 0.723897 -0.581886

O 0.263909 -1.096335 -0.780816
H 1.139756 -1.239165 -0.368071
H -0.335009 -1.106732 0.017725
Br -1.388012 -0.558457 1.989256
7

O -1.550866 0.475059 0.176870
H -1.282301 -0.269148 0.765626
H -0.717384 0.551920 -0.357200
O 1.019483 0.235067 -0.883906
H 1.418120 0.895775 -0.281602
H 0.952079 -0.562797 -0.288047
Br 0.393006 -2.018891 1.405533
7

O -0.367950 0.432166 -1.253595
H -1.291981 0.563904 -0.958342
H 0.131803 0.987900 -0.592291
O 0.205263 -1.420721 0.749746
H -0.027824 -0.956789 -0.096994
H 0.527662 -0.643176 1.263893
Br 1.066791 1.799785 1.354945
7

O -0.097125 1.219469 1.054855
H -0.435583 0.808087 0.216018
H 0.437028 0.461560 1.388637
O -0.608228 -0.358022 -1.178323
H 0.108000 0.020744 -1.727598
H -0.101924 -0.992178 -0.596868
Br 1.251815 -1.907480 1.016777

Br -4 water molecules

13

O 1.575435 -0.267649 -1.228428
H 1.888703 0.435234 -0.630861
H 1.186528 -0.908273 -0.579107
O -1.874441 -0.277641 0.697552
H -1.471555 0.319739 1.354159
H -1.598103 0.167729 -0.143505
O 0.497508 -1.649902 0.845311
H 0.868510 -0.925521 1.386369

H	-0.436456	-1.336274	0.747348
O	-0.739571	1.179778	-1.313609
H	-0.422935	1.750927	-0.588065
H	0.053943	0.606255	-1.457058
Br	0.870157	1.635676	1.635421

13

O	1.294004	0.119472	-1.537236
H	1.479770	0.852598	-0.919749
H	1.185714	-0.630514	-0.896864
O	-1.527382	-0.578789	1.179847
H	-1.605738	-0.149754	0.291016
H	-1.014026	0.101161	1.658912
O	0.956145	-1.557071	0.550897
H	1.420108	-0.892526	1.090531
H	0.012290	-1.361163	0.779127
O	-1.297008	0.913746	-1.087314
H	-0.974255	1.600031	-0.473605
H	-0.440123	0.549135	-1.421831
Br	0.850973	1.808519	1.426218

13

O	1.898744	-0.478048	-0.903397
H	1.543169	0.321043	-0.427424
H	1.577584	-0.351801	-1.810590
O	-1.130846	0.215877	1.697914
H	-0.787935	-0.602361	1.261037
H	-1.768678	0.521712	1.023893
O	-0.355970	-1.824348	-0.003653
H	-0.978343	-1.359044	-0.598381
H	0.514726	-1.460096	-0.300607
O	0.699170	1.616906	0.259120
H	0.150506	1.184582	0.960797
H	0.037493	1.681257	-0.460136
Br	-2.029169	0.759396	-1.497763

13

O	1.235993	-0.766707	-1.220031
H	1.692338	-0.193679	-0.568959
H	0.493185	-0.178228	-1.507460
O	-1.453559	0.636515	1.034805
H	-1.152255	-0.305899	1.060032
H	-0.634797	1.087143	1.329600
O	-0.093881	-1.743064	0.964334
H	0.533490	-1.353283	1.596705
H	0.336765	-1.520359	0.098890
O	-0.768757	1.037578	-1.570586
H	-1.121623	0.869479	-0.656919
H	-0.162945	1.782232	-1.424234
Br	1.816698	1.272932	1.354149

13

O	1.355738	-0.553698	-1.456633
H	2.034744	-0.037690	-0.992208
H	0.935813	-1.063859	-0.712990
O	-1.930900	-0.068427	0.668301
H	-1.576079	0.399871	1.444720
H	-1.533528	0.456831	-0.072585
O	0.295250	-1.664710	0.749057
H	0.768126	-1.002213	1.294326
H	-0.603681	-1.251856	0.706443
O	-0.467487	1.442461	-1.075283
H	-0.018860	1.743081	-0.257275
H	0.160176	0.744433	-1.387941
Br	1.101396	1.357876	1.882973

13

O	1.516576	-0.229937	-1.176410
H	1.765121	0.473896	-0.529455
H	1.143170	-0.914155	-0.533128
O	-1.788564	-0.278941	0.673398
H	-1.350376	0.319816	1.324322
H	-1.529206	0.192840	-0.182401
O	0.490300	-1.682208	0.840883
H	0.880802	-0.966306	1.397905
H	-0.443385	-1.309041	0.729425
O	-0.769998	1.172095	-1.341504
H	-0.450899	1.767754	-0.621460
H	0.047021	0.585651	-1.444109
Br	0.887162	1.598614	1.588059

13

O	1.186653	0.107652	-1.483408
H	1.398247	0.840145	-0.852625
H	1.127777	-0.656803	-0.825328
O	-1.444356	-0.599703	1.094442
H	-1.538949	-0.116374	0.211583
H	-0.951364	0.094134	1.598926
O	0.994200	-1.591014	0.591897
H	1.441505	-0.889789	1.118244
H	0.027851	-1.352907	0.778556
O	-1.330706	0.941527	-1.098972

H -1.011646 1.645073 -0.487194
H -0.440613 0.569834 -1.403046
Br 0.881873 1.783069 1.396876
13

O 1.668670 -0.429667 -0.992233
H 1.456189 0.372044 -0.412060
H 1.032938 -0.270573 -1.728128
O -1.031597 0.179843 1.683959
H -0.738365 -0.659784 1.198904
H -1.725035 0.507090 1.070345
O -0.353186 -1.848500 0.076629
H -0.972559 -1.428350 -0.572587
H 0.512438 -1.441677 -0.247378
O 0.744781 1.695400 0.363715
H 0.160714 1.173161 1.002820
H 0.118804 1.772501 -0.400047
Br -1.503339 0.603584 -1.843129
13

O 1.114339 -0.888357 -1.275971
H 1.695943 -0.327528 -0.704853
H 0.398779 -0.206354 -1.489360
O -1.568021 0.519546 0.963911
H -1.128664 -0.391511 0.982951
H -0.815948 1.061279 1.309849
O -0.007579 -1.663709 1.033223
H 0.598138 -1.092317 1.559671
H 0.371806 -1.505001 0.108103
O -0.613861 1.155937 -1.458596
H -1.108846 0.921139 -0.606897
H 0.120269 1.690886 -1.078991
Br 1.664298 1.350652 1.147287
13

O 1.404421 -0.417043 -1.280350
H 1.844676 0.175566 -0.626653
H 0.960343 -1.064378 -0.643166
O -1.807197 -0.016691 0.727387
H -1.266234 0.429714 1.421162
H -1.480643 0.488613 -0.085245
O 0.197005 -1.798653 0.680314
H 0.721377 -1.216636 1.282225
H -0.658743 -1.261089 0.644536
O -0.574671 1.392003 -1.194380
H -0.135918 1.852497 -0.439105
H 0.119184 0.678435 -1.374855
Br 1.197108 1.259761 1.679036

Br -8 water molecules

25

O 0.911185 1.759778 0.089360
H 0.861390 1.416783 -0.845657
H 0.201621 1.256803 0.543680
O -1.232689 3.540912 -0.237026
H -0.351761 3.125353 -0.096022
H -1.740038 3.239831 0.534118
O 2.374119 -0.721989 0.440851
H 2.125808 0.223502 0.393339
H 1.997704 -1.017805 1.308285
O 0.595322 0.666819 -2.384317
H 0.542049 -0.274316 -2.116985
H -0.355597 0.948662 -2.360821
O -0.495759 -3.429228 1.216179
H -0.206760 -3.065583 0.350682
H -1.318054 -2.936767 1.381700
O -1.942085 1.412497 -1.849678
H -2.066919 0.814885 -1.086247
H -1.774205 2.274613 -1.395705
O 0.962023 -1.564687 2.646421
H 0.278855 -0.876191 2.537881
H 0.521606 -2.341502 2.222538
O 0.236749 -1.738856 -0.923242
H 1.069426 -1.431703 -0.469873
H -0.458833 -1.235016 -0.447917
Br -1.702848 -0.025489 1.184366
25

O 0.500637 1.579655 1.110854
H -0.218212 0.910567 1.133775
H -0.008177 2.434621 1.105843
O -1.138059 3.667418 0.680588
H -1.566051 3.146583 -0.051310
H -1.808140 3.689151 1.381258
O 2.195408 -0.753550 0.746565
H 1.837518 0.093182 1.075812
H 1.694231 -1.442199 1.255510
O 0.644986 1.580372 -1.628268

H	0.725810	1.630395	-0.645556
H	0.652513	0.611299	-1.786472
O	0.392061	-3.815404	-0.759589
H	0.501274	-2.917898	-1.155311
H	-0.557172	-3.991473	-0.856715
O	-1.988052	2.047444	-1.290756
H	-1.048211	1.876227	-1.563961
H	-2.200174	1.264115	-0.746024
O	0.554934	-2.705039	1.747895
H	-0.246511	-2.146674	1.696106
H	0.518425	-3.216056	0.901722
O	0.552255	-1.167773	-1.327443
H	-0.286728	-1.043412	-0.827965
H	1.246078	-1.008544	-0.625615
Br	-1.953523	-0.645180	0.780077

25

O	-0.197585	2.806217	1.566464
H	0.626647	2.277058	1.474161
H	-0.817534	2.150096	1.933056
O	-0.813315	2.796198	-1.110041
H	-0.026797	2.349930	-1.468526
H	-0.611636	2.883493	-0.143963
O	1.595275	0.718823	1.147047
H	1.325309	0.596294	0.192949
H	0.827598	0.335087	1.623902
O	0.709685	0.301421	-1.355158
H	0.988010	-0.645719	-1.492940
H	-0.257368	0.220335	-1.199005
O	-1.474243	-2.354211	-0.725068
H	-1.780773	-1.501887	-1.092891
H	-1.414167	-2.139484	0.227213
O	-2.057087	0.410974	-0.870183
H	-2.020159	0.303050	0.103482
H	-1.790044	1.355975	-1.015170
O	1.857134	-2.112228	1.265006
H	0.968293	-2.094632	1.664653
H	2.100893	-1.163255	1.268784
O	1.175289	-2.334627	-1.398485
H	1.511510	-2.354206	-0.469877
H	0.205911	-2.464893	-1.257298
Br	-1.234880	-0.580889	2.216860

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O	2.124408	0.718026	-2.348097
H	1.308164	1.153904	-2.693796
H	1.778293	-0.159920	-2.096632
O	1.842848	1.842405	0.137519
H	2.127089	1.459280	-0.729457
H	0.870620	1.928300	0.000418
O	-2.307943	-1.910723	1.344046
H	-1.481950	-2.350818	1.658074
H	-2.127257	-1.815416	0.390354
O	0.222761	-2.964613	1.860076
H	0.351568	-3.121342	0.908666
H	0.722700	-2.138834	2.010617
O	-0.382321	1.713806	-3.064036
H	-0.764474	0.829076	-3.188825
H	-0.700870	1.961335	-2.172961
O	1.076300	-0.363553	1.449122
H	1.552671	0.445680	1.120522
H	0.719662	-0.733491	0.612863
O	-0.861893	1.552323	-0.353913
H	-0.709297	0.637113	-0.676680
H	-1.251370	1.373885	0.546489
O	-1.497543	0.603389	2.050243
H	-1.948395	-0.249820	1.827098
H	-0.553632	0.322139	2.046328
Br	-0.241207	-1.559112	-1.395499

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O	-1.043528	0.880320	2.613644
H	-0.228966	1.173646	2.145601
H	-0.922388	-0.088376	2.616166
O	1.057704	1.082322	0.843397
H	0.512429	1.376842	0.048855
H	0.902484	0.114639	0.893985
O	2.087765	-1.350960	-1.252684
H	1.720915	-1.773367	-0.451366
H	2.668620	-0.638268	-0.887351
O	-0.501617	1.734622	-1.178165
H	-0.440309	0.903627	-1.716294
H	-1.338758	1.614188	-0.659172
O	-2.634101	1.159590	0.416656
H	-2.681226	0.217294	0.142638
H	-2.137562	1.104125	1.270810
O	3.584074	0.581324	0.001778
H	4.015131	0.103827	0.727434
H	2.753420	0.934261	0.405359
O	-2.244558	-1.452261	-0.368845
H	-1.557496	-1.797237	0.247917
H	-2.819948	-2.209689	-0.558155

O	-0.365220	-0.713517	-2.323805
H	0.518833	-0.946950	-1.947718
H	-1.028218	-1.070063	-1.693851
Br	0.304269	-2.106417	1.537608

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O	0.847314	1.646774	0.033286
H	0.721882	1.279407	-0.915264
H	0.098087	1.200143	0.516215
O	-0.806182	3.698280	-0.600913
H	-0.081821	3.079318	-0.285406
H	-1.311813	3.880707	0.216457
O	2.248546	-0.656593	0.656286
H	1.931122	0.279668	0.533483
H	1.778379	-0.954185	1.501402
O	0.302500	0.599807	-2.336971
H	0.260983	-0.331629	-1.987071
H	-0.650145	0.928958	-2.253650
O	0.124285	-3.676092	1.068502
H	0.129056	-3.079885	0.261441
H	-0.827031	-3.857644	1.205103
O	-2.108026	1.632353	-1.761088
H	-2.225204	1.092267	-0.939334
H	-1.697578	2.474665	-1.386452
O	0.731178	-1.586762	2.659664
H	-0.053875	-1.025474	2.440373
H	0.515774	-2.437796	2.160820
O	0.260199	-1.678093	-0.761157
H	1.096753	-1.328117	-0.283363
H	-0.462027	-1.195643	-0.272696
Br	-1.790044	0.036871	1.166242

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O	0.504425	1.452303	0.993481
H	-0.226811	0.780941	0.918955
H	-0.018905	2.322132	1.077285
O	-1.104408	3.525029	0.870542
H	-1.512687	3.087650	0.048014
H	-1.779319	3.383149	1.564139
O	2.150704	-0.731351	0.757413
H	1.761640	0.139775	1.026201
H	1.601759	-1.406007	1.276774
O	0.633512	1.563418	-1.737119
H	0.743578	1.613691	-0.740832
H	0.652464	0.575270	-1.871209
O	0.414796	-3.761342	-0.627983
H	0.516437	-2.866015	-1.072149
H	-0.542102	-3.941941	-0.722020
O	-1.939510	2.154739	-1.250007
H	-1.001181	1.942100	-1.566607
H	-2.174927	1.321012	-0.771388
O	0.497270	-2.557068	1.795541
H	-0.315415	-2.005150	1.675537
H	0.485376	-3.111836	0.953067
O	0.611468	-1.163197	-1.352768
H	-0.255803	-0.997286	-0.889349
H	1.283877	-0.984203	-0.599274
Br	-1.989120	-0.657985	0.594774

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O	-0.074277	2.878393	1.384773
H	0.623278	2.153190	1.388561
H	-0.816050	2.462705	1.870494
O	-0.841934	2.737343	-1.176484
H	-0.080967	2.233056	-1.544111
H	-0.557614	2.882769	-0.216060
O	1.449386	0.658299	1.203673
H	1.223382	0.568854	0.207015
H	0.667435	0.195064	1.617853
O	0.706270	0.334689	-1.294606
H	0.997079	-0.636953	-1.442561
H	-0.266492	0.221713	-1.098439
O	-1.489214	-2.298865	-0.853414
H	-1.761454	-1.372737	-1.086467
H	-1.393403	-2.202121	0.129063
O	-2.015118	0.413320	-0.717485
H	-1.892162	0.304958	0.260723
H	-1.732728	1.369686	-0.919103
O	1.909331	-2.089967	1.257356
H	1.007448	-2.130724	1.658900
H	2.071722	-1.109186	1.291773
O	1.174671	-2.232884	-1.359315
H	1.503840	-2.256959	-0.409677
H	0.184364	-2.371376	-1.245845
Br	-1.200825	-0.953349	2.178358

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O	1.934813	0.734326	-2.462779
H	1.225630	1.402470	-2.721382
H	1.395683	-0.078008	-2.290002
O	1.716711	1.603669	0.079401
H	1.989628	1.272998	-0.835068

H	0.733128	1.707314	-0.079367
O	-2.152386	-2.033081	1.237464
H	-1.397721	-2.365759	1.817192
H	-1.729149	-2.005635	0.342929
O	0.027353	-2.631602	2.726104
H	0.436414	-3.425275	2.327349
H	0.576303	-1.886856	2.354987
O	-0.102132	2.471157	-2.879380
H	-0.682558	2.045218	-3.540971
H	-0.550228	2.258803	-2.015345
O	1.115398	-0.647951	1.259831
H	1.497887	0.230942	0.898817
H	0.751116	-1.059283	0.429349
O	-0.952246	1.393548	-0.562992
H	-0.803655	0.485802	-0.945725
H	-1.265842	1.158711	0.383166
O	-1.369440	0.464791	1.836450
H	-1.841166	-0.407051	1.638671
H	-0.423170	0.143951	1.791089
Br	-0.261438	-1.660183	-1.547253

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O	-1.107765	0.991836	2.646582
H	-0.262134	1.253183	2.182723
H	-0.970569	0.017275	2.717599
O	1.054505	1.099074	0.970578
H	0.467759	1.374008	0.151478
H	0.881311	0.122402	1.057258
O	1.974865	-1.594930	-1.163811
H	1.526650	-1.867317	-0.324216
H	2.518187	-0.792165	-0.879317
O	-0.449272	1.729921	-1.020067
H	-0.339749	0.906523	-1.604823
H	-1.331818	1.557853	-0.555058
O	-2.627540	1.062929	0.396706
H	-2.557130	0.113576	0.098352
H	-2.137084	1.054424	1.274879
O	3.339447	0.555929	-0.290939
H	3.929715	0.181379	0.393381
H	2.553247	0.891808	0.245352
O	-2.020795	-1.435296	-0.530895
H	-1.376451	-1.735614	0.174932
H	-2.654334	-2.175506	-0.619966
O	-0.193900	-0.558567	-2.358603
H	0.646555	-0.933440	-1.940284
H	-0.916074	-0.986992	-1.822351
Br	0.234123	-1.998768	1.674958

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O	2.063769	1.865891	-0.241546
H	2.814443	1.853096	0.396110
H	2.014770	0.940973	-0.581066
O	-2.847393	-2.010757	0.108273
H	-2.590413	-1.110727	0.403026
H	-2.086418	-2.558341	0.408989
O	-1.579644	3.014275	0.886296
H	-0.805042	3.023528	1.490763
H	-1.155887	3.081340	-0.007331
O	0.788566	2.427888	2.150990
H	1.095483	2.177142	1.245308
H	0.648212	1.558510	2.572062
O	-2.035314	-2.013166	-2.491447
H	-2.440276	-2.060151	-1.587888
H	-1.189903	-2.513891	-2.383903
O	-1.535780	0.341457	0.783704
H	-1.649928	1.325396	0.919555
H	-0.787401	0.060550	1.350108
O	-0.205096	2.889142	-1.501727
H	0.684244	2.726685	-1.125446
H	-0.484789	1.996780	-1.802698
O	-0.744272	0.208801	-1.770093
H	-1.092575	0.255491	-0.839833
H	-1.279526	-0.524156	-2.187391
O	1.590156	-0.767182	-1.002292
H	1.481952	-0.954433	-0.045616
H	0.699731	-0.429560	-1.306849
O	-0.515546	-3.311121	0.701628
H	-0.584563	-4.123767	1.228194
H	-0.003242	-2.691259	1.266391
O	0.392751	-3.193845	-1.906680
H	0.986550	-2.426921	-1.768499
H	0.108589	-3.397169	-0.987083
O	3.571575	1.669868	2.076066
H	2.809107	2.169232	2.425582
H	3.289953	0.747465	2.219460
Br	1.156672	-0.926756	2.321797

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O	1.912187	-0.210580	0.088440
H	1.180352	-0.072910	-0.580413
H	1.431248	-0.472095	0.902306
O	1.503054	2.496142	0.541424
H	1.729371	2.608589	1.495636
H	1.782563	1.568318	0.354031
O	-2.574887	2.313000	-0.401276
H	-2.616418	1.337741	-0.476496
H	-2.156053	2.429473	0.483719
O	-0.201444	2.901786	-1.653418
H	-1.108564	2.828701	-1.260602
H	0.387341	3.019069	-0.879675
O	0.133452	-2.129333	-2.917633
H	0.047462	-1.175019	-2.694238
H	0.929615	-2.387535	-2.389403
O	1.519093	2.402142	3.270072
H	0.595011	2.712532	3.230684
H	1.405555	1.435369	3.322369
O	-0.963327	2.371735	1.810324
H	-0.156125	2.416897	1.245751
H	-0.960872	1.444146	2.124405
O	-2.129234	-0.471771	-0.137331
H	-1.708276	-0.549201	0.742892
H	-2.104416	-1.406670	-0.500472
O	2.196814	-2.716233	-1.164299
H	2.355038	-1.819339	-0.797287
H	1.601433	-3.097652	-0.481288
O	0.334653	-3.400650	0.753623
H	0.365490	-4.202319	1.299886
H	0.187497	-2.669269	1.393778
O	-1.699037	-2.928960	-1.062863
H	-1.097039	-2.695229	-1.818807
H	-1.064555	-3.214906	-0.367869
O	-0.017599	0.257965	-1.641381
H	-0.052777	1.247259	-1.768278
H	-0.828936	0.027056	-1.118685
Br	-0.165276	-0.747631	2.651525

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O	3.057350	1.596548	-0.889207
H	3.224086	1.650769	0.082931
H	2.611217	0.723116	-0.985902
O	-2.755270	-2.305524	-0.003065
H	-2.698700	-1.418137	0.408413
H	-1.920168	-2.744586	0.279365
O	-2.160559	2.806333	1.523835
H	-1.187029	2.829791	1.690808
H	-2.251196	3.197287	0.640607
O	0.531572	2.392858	1.597231
H	0.559833	2.537293	0.604676
H	0.501988	1.422348	1.724864
O	-1.773605	-1.730327	-2.481406
H	-2.240451	-1.996675	-1.648805
H	-0.918189	-2.226087	-2.425150
O	-2.043365	0.153289	1.090531
H	-2.224598	1.106119	1.317574
H	-1.286860	-0.110966	1.653555
O	0.608117	2.780099	-1.031652
H	1.542094	2.448388	-1.097975
H	0.058344	2.026101	-1.336887
O	-0.892179	0.489510	-1.337899
H	-1.346609	0.386266	-0.462652
H	-1.268410	-0.255181	-1.891819
O	1.489983	-0.626249	-0.888649
H	1.470626	-0.824980	0.072037
H	0.606810	-0.187942	-1.051197
O	-0.275751	-3.344578	0.565219
H	-0.291726	-4.172754	1.071515
H	0.124148	-2.687511	1.176723
O	0.640732	-2.970586	-2.019702
H	1.108811	-2.143645	-1.760098
H	0.345078	-3.294348	-1.140597
O	3.230913	1.733726	1.863048
H	2.362617	2.187462	1.930931
H	3.000535	0.822666	2.121350
Br	0.909712	-0.852649	2.371007

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O	2.000756	-0.345012	0.229571
H	1.378937	-0.108669	-0.518212
H	1.404934	-0.499582	0.990460
O	2.531090	2.378210	0.425721
H	1.905815	2.448142	1.182503
H	2.554568	1.403421	0.300305
O	-1.736057	2.463891	0.315725
H	-1.987386	1.599533	-0.073432
H	-2.162276	2.466773	1.205871
O	0.522918	3.013627	-1.327766
H	-0.254961	3.063381	-0.737189
H	1.296102	2.905086	-0.715636
O	0.725301	-2.149981	-2.813369

H	0.717010	-1.184768	-2.641361
H	1.328577	-2.495251	-2.108754
O	0.396054	2.188724	2.102571
H	-0.235369	2.285540	1.352043
H	0.335942	1.233690	2.316546
O	-2.287555	2.227511	2.995331
H	-2.246919	1.256232	3.056464
H	-1.344062	2.473434	3.067626
O	-1.977209	-0.188920	-0.474044
H	-1.680141	-0.465088	0.419540
H	-2.060619	-1.042559	-0.990111
O	2.242189	-2.956428	-0.667473
H	2.348974	-2.045017	-0.311131
H	1.415277	-3.252729	-0.222565
O	-0.259021	-3.409362	0.403210
H	-0.372891	-2.713941	1.089833
H	-0.466179	-4.236521	0.867729
O	-1.760761	-2.527772	-1.736692
H	-0.918813	-2.403679	-2.247660
H	-1.409425	-2.984716	-0.939334
O	0.355212	0.361268	-1.726472
H	0.425518	1.354845	-1.723978
H	-0.520566	0.169642	-1.304672
Br	-0.577377	-0.911944	2.479691

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O	1.969709	1.770255	-0.772843
H	2.791634	1.854322	-0.231983
H	1.895712	0.814385	-0.970139
O	-2.776355	-2.119459	0.491551
H	-2.570702	-1.180193	0.683865
H	-1.983039	-2.575750	0.853483
O	-1.545826	3.015044	0.734162
H	-0.711862	3.132397	1.238441
H	-1.223487	3.035803	-0.203767
O	1.046420	2.684075	1.684038
H	1.184301	2.306948	0.781180
H	0.968474	1.873380	2.225666
O	-2.131400	-2.334057	-2.162428
H	-1.768208	-1.420996	-2.219586
H	-2.486706	-2.330586	-1.237695
O	-1.574598	0.351447	0.956500
H	-1.631627	1.348702	0.951859
H	-0.747773	0.129970	1.431808
O	-0.400163	2.782302	-1.792771
H	0.535496	2.665196	-1.527979
H	-0.679980	1.844158	-1.919595
O	-0.946166	0.111751	-1.680260
H	-1.294312	0.173995	-0.754534
H	-0.041117	-0.256974	-1.512608
O	1.426189	-0.991957	-0.943489
H	1.123495	-1.915224	-1.182871
H	1.434962	-0.980051	0.037236
O	-0.371672	-3.149106	1.322933
H	-0.361799	-3.876263	1.965711
H	0.153789	-2.435179	1.747429
O	0.279460	-3.372409	-1.352724
H	-0.589233	-3.073356	-1.728120
H	0.089101	-3.465429	-0.393131
O	3.736367	2.014238	1.269368
H	2.997222	2.528468	1.652674
H	3.557713	1.122363	1.618064
Br	1.391702	-0.543451	2.365970

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O	2.223855	1.960561	-0.421118
H	2.939761	1.866993	0.272651
H	2.050887	1.003409	-0.681544
O	-2.914889	-2.108766	-0.062155
H	-2.742559	-1.195130	0.288032
H	-2.150160	-2.623240	0.322366
O	-1.555605	2.856161	0.930015
H	-0.730174	2.812969	1.492189
H	-1.139185	2.979804	0.017745
O	0.913434	2.357876	1.958043
H	1.261377	2.255111	1.020253
H	0.778714	1.410217	2.224930
O	-1.764749	-1.928262	-2.496145
H	-2.287293	-2.046695	-1.638532
H	-0.903654	-2.415202	-2.291126
O	-1.870666	0.272253	0.846033
H	-1.851055	1.300692	0.933222
H	-1.113234	-0.044764	1.402018
O	-0.222590	2.917342	-1.423379
H	0.707123	2.792265	-1.104781
H	-0.477830	1.987035	-1.687532
O	-0.800823	0.294989	-1.586482
H	-1.250185	0.285104	-0.679489
H	-1.222081	-0.509440	-2.075956
O	1.534889	-0.604673	-0.880719
H	1.427410	-0.780554	0.093175
H	0.605454	-0.265650	-1.161580

O	-0.601677	-3.292943	0.752485
H	-0.607945	-4.128111	1.263360
H	-0.128213	-2.646218	1.344627
O	0.561915	-3.069857	-1.702845
H	1.080461	-2.239594	-1.516382
H	0.202288	-3.289013	-0.797833
O	3.597257	1.480168	1.879014
H	2.852221	1.998728	2.271989
H	3.259023	0.561609	1.978335
Br	0.922014	-0.884872	2.334032

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O	3.087784	1.627886	-0.983100
H	3.205731	1.725079	0.010972
H	2.686582	0.713209	-1.054828
O	-2.890216	-2.194182	-0.145450
H	-2.756080	-1.314858	0.302385
H	-2.107871	-2.705825	0.203928
O	-2.188306	2.556743	1.877203
H	-1.189615	2.686203	1.824622
H	-2.529031	3.101773	1.139224
O	0.468824	2.442024	1.554884
H	0.517533	2.562312	0.523831
H	0.458529	1.460546	1.699928
O	-1.670836	-1.673519	-2.492646
H	-2.215756	-1.902042	-1.671282
H	-0.839686	-2.231945	-2.351095
O	-1.944975	0.101069	0.976707
H	-2.165077	1.029860	1.339283
H	-1.196426	-0.215089	1.545977
O	0.668777	2.738098	-1.008291
H	1.613691	2.372908	-1.094200
H	0.105427	1.977818	-1.326710
O	-0.685497	0.442752	-1.357880
H	-1.159789	0.356476	-0.470303
H	-1.107468	-0.311679	-1.920506
O	1.658353	-0.679753	-0.959124
H	1.638837	-0.830614	0.024096
H	0.755736	-0.220881	-1.114084
O	-0.504818	-3.281201	0.630113
H	-0.458160	-4.106539	1.154195
H	-0.044626	-2.604514	1.197906
O	0.588395	-3.014997	-1.860572
H	1.122425	-2.199258	-1.633394
H	0.243687	-3.271528	-0.960676
O	3.142618	1.852498	1.725874
H	2.244909	2.286782	1.781678
H	2.916131	0.931844	1.992256
Br	0.980168	-0.810210	2.232638

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O	1.879135	-0.091962	-0.016254
H	1.154209	0.034247	-0.732617
H	1.352044	-0.327331	0.795279
O	1.470405	2.539868	0.526117
H	1.722199	2.594030	1.495638
H	1.741983	1.601869	0.289912
O	-2.566582	2.229158	-0.293422
H	-2.549278	1.238090	-0.370590
H	-2.122790	2.359070	0.595340
O	-0.329989	2.886491	-1.624765
H	-1.212451	2.722096	-1.156583
H	0.318906	2.994015	-0.885293
O	0.248090	-2.185503	-2.819892
H	0.169728	-1.203650	-2.666293
H	1.010827	-2.420926	-2.202023
O	1.576610	2.329698	3.228223
H	0.636611	2.629020	3.209878
H	1.460205	1.350999	3.247491
O	-0.930454	2.386291	1.848758
H	-0.127967	2.467719	1.249227
H	-0.875425	1.437659	2.134232
O	-1.979412	-0.470682	-0.192676
H	-1.533004	-0.564225	0.686886
H	-2.007130	-1.433000	-0.571604
O	2.155430	-2.678560	-0.964338
H	2.257851	-1.744426	-0.630135
H	1.515551	-3.058978	-0.299362
O	0.149460	-3.417916	0.735478
H	0.199953	-4.234718	1.272470
H	0.064658	-2.685136	1.403874
O	-1.730652	-2.866281	-1.147372
H	-1.034259	-2.656531	-1.858258
H	-1.150461	-3.207554	-0.410130
O	-0.000636	0.287499	-1.773029
H	-0.091173	1.299757	-1.866483
H	-0.794502	0.022705	-1.199381
Br	-0.055297	-0.712279	2.560849

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O	2.131964	-0.384241	0.203518
H	1.468864	-0.100897	-0.524478

H	1.540305	-0.581998	0.975827
O	2.468001	2.353661	0.566851
H	1.778598	2.411610	1.287279
H	2.530681	1.364444	0.441651
O	-1.657704	2.428512	0.164601
H	-1.845353	1.486856	-0.114350
H	-2.169242	2.519064	1.024061
O	0.633076	2.952423	-1.323794
H	-0.189677	3.018282	-0.774723
H	1.369402	2.817532	-0.642663
O	0.463191	-1.987096	-2.925493
H	0.489965	-1.022588	-2.672369
H	1.110621	-2.376960	-2.253306
O	0.232075	2.207547	2.112314
H	-0.328782	2.244262	1.277597
H	0.244457	1.231039	2.308941
O	-2.454703	2.377896	2.742042
H	-2.590609	1.413927	2.855457
H	-1.471835	2.464641	2.866829
O	-1.809930	-0.219126	-0.262278
H	-1.426261	-0.513502	0.607812
H	-1.917685	-1.100270	-0.794536
O	2.059590	-2.896629	-0.945696
H	2.257958	-2.016011	-0.518362
H	1.298210	-3.227959	-0.391540
O	-0.203965	-3.486945	0.461823
H	-0.235501	-2.805334	1.189092
H	-0.324219	-4.342079	0.922306
O	-1.762731	-2.482041	-1.527090
H	-0.970208	-2.322858	-2.146380
H	-1.324181	-2.982520	-0.782840
O	0.422377	0.361478	-1.625257
H	0.484523	1.383344	-1.635824
H	-0.436549	0.152302	-1.139368
Br	-0.237134	-0.968757	2.513234

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O	2.097258	1.854383	-0.921701
H	2.873553	1.819324	-0.286865
H	1.920162	0.889239	-1.098525
O	-2.791018	-2.170793	0.567837
H	-2.622056	-1.206602	0.740394
H	-1.965529	-2.600593	0.930063
O	-1.533111	2.963590	0.712953
H	-0.650230	3.003670	1.178925
H	-1.218087	3.006413	-0.248227
O	1.049732	2.612118	1.505681
H	1.280345	2.340258	0.566615
H	0.926233	1.727846	1.940778
O	-1.945959	-2.325621	-1.996077
H	-1.657905	-1.368640	-2.055213
H	-2.346300	-2.332461	-1.069220
O	-1.783779	0.376010	0.898058
H	-1.781761	1.408238	0.892389
H	-0.964137	0.127573	1.399637
O	-0.435056	2.803178	-1.742911
H	0.520833	2.734988	-1.498159
H	-0.677241	1.829820	-1.842187
O	-0.982064	0.182360	-1.626853
H	-1.369455	0.246947	-0.691889
H	-0.058822	-0.173620	-1.409874
O	1.398995	-0.767058	-0.900417
H	1.154580	-1.749869	-1.118905
H	1.366097	-0.735655	0.093866
O	-0.373232	-3.220735	1.290055
H	-0.320089	-3.976893	1.909037
H	0.114255	-2.482525	1.747627
O	0.496260	-3.159962	-1.292246
H	-0.427235	-2.908352	-1.637478
H	0.291836	-3.347395	-0.333647
O	3.692670	1.649460	1.262557
H	3.010143	2.251124	1.651509
H	3.345223	0.772328	1.544345
Br	1.110617	-0.533333	2.363481

Br -16 water molecules

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O	-2.474955	1.111501	1.273802
H	-2.683406	0.317027	1.844395
H	-1.619492	1.439927	1.615736
O	-1.605205	-0.525584	-0.669319
H	-1.900496	0.151115	-0.006695
H	-2.021242	-0.259554	-1.535293
O	-3.066155	2.515733	-1.099802
H	-2.099488	2.710432	-1.123040
H	-3.145071	2.046341	-0.244359
O	0.673982	-3.679458	-0.725693
H	0.698329	-2.831149	-1.229528

H	1.482028	-3.589007	-0.176718
O	0.827045	-1.681817	2.383682
H	0.920039	-0.734465	2.141472
H	0.034067	-1.989540	1.858881
O	-2.497090	0.579359	-2.917816
H	-2.828307	1.329937	-2.360227
H	-1.635204	0.890497	-3.251681
O	-1.209819	-2.617284	0.910190
H	-1.491852	-1.926338	0.259910
H	-0.597273	-3.183878	0.369029
O	0.430387	1.020415	-3.232466
H	0.529426	0.128490	-2.815987
H	1.336791	1.393361	-3.070451
O	-2.760787	-1.089092	2.751346
H	-2.346415	-1.805468	2.232724
H	-2.083471	-0.870738	3.440601
O	2.900818	-0.146632	-0.170172
H	2.461590	0.366440	0.538524
H	3.066190	-1.044813	0.216804
O	-0.337306	2.524387	-1.130736
H	-0.100731	1.927187	-1.892157
H	-0.096971	2.030389	-0.319521
O	2.837730	1.760185	-2.247666
H	2.995635	1.043851	-1.600504
H	2.648538	2.552061	-1.690194
O	2.789542	-2.651754	0.812714
H	2.138400	-2.393081	1.516801
H	3.507432	-3.100169	1.286947
O	-0.703778	-0.455237	4.414266
H	-0.433114	0.430072	4.113281
H	-0.077653	-1.036594	3.929279
O	2.010375	3.872050	-0.629453
H	2.087837	3.471675	0.254323
H	1.095244	3.615380	-0.886224
O	0.792795	-1.093620	-1.603105
H	1.552441	-0.723757	-1.087591
H	-0.028898	-0.817492	-1.116981
Br	0.818273	1.579769	1.841384

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O	-2.579400	1.124828	1.027061
H	-2.865578	0.330064	1.567203
H	-1.755136	1.435689	1.452429
O	-1.476846	-0.572851	-0.785521
H	-1.821104	0.109293	-0.154288
H	-1.867038	-0.312371	-1.665656
O	-2.909573	2.560312	-1.335169
H	-1.939293	2.729795	-1.320762
H	-3.035410	2.080848	-0.489029
O	1.009115	-3.579130	-0.406174
H	1.003140	-2.829922	-1.050543
H	0.149737	-3.469345	0.059151
O	0.577088	-1.548154	2.713658
H	0.670719	-0.616527	2.413090
H	1.422332	-1.972367	2.419070
O	-2.288842	0.554786	-3.059360
H	-2.628986	1.326031	-2.534972
H	-1.415959	0.848044	-3.380016
O	-1.234933	-2.619515	0.970568
H	-0.583437	-2.190608	1.581572
H	-1.390291	-1.959513	0.252345
O	0.647218	0.932312	-3.372612
H	0.722698	0.037340	-2.961442
H	1.533661	1.309604	-3.134399
O	-3.078688	-1.057505	2.429736
H	-2.588080	-1.761683	1.953356
H	-2.507477	-0.867877	3.216444
O	2.804121	-0.157468	-0.043314
H	2.966480	-0.992528	0.466462
H	2.271365	0.396695	0.565331
O	-0.174930	2.455265	-1.261388
H	0.075277	1.853127	-2.010314
H	-0.009140	1.952488	-0.437045
O	2.970213	1.682368	-2.173769
H	3.084209	0.974661	-1.508725
H	2.781392	2.484218	-1.631505
O	2.679208	-2.472172	1.320362
H	3.383381	-3.075116	1.604104
H	2.112771	-2.994538	0.675448
O	-1.291080	-0.476381	4.401835
H	-1.009486	0.428292	4.185392
H	-0.557805	-1.021534	4.043677
O	2.122476	3.817610	-0.597583
H	2.155757	3.433095	0.295471
H	1.227405	3.545079	-0.904727
O	0.940438	-1.185651	-1.699509
H	1.650226	-0.783400	-1.136332
H	0.093920	-0.905259	-1.261335
Br	0.637097	1.606231	1.840086

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O	-2.479138	1.094940	1.181453

H	-2.755783	0.289323	1.708869
H	-1.625402	1.363037	1.578572
O	-1.641037	-0.531471	-0.813265
H	-1.935776	0.137816	-0.142631
H	-1.929574	-0.185692	-1.692979
O	-2.680265	2.620943	-1.172041
H	-1.707517	2.769731	-1.089575
H	-2.879919	2.117900	-0.355753
O	0.747835	-3.762024	-0.854058
H	0.823628	-2.861433	-1.250202
H	-0.045826	-3.657016	-0.285772
O	0.660299	-1.761307	2.404437
H	0.851634	-0.819897	2.213036
H	1.432405	-2.270847	2.026181
O	-2.119004	0.886702	-3.118837
H	-2.851463	0.665636	-3.713764
H	-2.473517	1.580355	-2.495638
O	-1.311690	-2.697970	0.804055
H	-0.591114	-2.292142	1.352432
H	-1.520377	-2.026195	0.116209
O	0.651832	1.015840	-3.046324
H	-0.289197	0.990124	-3.333807
H	0.785426	0.143664	-2.596002
O	-2.927671	-1.142316	2.541705
H	-2.283660	-0.981366	3.276937
H	-2.492937	-1.829113	1.991572
O	3.255973	1.587625	-1.683863
H	2.561484	1.474896	-2.357267
H	3.018631	2.436389	-1.231817
O	0.036285	2.565133	-0.955061
H	0.313451	1.971445	-1.708018
H	0.178091	2.054522	-0.129631
O	2.873314	-0.259605	0.235074
H	2.424988	0.317527	0.887240
H	3.136579	0.374862	-0.488623
O	2.571605	-2.991298	1.016047
H	2.875543	-2.141784	0.636299
H	1.969533	-3.367280	0.322910
O	-0.960322	-0.641093	4.360144
H	-0.643535	0.242712	4.100755
H	-0.309799	-1.228339	3.919151
O	2.372005	3.809543	-0.333349
H	2.387645	3.480951	0.581676
H	1.457481	3.577418	-0.621971
O	0.884220	-1.092904	-1.399661
H	1.553197	-0.804260	-0.728451
H	-0.007653	-0.832029	-1.046778
Br	0.742809	1.537968	2.081896

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O	-2.685985	0.915883	1.096310
H	-2.988776	0.086465	1.569107
H	-1.822094	1.130562	1.506430
O	-1.790356	-0.802872	-0.809538
H	-2.102985	-0.117568	-0.167412
H	-1.999628	-0.421573	-1.709260
O	-2.709889	2.526751	-1.207772
H	-1.799271	2.879601	-1.128374
H	-2.842583	2.012282	-0.383828
O	0.824877	-3.710129	-0.840318
H	0.842823	-2.802831	-1.226068
H	0.005651	-3.686566	-0.299836
O	0.465264	-1.804056	2.431559
H	0.571745	-0.859623	2.187980
H	1.291305	-2.244756	2.079768
O	-2.136421	0.596740	-3.038230
H	-1.197269	0.807644	-3.232869
H	-2.430151	1.354120	-2.469078
O	-1.389898	-2.944326	0.776015
H	-0.725274	-2.492686	1.356567
H	-1.618421	-2.271385	0.092478
O	0.645104	1.135726	-2.957129
H	0.409405	1.776457	-2.239621
H	0.719947	0.272514	-2.474876
O	-3.156329	-1.366762	2.371176
H	-2.547620	-1.180001	3.129365
H	-2.693867	-2.065913	1.861885
O	3.275283	1.324401	-1.957319
H	2.461175	1.248814	-2.501149
H	3.175790	2.207331	-1.534990
O	0.026569	2.896136	-0.959664
H	0.061973	2.405601	-0.107787
H	0.866475	3.410912	-0.928310
O	2.795297	-0.163447	0.233941
H	2.308093	0.456538	0.814608
H	3.072262	0.373471	-0.561820
O	2.536025	-2.831280	1.109002
H	2.806787	-1.966041	0.736194
H	1.990313	-3.246646	0.393670
O	-1.289841	-0.757095	4.268715
H	-1.013630	0.147401	4.040454
H	-0.586626	-1.303560	3.855826

O	2.618407	3.603947	-0.598264
H	3.050394	4.451449	-0.794144
H	2.743051	3.483773	0.358129
O	0.788625	-1.021900	-1.359416
H	1.448875	-0.739458	-0.679167
H	-0.121603	-0.873106	-0.986958
Br	0.473242	1.474155	1.979737

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O	-2.194163	1.165855	1.598516
H	-2.460870	0.334436	2.093629
H	-1.299916	1.387407	1.929095
O	-1.637063	-0.538828	-0.472001
H	-1.783596	0.132592	0.237843
H	-2.070103	-0.166328	-1.289334
O	-2.815089	2.592053	-0.616392
H	-3.274168	3.437578	-0.497187
H	-2.793836	2.161414	0.272001
O	0.571990	-3.737404	-1.062761
H	0.586888	-2.826272	-1.446267
H	-0.164723	-3.675460	-0.417555
O	0.881459	-1.842644	2.111012
H	1.026980	-0.900740	1.885491
H	1.621034	-2.334428	1.652200
O	-2.511053	0.758173	-2.638056
H	-1.624151	0.961825	-3.002101
H	-2.731786	1.527696	-2.068534
O	-1.337323	-2.833444	0.890356
H	-0.524331	-2.477301	1.332558
H	-1.583970	-2.105346	0.272913
O	0.325512	1.148372	-3.171432
H	0.184501	1.686549	-2.351912
H	0.469969	0.247133	-2.789804
O	-2.622961	-1.140713	2.824144
H	-1.871149	-1.022777	3.460016
H	-2.309104	-1.838270	2.210144
O	3.060778	1.431515	-2.312378
H	2.216628	1.352179	-2.805053
H	2.933555	2.253276	-1.775065
O	-0.121659	2.500771	-0.898755
H	-1.085908	2.709169	-0.805234
H	0.123226	2.047469	-0.064053
O	2.832877	-0.293502	-0.277495
H	2.512971	0.298228	0.433545
H	3.035274	0.316626	-1.044258
O	2.664603	-3.032027	0.523576
H	2.920375	-2.173797	0.128106
H	1.962873	-3.382910	-0.084381
O	-0.397247	-0.738511	4.306950
H	-0.079346	0.152681	4.076619
H	0.173312	-1.309984	3.748470
O	2.409188	3.541284	-0.683114
H	2.502299	3.170495	0.211592
H	1.444097	3.454718	-0.844630
O	0.653160	-1.076428	-1.618276
H	1.427650	-0.803555	-1.062947
H	-0.148835	-0.830169	-1.083116
Br	1.117765	1.490655	1.994006

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O	-2.270372	0.891272	1.296357
H	-2.537865	0.077268	1.863881
H	-1.389573	1.181983	1.643158
O	-1.674593	-0.662706	-0.751690
H	-1.849843	0.005469	-0.010438
H	-2.070795	-0.241095	-1.592465
O	-2.911661	2.536007	-0.872240
H	-1.941318	2.776765	-0.946982
H	-2.902733	1.972689	-0.054558
O	0.838227	-3.651326	-0.510903
H	0.798524	-2.863598	-1.130724
H	1.605912	-3.383910	0.066981
O	0.574325	-1.431152	2.301906
H	0.623017	-0.471127	2.031808
H	-0.165146	-1.852681	1.726446
O	-2.480165	0.740656	-2.815594
H	-2.742062	1.471070	-2.164274
H	-1.580684	1.011937	-3.119497
O	-1.215726	-2.702077	0.867099
H	-1.528697	-2.063929	0.158885
H	-0.480687	-3.220209	0.384709
O	0.380458	1.061197	-3.079185
H	0.467288	0.124005	-2.718512
H	1.351702	1.367473	-3.036476
O	-2.815237	-1.250400	2.697713
H	-2.386019	-1.968514	2.170049
H	-2.171669	-1.118051	3.465344
O	2.681083	-0.049421	-0.363154
H	2.255393	0.541048	0.313600
H	2.904332	-0.885562	0.156827
O	-0.231386	2.669461	-1.092461
H	-0.037572	1.978732	-1.823996

H	0.001678	2.217456	-0.237429
O	2.903790	1.680475	-2.531383
H	3.004675	0.971937	-1.844081
H	2.754259	2.498907	-1.961279
O	2.698702	-2.322922	1.013915
H	1.964817	-2.026118	1.646990
H	3.420704	-2.648310	1.587630
O	-0.864699	-0.824807	4.483943
H	-0.750836	0.147495	4.482045
H	-0.207713	-1.126648	3.786542
O	2.240175	3.735662	-0.914801
H	2.413666	3.378312	-0.017494
H	1.266396	3.521002	-1.030716
O	0.686124	-1.213979	-1.715720
H	1.419739	-0.768785	-1.184640
H	-0.171171	-0.962192	-1.233366
Br	0.913994	1.712300	1.780942

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O	-2.404586	0.931406	1.029822
H	-2.734655	0.155026	1.622873
H	-1.564949	1.251209	1.446703
O	-1.569026	-0.730936	-0.844707
H	-1.836540	-0.036243	-0.156375
H	-1.897742	-0.356084	-1.734957
O	-2.835997	2.465442	-1.241001
H	-1.863973	2.711775	-1.234784
H	-2.899293	1.940232	-0.399305
O	0.999594	-3.588499	-0.311337
H	0.970291	-2.815121	-0.954451
H	0.118927	-3.496354	0.149073
O	0.387218	-1.330500	2.412579
H	0.490247	-0.372675	2.152857
H	1.287844	-1.734771	2.183828
O	-2.218808	0.568305	-3.031488
H	-2.544416	1.327074	-2.443667
H	-1.306358	0.845801	-3.285305
O	-1.357424	-2.715806	0.930056
H	-0.702641	-2.160526	1.461943
H	-1.554565	-2.121303	0.147650
O	0.656267	0.974372	-3.088708
H	0.715764	0.054794	-2.680638
H	1.615727	1.291593	-2.961557
O	-3.080190	-1.127119	2.471896
H	-2.623519	-1.851901	1.962124
H	-2.480069	-1.005260	3.275084
O	2.714520	-0.014015	-0.092905
H	2.873635	-0.843822	0.456778
H	2.212233	0.586410	0.519175
O	-0.148034	2.623920	-1.213624
H	0.121280	1.920944	-1.909709
H	0.011775	2.195029	-0.330164
O	3.109811	1.636126	-2.312463
H	3.166728	0.958179	-1.590591
H	2.901015	2.474077	-1.790878
O	2.558437	-2.278417	1.302455
H	3.249853	-2.824793	1.725553
H	2.021360	-2.906525	0.683970
O	-1.266675	-0.726168	4.413294
H	-1.136641	0.243966	4.413946
H	-0.524628	-1.049024	3.823189
O	2.275219	3.741545	-0.850435
H	2.376144	3.418657	0.070848
H	1.319210	3.500609	-1.042466
O	0.864068	-1.224330	-1.598361
H	1.541573	-0.743806	-1.025130
H	-0.038546	-0.984039	-1.190885
Br	0.713467	1.808210	1.798556

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O	-2.385049	0.972752	1.111594
H	-2.716353	0.178155	1.681752
H	-1.529319	1.241661	1.533138
O	-1.573747	-0.675079	-0.771581
H	-1.844948	0.011059	-0.072814
H	-1.886562	-0.284054	-1.647133
O	-2.622287	2.609102	-1.114459
H	-1.647211	2.837888	-1.044638
H	-2.753326	2.066617	-0.290925
O	0.807481	-3.705045	-0.619525
H	0.838114	-2.822491	-1.099013
H	-0.047296	-3.622225	-0.118149
O	0.460036	-1.666231	2.204653
H	0.562161	-0.708728	1.955761
H	1.347375	-2.097685	1.906451
O	-2.040558	0.805906	-2.910477
H	-2.730357	0.662376	-3.587952
H	-2.391329	1.548532	-2.294468
O	-1.494320	-2.822793	0.822474
H	-0.743131	-2.388061	1.342430
H	-1.654608	-2.152605	0.096572
O	0.638189	1.060380	-2.896050

H	-0.328083	1.007225	-3.157567
H	0.792550	0.160384	-2.460800
O	-2.991976	-1.133880	2.509525
H	-2.308817	-1.013563	3.242932
H	-2.597089	-1.862976	1.954090
O	3.275140	1.579640	-1.860689
H	2.482386	1.502274	-2.442886
H	3.082508	2.413932	-1.320537
O	0.066390	2.719316	-0.920780
H	0.328536	2.051355	-1.648132
H	0.163891	2.222941	-0.063501
O	2.830331	-0.160728	0.046942
H	2.378339	0.423840	0.708289
H	3.100047	0.483391	-0.705707
O	2.578311	-2.713905	1.142674
H	2.873130	-1.886081	0.680803
H	1.992298	-3.177492	0.458093
O	-0.974985	-0.761635	4.264853
H	-0.718327	0.171685	4.103170
H	-0.330147	-1.247689	3.672794
O	2.527486	3.646693	-0.343129
H	2.527612	3.258912	0.558771
H	1.569464	3.516508	-0.612077
O	0.879716	-1.150200	-1.455631
H	1.571651	-0.800356	-0.805867
H	-0.027642	-0.912427	-1.059123
Br	0.768041	1.543030	2.017361

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O	-2.437369	0.924114	1.044659
H	-2.786878	0.126924	1.598373
H	-1.601734	1.199700	1.498822
O	-1.598356	-0.729600	-0.842645
H	-1.865246	-0.047451	-0.143273
H	-1.885968	-0.318193	-1.733421
O	-2.703680	2.541442	-1.206742
H	-1.744246	2.801642	-1.128890
H	-2.818298	1.993911	-0.385118
O	0.757508	-3.768219	-0.617977
H	0.801791	-2.892721	-1.110341
H	-0.109291	-3.677170	-0.139400
O	0.333557	-1.681074	2.174796
H	0.436833	-0.724356	1.925437
H	1.227937	-2.114134	1.897931
O	-2.107020	0.630912	-3.018352
H	-1.149117	0.818807	-3.208536
H	-2.392330	1.403551	-2.432126
O	-1.578745	-2.864598	0.757469
H	-0.844644	-2.419894	1.292804
H	-1.722243	-2.194071	0.026315
O	0.721829	0.993774	-2.973043
H	0.429969	1.569026	-2.198193
H	0.795675	0.081139	-2.549029
O	-3.106067	-1.183210	2.417666
H	-2.442701	-1.064588	3.168996
H	-2.699168	-1.911551	1.869549
O	3.250253	1.481060	-1.885008
H	2.434538	1.333176	-2.443022
H	3.048269	2.333956	-1.412385
O	-0.017448	2.579479	-0.946726
H	0.039814	2.112161	-0.068645
H	0.760933	3.205968	-0.862551
O	2.766152	-0.202115	0.060523
H	2.295217	0.384630	0.705940
H	3.060509	0.432357	-0.691205
O	2.474586	-2.732295	1.171744
H	2.775028	-1.909698	0.702905
H	1.907436	-3.211937	0.482786
O	-1.133330	-0.813643	4.223003
H	-0.881053	0.125607	4.095643
H	-0.474664	-1.281773	3.630851
O	2.372729	3.607729	-0.388092
H	2.670680	4.539944	-0.406664
H	2.343341	3.371971	0.565811
O	0.853287	-1.229789	-1.492095
H	1.532451	-0.864273	-0.840103
H	-0.060807	-0.983465	-1.111319
Br	0.696320	1.531931	2.018597

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O	-2.049634	0.962596	1.439202
H	-2.360894	0.166822	2.027225
H	-1.137530	1.181706	1.760245
O	-1.701860	-0.654799	-0.639863
H	-1.770922	0.011330	0.116898
H	-2.113238	-0.188737	-1.447883
O	-2.643963	2.599486	-0.572478
H	-3.152579	3.407375	-0.362643
H	-2.623315	2.057407	0.273465
O	0.609470	-3.748344	-0.828312
H	0.588256	-2.870523	-1.317223
H	-0.160428	-3.644747	-0.208035

O	0.741134	-1.706206	2.041659
H	0.870499	-0.739425	1.850641
H	1.557190	-2.165826	1.609883
O	-2.484210	0.824107	-2.669560
H	-1.551179	0.992907	-2.981584
H	-2.667718	1.585000	-2.055093
O	-1.425658	-2.791866	0.932880
H	-0.601827	-2.363373	1.331810
H	-1.684993	-2.123466	0.234346
O	0.285097	1.095875	-3.030842
H	0.173921	1.632961	-2.182862
H	0.426226	0.162089	-2.678237
O	-2.616570	-1.129270	2.849087
H	-1.840561	-1.078152	3.494767
H	-2.333552	-1.855068	2.223517
O	2.988400	1.482399	-2.342418
H	2.096445	1.388226	-2.776434
H	2.879656	2.319133	-1.789188
O	-0.023654	2.605175	-0.860168
H	-1.011244	2.794299	-0.751584
H	0.232862	2.161586	-0.005970
O	2.742116	-0.259626	-0.417898
H	2.411614	0.323789	0.312944
H	2.939897	0.393893	-1.189387
O	2.640576	-2.805208	0.666413
H	2.869135	-1.971041	0.176448
H	1.948074	-3.247833	0.075008
O	-0.381402	-0.950887	4.334822
H	-0.109739	-0.012315	4.258290
H	0.170023	-1.386195	3.619614
O	2.474713	3.576425	-0.723817
H	2.591628	3.173092	0.164216
H	1.486696	3.498699	-0.842454
O	0.609674	-1.206203	-1.702630
H	1.378639	-0.871082	-1.138786
H	-0.232162	-0.957339	-1.188852
Br	1.183507	1.510465	1.921516

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O	-1.318212	-2.427814	1.981897
H	-2.103967	-2.434909	1.385222
H	-0.646028	-1.991729	1.413951
O	0.189289	-1.111983	-3.573117
H	-0.594263	-0.641497	-3.218313
H	-0.096892	-1.438752	-4.441932
O	3.243470	2.946059	0.915000
H	3.492258	2.184597	1.498389
H	3.350267	2.595930	0.008252
O	0.200681	-1.005177	0.164993
H	0.386897	-1.766945	-0.472917
H	-0.509049	-0.502747	-0.286106
O	-1.880478	3.682028	1.206155
H	-0.944115	3.385074	1.281040
H	-1.997351	3.841572	0.237295
O	0.181327	2.170830	-1.441961
H	-0.412737	1.424013	-1.655150
H	0.249193	2.193878	-0.444073
O	3.664762	0.685197	2.430420
H	3.540873	0.182183	1.589765
H	2.774414	0.601479	2.826579
O	-1.382553	-4.292290	-0.385866
H	-1.041360	-4.229813	0.523313
H	-2.217093	-3.782604	-0.322584
O	0.610659	-2.930415	-1.563858
H	-0.145804	-3.511006	-1.284938
H	0.343482	-2.446955	-2.381625
O	0.911560	0.273319	2.652863
H	0.843535	-0.331938	1.890385
H	0.005793	0.205889	3.067411
O	-3.364730	-2.401832	0.140633
H	-3.092479	-1.714021	-0.501661
H	-3.940918	-1.906327	0.782482
O	-2.939503	1.260312	1.233971
H	-2.718374	0.987663	0.320240
H	-2.637113	2.216019	1.292334
O	2.842488	1.639194	-1.655990
H	2.943291	0.991897	-2.410503
H	1.882391	1.871438	-1.682271
O	2.907717	-0.382631	0.054866
H	1.945860	-0.565931	0.120891
H	2.941134	0.392249	-0.575767
O	2.843702	-0.330559	-3.445772
H	1.883584	-0.489387	-3.579874
H	3.114973	-1.120922	-2.915813
O	-4.564638	-0.809766	1.954232
H	-4.159219	0.056038	1.715550
H	-4.165035	-1.008483	2.816402

O	-2.091856	3.767037	-1.525299
H	-1.202205	3.363795	-1.648918
H	-2.685347	3.022457	-1.721196
O	3.348944	-2.449057	-1.732217
H	2.449149	-2.835424	-1.678777
H	3.339028	-1.788632	-1.001279
O	0.588481	2.474708	1.145123
H	1.525984	2.808433	1.085440
H	0.669327	1.680671	1.735587
O	-1.658087	-0.038917	3.283866
H	-1.611883	-0.969840	2.956055
H	-2.058537	0.448970	2.523867
Br	-2.324572	0.091918	-1.810919

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O	-1.399889	-2.580107	2.083002
H	-2.310062	-2.226847	1.934779
H	-0.849891	-2.022944	1.487847
O	-0.054484	-1.102243	-3.455837
H	-0.802495	-0.573043	-3.104949
H	-0.362957	-1.418519	-4.320788
O	3.329064	2.974252	0.830504
H	3.590574	2.201278	1.393338
H	3.402315	2.637828	-0.084197
O	0.041360	-0.973544	0.279207
H	0.220485	-1.732918	-0.364548
H	-0.644314	-0.443989	-0.175506
O	-1.806416	3.661351	1.364239
H	-0.850517	3.423516	1.374531
H	-1.993268	3.825765	0.406938
O	0.177523	2.297854	-1.425884
H	-0.428601	1.563634	-1.648700
H	0.281756	2.270903	-0.432544
O	3.791967	0.679047	2.270773
H	3.576201	0.202579	1.434697
H	2.930020	0.608866	2.730938
O	-1.501025	-4.241429	-0.229790
H	-1.358701	-3.936696	0.690999
H	-2.306811	-3.722626	-0.488093
O	0.431045	-2.903322	-1.442384
H	-0.300076	-3.501792	-1.110754
H	0.119864	-2.438030	-2.253821
O	1.098096	0.301313	2.665195
H	0.943489	-0.302794	1.914169
H	0.280848	0.160761	3.220301
O	-3.616942	-2.607621	-0.816661
H	-3.252022	-1.876709	-1.350341
H	-3.815051	-2.158806	0.035837
O	-2.404878	1.093359	1.486163
H	-2.292876	0.904150	0.531967
H	-2.307502	2.090573	1.535724
O	2.817539	1.725932	-1.771827
H	2.842862	1.046426	-2.504301
H	1.871196	2.009195	-1.766954
O	2.732377	-0.292685	-0.056890
H	1.768857	-0.449095	0.040294
H	2.792668	0.494417	-0.669019
O	2.596549	-0.293141	-3.501749
H	1.626449	-0.436897	-3.564719
H	2.883270	-1.084163	-2.981115
O	-3.772520	-1.251857	1.621878
H	-3.513343	-0.302409	1.656425
H	-4.463232	-1.357998	2.294071
O	-2.153571	3.855854	-1.349471
H	-1.255531	3.494909	-1.525066
H	-2.717961	3.084631	-1.532388
O	3.136901	-2.404246	-1.790116
H	2.241690	-2.792981	-1.688669
H	3.142320	-1.717028	-1.084181
O	0.677965	2.510710	1.160420
H	1.613316	2.837848	1.059232
H	0.775351	1.727487	1.762158
O	-1.302901	-0.165946	3.649025
H	-1.335651	-1.106785	3.379442
H	-1.689369	0.301586	2.870555
Br	-2.409581	0.347716	-1.709741

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O	-1.436666	-2.477135	2.146537
H	-2.279543	-2.187257	1.727922
H	-0.760332	-1.902538	1.722776
O	-0.338557	-1.275274	-3.086015
H	-1.009858	-0.696563	-2.671385
H	-0.735266	-1.549163	-3.929045
O	3.541416	3.217757	0.021877
H	3.753451	2.629171	0.788763
H	3.526931	2.610612	-0.746804
O	0.277021	-0.978484	0.544277
H	0.357988	-1.783454	-0.064326
H	-0.372475	-0.407679	0.079352
O	-1.528962	3.787804	1.305401
H	-0.567814	3.672024	1.128819

H	-1.896053	3.812079	0.387452
O	0.188379	2.270119	-1.931188
H	-0.447463	1.531595	-1.894452
H	0.383810	2.463017	-0.968953
O	3.749760	1.418975	2.076333
H	3.628993	0.672186	1.443562
H	2.867806	1.465716	2.491737
O	-1.380037	-4.442476	0.148629
H	-1.317085	-3.934676	0.988638
H	-2.161291	-4.025628	-0.293025
O	0.411350	-2.968494	-1.110696
H	-0.243211	-3.627007	-0.733848
H	0.015438	-2.543196	-1.908505
O	0.921937	0.932398	2.437529
H	0.907412	0.092992	1.937922
H	-0.044410	1.121195	2.551439
O	-3.413716	-2.977982	-0.932828
H	-3.016896	-2.183600	-1.333869
H	-3.796691	-2.621587	-0.106018
O	-1.754160	1.329028	2.238001
H	-1.949743	0.905551	1.378911
H	-1.793716	2.303764	1.987846
O	2.796390	1.364904	-1.941002
H	2.807698	0.619832	-2.608339
H	1.877459	1.711540	-2.032104
O	2.983908	-0.372291	0.101210
H	2.045300	-0.572385	0.308324
H	2.917258	0.309666	-0.624477
O	2.440273	-0.754566	-3.459916
H	1.463747	-0.828814	-3.422404
H	2.740477	-1.483390	-2.854832
O	-3.912068	-1.418441	1.342814
H	-3.715127	-0.644635	0.782687
H	-3.822332	-1.088578	2.272713
O	-2.255085	3.716873	-1.367921
H	-1.383402	3.455168	-1.732202
H	-2.735446	2.870061	-1.376962
O	3.068803	-2.584681	-1.578412
H	2.163320	-2.911863	-1.377718
H	3.206853	-1.879692	-0.906080
O	0.926030	2.854497	0.518682
H	1.865796	3.148423	0.358152
H	1.000057	2.118663	1.177415
O	-2.975508	-0.608871	3.783963
H	-2.292325	-1.284731	3.611483
H	-2.582337	0.208859	3.401878
Br	-2.331592	0.332314	-0.980133
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O	-1.574704	-2.584574	1.806016
H	-2.450423	-2.229850	1.517483
H	-0.932238	-2.036128	1.305781
O	0.579927	-0.850446	-3.536746
H	-0.218023	-0.371358	-3.228643
H	0.354312	-1.158698	-4.429509
O	3.021140	2.919856	1.377970
H	3.197342	2.146476	1.976784
H	3.242337	2.581158	0.488335
O	0.194761	-1.014033	0.258460
H	0.447392	-1.728540	-0.409344
H	-0.389811	-0.423109	-0.261198
O	-2.091419	3.595563	1.172041
H	-1.156166	3.338513	1.349307
H	-2.094161	3.800925	0.205193
O	0.425001	2.368189	-1.295178
H	-0.180383	1.673337	-1.625276
H	0.325051	2.340484	-0.302337
O	3.292634	0.641394	2.844056
H	3.329474	0.123241	2.004528
H	2.356170	0.507479	3.102663
O	-1.478948	-3.926602	-0.791453
H	-1.452214	-3.740843	0.168897
H	-2.283349	-3.426878	-1.090944
O	0.770395	-2.796524	-1.583450
H	-0.072026	-3.310060	-1.412945
H	0.616092	-2.229072	-2.375296
O	0.582130	0.194187	2.773078
H	0.533891	-0.391986	1.992107
H	-0.309771	0.078673	3.207824
O	-3.696804	-2.462436	-1.435183
H	-3.300437	-1.693022	-1.885396
H	-3.922891	-2.091977	-0.551377
O	-2.816157	1.054340	1.222812
H	-2.465999	0.817218	0.339216
H	-2.691450	2.050253	1.254682
O	3.024394	1.587074	-1.213602
H	3.214881	0.974053	-1.979272
H	2.089643	1.875909	-1.356261
O	2.940902	-0.481598	0.411327
H	1.978484	-0.670341	0.417177
H	3.000718	0.331633	-0.169609
O	3.252234	-0.288532	-3.085762

H	2.305793	-0.389470	-3.326371
H	3.433935	-1.106391	-2.556967
O	-3.941378	-1.412419	1.123134
H	-3.836584	-0.437286	1.200635
H	-4.715870	-1.635599	1.662600
O	-1.923620	3.922764	-1.569224
H	-0.993149	3.610761	-1.608309
H	-2.408779	3.138260	-1.878773
O	3.525861	-2.455866	-1.430997
H	2.611137	-2.805300	-1.492761
H	3.461950	-1.832195	-0.670217
O	0.384298	2.483898	1.373522
H	1.328492	2.803215	1.419465
H	0.395140	1.652387	1.915287
O	-1.932338	-0.177903	3.479665
H	-1.935520	-1.115799	3.205728
H	-2.262846	0.294930	2.675176
Br	-2.017276	0.354800	-1.903129

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O	-1.477666	-2.689723	1.923374
H	-2.326225	-2.352476	1.549802
H	-0.825225	-2.110788	1.476253
O	-0.331713	-1.257226	-3.467582
H	0.553700	-0.818080	-3.494234
H	-0.926975	-0.588722	-3.079689
O	3.410062	2.905209	1.143192
H	3.597613	2.100846	1.691679
H	3.552930	2.611997	0.224299
O	-0.032807	-0.852079	0.326319
H	0.083434	-1.613383	-0.331370
H	-0.738708	-0.298680	-0.068910
O	-1.405931	3.966876	1.638486
H	-0.525978	3.523488	1.604137
H	-1.630651	4.103823	0.686066
O	0.291620	2.378885	-1.284247
H	-0.305842	1.658130	-1.563392
H	0.381724	2.277132	-0.294232
O	3.572283	0.528710	2.489618
H	3.380527	0.121768	1.610740
H	2.698763	0.449400	2.922541
O	-1.432766	-4.537801	-0.307046
H	-1.431160	-4.090986	0.566295
H	-2.159364	-4.080000	-0.798266
O	0.279938	-2.786384	-1.369464
H	-0.309485	-3.538272	-1.084523
H	-0.059370	-2.387900	-2.216336
O	0.820621	0.100600	2.825686
H	0.679295	-0.408616	2.002504
H	-0.074757	0.036316	3.261434
O	-3.241899	-2.947763	-1.591923
H	-2.776018	-2.225693	-2.045243
H	-3.575421	-2.509537	-0.777290
O	-2.564161	1.547062	1.669363
H	-2.470435	1.334865	0.722895
H	-2.176089	2.460322	1.750965
O	2.932478	1.811426	-1.649133
H	2.882187	1.147729	-2.378586
H	2.001223	2.141253	-1.619033
O	2.658917	-0.242062	0.040482
H	1.683866	-0.338885	0.116549
H	2.793107	0.556345	-0.539921
O	2.255801	-0.279558	-3.319356
H	2.584709	-1.081823	-2.819690
H	2.672538	-0.342173	-4.193745
O	-3.655296	-1.560188	0.751950
H	-3.518108	-0.700202	0.309285
H	-4.520190	-1.496949	1.187932
O	-1.918386	4.024727	-1.048013
H	-1.062670	3.591814	-1.271936
H	-2.556998	3.308351	-1.205753
O	2.929202	-2.318482	-1.724949
H	2.027623	-2.689733	-1.585612
H	2.999823	-1.656519	-0.997535
O	0.768559	2.367711	1.318126
H	1.716764	2.669949	1.297239
H	0.755841	1.582117	1.922843
O	-1.738423	-0.198239	3.530054
H	-1.797759	-1.101577	3.164348
H	-2.074588	0.399584	2.810619
Br	-2.429874	0.528016	-1.530579

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O	-1.335281	-2.460474	1.813284
H	-2.145592	-2.344418	1.216914
H	-0.642443	-1.960414	1.297787
O	0.123052	-1.304190	-3.502894
H	-0.621679	-0.748075	-3.152532
H	-0.211342	-1.646480	-4.357114
O	3.161701	2.986988	0.808748
H	3.385500	2.227998	1.443297
H	3.279038	2.578550	-0.083377

O	0.336580	-1.011401	0.184280
H	0.485107	-1.824806	-0.464549
H	-0.340186	-0.471443	-0.305873
O	-1.967152	3.553071	1.295359
H	-0.983391	3.383017	1.362890
H	-2.076409	3.701290	0.303183
O	0.331545	2.355823	-1.418271
H	-0.250586	1.577120	-1.611008
H	0.365685	2.397106	-0.390571
O	3.495703	0.836776	2.370825
H	3.473172	0.264698	1.546027
H	2.559086	0.723191	2.684794
O	-1.356480	-4.296019	-0.283378
H	-1.164011	-3.948427	0.627488
H	-2.221285	-3.847622	-0.446633
O	0.591249	-2.938178	-1.452555
H	-0.172070	-3.532774	-1.135962
H	0.301745	-2.478825	-2.299361
O	0.781344	0.407486	2.511778
H	0.735225	-0.210450	1.737393
H	-0.081430	0.180242	3.020676
O	-3.340032	-2.293667	0.055564
H	-3.023617	-1.614885	-0.592442
H	-3.984418	-1.760888	0.634516
O	-2.705867	1.084533	1.433342
H	-2.423462	0.785987	0.532695
H	-2.484233	2.100018	1.425427
O	2.889437	1.554664	-1.687527
H	2.898649	0.874468	-2.450643
H	1.936279	1.873405	-1.677188
O	3.009887	-0.419090	0.037699
H	2.037196	-0.613255	0.138769
H	2.993321	0.381849	-0.599645
O	2.739398	-0.391324	-3.463123
H	1.768965	-0.573485	-3.578571
H	3.021715	-1.183975	-2.903198
O	-4.698677	-0.686461	1.659892
H	-4.087984	0.109800	1.607063
H	-4.538422	-1.028242	2.562653
O	-2.051147	3.711047	-1.391492
H	-1.111051	3.397443	-1.522824
H	-2.554683	2.897700	-1.614126
O	3.303837	-2.415931	-1.767988
H	2.401150	-2.814199	-1.660629
H	3.328491	-1.750489	-1.018510
O	0.573405	2.659590	1.144429
H	1.556758	2.927274	1.064483
H	0.601357	1.808056	1.697710
O	-1.558782	-0.281966	3.436647
H	-1.529182	-1.186653	3.006299
H	-2.007507	0.263549	2.718809
Br	-2.087061	0.222311	-1.672966

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O	-1.422950	-2.382261	1.964635
H	-2.346013	-2.025259	1.781496
H	-0.828335	-1.836865	1.375962
O	-0.031451	-1.259703	-3.435791
H	-0.732369	-0.657694	-3.068740
H	-0.401521	-1.579917	-4.283793
O	3.202217	2.998278	0.694429
H	3.466941	2.238866	1.313615
H	3.275328	2.589798	-0.202483
O	0.263052	-0.970186	0.274952
H	0.389322	-1.790709	-0.377574
H	-0.375123	-0.399767	-0.232642
O	-1.903095	3.537920	1.510813
H	-0.915858	3.375497	1.515787
H	-2.065223	3.696424	0.527226
O	0.293400	2.429442	-1.400676
H	-0.304036	1.663498	-1.598651
H	0.358041	2.435673	-0.375190
O	3.658590	0.848976	2.221938
H	3.565084	0.270922	1.406336
H	2.745748	0.740643	2.602793
O	-1.575744	-4.052204	-0.249623
H	-1.452862	-3.676258	0.665226
H	-2.397536	-3.545069	-0.554013
O	0.452102	-2.891393	-1.369131
H	-0.352165	-3.439315	-1.021300
H	0.163761	-2.425381	-2.210599
O	0.972899	0.429571	2.532101
H	0.825682	-0.191315	1.770827
H	0.166542	0.222883	3.128821
O	-3.685309	-2.543332	-0.930657
H	-3.256125	-1.794309	-1.409983
H	-3.905088	-2.104183	-0.061977
O	-2.517777	1.033531	1.629378
H	-2.193037	0.804007	0.722976
H	-2.379998	2.062383	1.651743
O	2.817317	1.547595	-1.771623
H	2.787865	0.856743	-2.525121

H	1.875368	1.894780	-1.729625
O	2.958920	-0.425185	-0.043683
H	1.990012	-0.590852	0.116478
H	2.935975	0.366339	-0.692035
O	2.598811	-0.426567	-3.505062
H	1.620480	-0.587663	-3.586966
H	2.877862	-1.219959	-2.944679
O	-3.843602	-1.271698	1.491174
H	-3.612281	-0.301107	1.589865
H	-4.499577	-1.459726	2.191912
O	-2.120714	3.738793	-1.167388
H	-1.181419	3.473068	-1.377664
H	-2.600698	2.907426	-1.379723
O	3.156234	-2.460135	-1.809984
H	2.244989	-2.825714	-1.659643
H	3.223566	-1.777560	-1.078468
O	0.628914	2.663093	1.164220
H	1.602509	2.942826	1.033041
H	0.707559	1.816759	1.720809
O	-1.272795	-0.208912	3.686276
H	-1.281604	-1.137822	3.326618
H	-1.773910	0.277732	2.961899
Br	-2.135391	0.309085	-1.555211

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O	-1.492042	-2.312405	2.068190
H	-2.333550	-2.042982	1.602470
H	-0.784777	-1.780574	1.606229
O	-0.321725	-1.528001	-3.040818
H	-0.983458	-0.887777	-2.676246
H	-0.741431	-1.874011	-3.855045
O	3.508200	3.115092	0.073489
H	3.695884	2.461948	0.821780
H	3.454070	2.546338	-0.735739
O	0.335520	-1.012467	0.478256
H	0.466328	-1.880127	-0.103630
H	-0.360611	-0.506722	-0.023356
O	-1.444371	3.870886	1.428133
H	-0.468232	3.736510	1.260339
H	-1.803439	3.871692	0.484602
O	0.163643	2.353030	-1.704820
H	-0.424224	1.559305	-1.650450
H	0.422985	2.534263	-0.728050
O	3.643577	1.251873	2.010619
H	3.467372	0.567301	1.293029
H	2.754036	1.310132	2.433595
O	-1.256613	-4.371445	0.244126
H	-1.256424	-3.806161	1.067974
H	-2.059158	-3.988733	-0.230758
O	0.566234	-3.045482	-1.021391
H	-0.120656	-3.679150	-0.578243
H	0.129828	-2.655531	-1.835280
O	0.828965	0.872811	2.407045
H	0.813924	0.053119	1.849636
H	-0.157818	1.087910	2.462972
O	-3.311676	-3.031350	-0.849035
H	-2.898300	-2.240327	-1.264048
H	-3.721282	-2.631238	-0.037160
O	-1.775807	1.399903	2.117514
H	-1.946565	1.017465	1.221395
H	-1.746376	2.419343	1.919832
O	2.686302	1.414990	-2.053302
H	2.619685	0.621113	-2.696656
H	1.750567	1.777281	-2.041179
O	2.905343	-0.275219	-0.052391
H	1.956570	-0.501735	0.161805
H	2.816321	0.423833	-0.792335
O	2.334014	-0.755346	-3.498961
H	1.357186	-0.924164	-3.434288
H	2.711011	-1.456164	-2.873165
O	-3.992633	-1.395084	1.276299
H	-3.775694	-0.633132	0.690287
H	-3.832020	-1.027855	2.212071
O	-2.195037	3.678112	-1.159977
H	-1.313049	3.378188	-1.519204
H	-2.687399	2.827339	-1.138906
O	3.189435	-2.483441	-1.620382
H	2.309893	-2.886238	-1.388292
H	3.243857	-1.723998	-0.970255
O	0.972659	2.924765	0.690105
H	1.949208	3.143718	0.474370
H	1.016428	2.121203	1.300118
O	-3.048216	-0.490225	3.572222
H	-2.335320	-1.160706	3.418957
H	-2.642240	0.333310	3.172303
Br	-2.253009	0.246672	-1.026811

61

O	-1.709301	-2.457925	1.613359
H	-2.593566	-2.086037	1.309820
H	-1.031965	-1.896863	1.138174
O	0.472017	-1.116451	-3.436019

H	-0.279114	-0.534229	-3.142821
H	0.228310	-1.394557	-4.342499
O	3.068943	2.947031	1.294634
H	3.233522	2.170413	1.926427
H	3.262723	2.558013	0.406679
O	0.208954	-0.986776	0.279806
H	0.449118	-1.770563	-0.384226
H	-0.328826	-0.382772	-0.299447
O	-2.129157	3.458403	1.328239
H	-1.153418	3.308258	1.487504
H	-2.138200	3.670792	0.342319
O	0.483699	2.497119	-1.213960
H	-0.090688	1.748287	-1.519899
H	0.407510	2.467858	-0.188994
O	3.270717	0.745688	2.810072
H	3.314533	0.201641	1.968561
H	2.305950	0.628291	3.026661
O	-1.493241	-4.047161	-0.660070
H	-1.536965	-3.697158	0.272565
H	-2.240853	-3.518177	-1.092979
O	0.685592	-2.829563	-1.396829
H	-0.150481	-3.399712	-1.196385
H	0.516259	-2.333910	-2.253986
O	0.575488	0.335974	2.669230
H	0.558583	-0.246741	1.865813
H	-0.308966	0.090875	3.127163
O	-3.461223	-2.496164	-1.612511
H	-2.978129	-1.720309	-1.984805
H	-3.811829	-2.104304	-0.764054
O	-2.742655	0.947144	1.280712
H	-2.286560	0.745697	0.425129
H	-2.620864	1.974904	1.344145
O	3.022957	1.591142	-1.242797
H	3.113696	0.934970	-2.024010
H	2.087879	1.947015	-1.335839
O	2.929814	-0.435939	0.408893
H	1.952755	-0.627209	0.422245
H	2.973937	0.389791	-0.197426
O	3.086758	-0.282514	-3.087193
H	2.131520	-0.441512	-3.314127
H	3.290427	-1.098592	-2.525431
O	-4.032661	-1.334416	0.799451
H	-3.825791	-0.371547	0.987874
H	-4.790214	-1.558739	1.375871
O	-1.911761	3.840638	-1.334761
H	-0.956000	3.554081	-1.384433
H	-2.363703	3.042658	-1.687847
O	3.417109	-2.372562	-1.414651
H	2.497321	-2.747932	-1.416940
H	3.369710	-1.736353	-0.641247
O	0.456750	2.640636	1.377682
H	1.443791	2.905806	1.397261
H	0.444285	1.766671	1.893794
O	-1.800157	-0.380227	3.440240
H	-1.750538	-1.281987	3.016621
H	-2.189110	0.160577	2.686139
Br	-1.883512	0.404665	-1.831470

61

O	-1.593846	-2.436178	1.743786
H	-2.497781	-2.056860	1.516521
H	-0.957873	-1.887318	1.202173
O	-0.039813	-1.430462	-3.568400
H	0.845905	-0.952270	-3.572735
H	-0.652851	-0.768320	-3.164979
O	3.223217	2.881505	1.103982
H	3.412372	2.062297	1.673346
H	3.337539	2.546294	0.184066
O	0.216277	-1.013866	0.201876
H	0.360118	-1.825672	-0.468990
H	-0.364769	-0.405462	-0.332744
O	-1.954608	3.509957	1.600728
H	-0.969772	3.351998	1.664531
H	-2.055382	3.731335	0.621454
O	0.401006	2.574312	-1.196066
H	-0.183900	1.816526	-1.460389
H	0.418921	2.533383	-0.167458
O	3.483564	0.605498	2.484657
H	3.453473	0.089146	1.626319
H	2.532625	0.506412	2.765746
O	-1.633435	-4.094589	-0.482132
H	-1.569039	-3.723191	0.440686
H	-2.387948	-3.531210	-0.853987
O	0.471049	-2.902732	-1.451568
H	-0.329985	-3.474678	-1.148484
H	0.195377	-2.431080	-2.314827
O	0.780155	0.295108	2.548199
H	0.666698	-0.282862	1.747239
H	-0.056656	0.071669	3.096804
O	-3.562176	-2.422922	-1.313281
H	-3.066537	-1.665665	-1.707433
H	-3.859423	-2.018202	-0.450740

O -2.611870 1.014387 1.504100
H -2.222519 0.837408 0.610853
H -2.457560 2.034927 1.609033
O 2.885323 1.618460 -1.521431
H 2.830391 0.992695 -2.306703
H 1.958732 2.012359 -1.483080
O 2.919004 -0.477904 0.074834
H 1.939108 -0.642008 0.171014
H 2.938950 0.366949 -0.499118
O 2.424379 -0.339789 -3.318626
H 2.768927 -1.165177 -2.807580
H 2.913903 -0.352981 -4.165898
O -3.949127 -1.258087 1.131924
H -3.712388 -0.298501 1.299788
H -4.671273 -1.465514 1.757858
O -2.004269 3.887117 -1.065070
H -1.056429 3.610708 -1.221489
H -2.484169 3.085976 -1.371456
O 3.135356 -2.363736 -1.827235
H 2.247610 -2.791811 -1.684635
H 3.205908 -1.752167 -1.032266
O 0.610832 2.655244 1.385411
H 1.602443 2.893477 1.338601
H 0.616522 1.755797 1.858650
O -1.521638 -0.357183 3.562154
H -1.519875 -1.266106 3.151636
H -1.970712 0.176223 2.835873
Br -1.983851 0.471285 -1.677556

Mg – 1 water molecule

4

O 0.027338 0.036568 0.130447
H 0.695769 -0.408330 0.677774
H -0.634964 0.412712 0.733786
Mg -0.102240-0.046487 -1.801623
4

O -0.051141 -0.026161 -0.141138
H -0.011038 -0.946119 -0.452598
H 0.250306 0.538384 -0.871974
Mg -0.2022410.506604 1.717885
4

O 0.018008 0.022677 0.128123
H -0.541032 0.576628 0.698527
H 0.669455 -0.418408 0.697928
Mg -0.192294-0.205960 -1.784202
4

O 0.100730 0.050445 -0.142960
H 0.617341 -0.706682 -0.466215
H 0.737490 0.728849 0.138308
Mg -1.703534-0.096017 0.566990
4

O 0.038622 -0.112630 -0.052641
H -0.439312 -0.958124 -0.017507
H 0.768563 -0.216091 -0.685784
Mg -0.4444571.513021 0.881607
4

O 0.010015 0.007544 0.132337
H 0.706729 -0.399347 0.685778
H -0.631478 0.426198 0.741098
Mg -0.099363-0.039931 -1.818828
4

O -0.130248 -0.023444 -0.166601
H 0.019318 -0.950006 -0.447281
H 0.279617 0.537238 -0.857409
Mg -0.1828020.508920 1.723465
4

O -0.098491 -0.114279 0.178053
H -0.496989 0.627603 0.679232
H 0.711478 -0.364162 0.669735
Mg -0.161862-0.174226 -1.786644
4

O 0.096604 0.064628 -0.175639
H 0.622487 -0.713223 -0.455560
H 0.742832 0.725050 0.150106
Mg -1.709896-0.099861 0.577216
4

O 0.041122 -0.113507 -0.052200
H -0.440420 -0.964480 -0.020030
H 0.772732 -0.222732 -0.692435
Mg -0.4500191.526894 0.890339

Mg – 2 water molecules

7

O -0.007934 0.146052 1.960571
H -0.755138 -0.113514 2.525705
H 0.798865 -0.091948 2.448549
O -0.149905 -0.009384 -1.961806
H 0.190780 -0.775429 -2.454344
H 0.020856 0.769397 -2.518510
Mg -0.0975270.074827 -0.000166
7

O 0.028805 -0.165051 1.961026
H 0.813933 0.124593 2.455896
H -0.333447 -0.929082 2.440809
O -0.227046 0.180950 -1.937909
H 0.433617 -0.180575 -2.552067
H -0.618655 0.954742 -2.377793
Mg -0.1056700.011383 0.010268
7

O 0.498453 1.743096 -0.757395
H 0.996594 1.762528 -1.592550
H -0.149607 2.466882 -0.813692
O -0.517042 -1.672220 0.847092
H -0.269548 -2.520037 0.440665
H -0.548513 -1.824542 1.806720
Mg -0.0096600.044915 0.070684
7

O 1.695760 -0.205027 -0.908723
H 2.509696 -0.622332 -0.582359
H 1.896604 0.187399 -1.774354
O -1.726250 0.039883 0.939013
H -2.551768 0.204222 0.452308
H -1.836298 0.447842 1.814855
Mg 0.008178 -0.068400 0.047323
7

O -0.806928 -0.471654 1.735993
H -1.388683 0.153233 2.201523
H -1.225801 -1.345251 1.822079
O 0.925823 0.569725 -1.614772
H 1.885085 0.650306 -1.748539
H 0.543752 0.339550 -2.478690
Mg 0.112918 0.052876 0.086291
7

O -0.059513 -0.185690 1.965689
H -0.661374 0.331934 2.539677
H 0.822604 -0.127913 2.388012
O -0.152194 -0.059964 -1.972493
H 0.481632 -0.613061 -2.474620
H -0.189495 0.797242 -2.445217
Mg -0.241664-0.142546 -0.001048
7

O 0.267081 -0.171683 1.945624
H -0.470901 0.206720 2.467378
H 0.500584 -1.013337 2.389236
O 0.002352 0.160160 -1.967987
H -0.828484 -0.163362 -2.374218
H 0.218054 0.992839 -2.437123
Mg 0.302852 -0.014377 -0.022679
7

O 0.510172 1.724021 -0.812277
H 0.804900 1.784822 -1.744069
H 0.040575 2.562196 -0.622866
O -0.512574 -1.721441 0.814854
H -0.043902 -2.553242 0.597122
H -0.792886 -1.806726 1.749165
Mg -0.0056090.010991 0.019594
7

O 1.805250 -0.076117 -0.813561
H 2.275025 -0.934697 -0.770895
H 1.951329 0.260443 -1.721901
O -1.758551 0.313965 0.817142
H -2.426296 -0.379439 0.635808
H -1.929674 0.614912 1.733449
Mg 0.078838 0.184522 0.108022
7

O -1.066899 -0.353185 1.627885
H -0.635167 -0.126013 2.477558
H -1.406600 -1.265173 1.740649
O 0.804110 0.512578 -1.717158

H 1.505942 1.194365 -1.760660
H 1.116468 -0.229663 -2.274722
Mg -0.2716910.215874 -0.089667

Mg – 4 water molecules

13

O -1.374685 -1.324484 -0.653158
H -1.148713 -2.251966 -0.831649
H -2.121015 -1.112474 -1.237726
O 1.781470 -0.573776 -0.597266
H 2.150019 -0.616724 -1.493763
H 2.416414 -1.022382 -0.016043
O -0.084694 0.004779 1.910592
H 0.411231 0.582849 2.511314
H -0.682587 -0.523497 2.463612
O -0.440468 1.883773 -0.634839
H -0.977189 2.506507 -0.118067
H 0.103798 2.422507 -1.232117
Mg -0.0335840.024889 -0.070889
13

O 2.020898 0.024190 -0.174242
H 2.502114 -0.812904 -0.284860
H 2.527033 0.688744 -0.669199
O -0.514321 -1.847423 0.165426
H -0.997087 -2.327677 -0.527494
H -0.805596 -2.237682 1.006402
O -0.840523 0.819164 -1.617988
H -1.266182 1.692295 -1.634102
H -1.344579 0.269144 -2.240727
O -0.370349 1.108182 1.630203
H 0.288782 1.365211 2.295132
H -1.238266 1.203725 2.053484
Mg 0.037433 0.056348 -0.001073
13

O 0.395645 -1.335602 1.436668
H -0.325592 -1.711689 1.969295
H 1.151591 -1.258682 2.042191
O 1.691558 0.058064 -0.992155
H 2.217143 -0.721879 -1.233821
H 1.909858 0.741297 -1.647404
O -0.466683 1.881453 0.489613
H 0.028319 2.440063 1.111011
H -0.986912 2.487953 -0.063029
O -1.628591 -0.820016 -0.802992
H -2.508173 -0.407653 -0.787470
H -1.601992 -1.367831 -1.604834
Mg -0.0194740.003947 0.024656
13

O 1.893541 -0.140227 -0.443653
H 2.249689 -0.568154 -1.239839
H 2.587878 -0.220071 0.230630
O -0.824556 -1.624513 0.909641
H -0.260130 -2.298679 1.324015
H -1.615758 -1.564213 1.470268
O -0.114828 1.664926 0.977513
H -0.626924 1.838085 1.783984
H 0.617366 2.303692 0.979404
O -0.988189 0.182620 -1.772771
H -1.621988 -0.461652 -2.127303
H -1.292785 1.053512 -2.077573
Mg -0.051747-0.046784 -0.030539
13

O 1.641761 0.598360 -0.514746
H 2.049201 1.427310 -0.214814
H 2.047915 0.393122 -1.372408
O 0.114716 -2.035949 -0.496801
H -0.615341 -2.641745 -0.701848
H 0.932615 -2.549363 -0.597539
O -1.559721 0.561595 -0.794009
H -1.808559 0.260724 -1.684091
H -1.816499 1.497971 -0.757116
O -0.237966 0.863174 1.904783
H -1.120836 0.977361 2.295367
H 0.365132 0.757100 2.658626
Mg -0.021913-0.198928 0.231424
13

O -1.357888 -1.234203 -0.719505
H -1.165079 -2.128054 -1.067312
H -2.166157 -0.937478 -1.184673
O 1.818820 -0.510633 -0.619409
H 1.995348 -0.972675 -1.463278
H 2.558981 -0.752036 -0.026161
O -0.201584 0.034039 2.026509

H 0.234753 0.663962 2.634339
H -0.394079 -0.762196 2.561785
O -0.280890 1.899585 -0.528056
H -1.044464 2.448174 -0.257600
H -0.005048 2.245599 -1.400630
Mg 0.007289 0.005920 0.043993
13

O 1.911612 -0.010615 -0.509132
H 2.405882 -0.820897 -0.748113
H 2.572369 0.591364 -0.110556
O -0.787751 -1.825840 0.236187
H -0.518832 -2.609307 -0.284194
H -1.058624 -2.171535 1.110840
O -1.037289 0.954249 -1.464275
H -1.953333 0.713879 -1.710743
H -0.610032 1.241887 -2.296749
O -0.352029 1.040460 1.652698
H 0.146609 0.936612 2.487398
H -0.693514 1.957403 1.660088
Mg -0.0257110.003656 -0.022487
13

O 0.332371 -1.126901 1.556036
H -0.361298 -1.455711 2.162542
H 1.149537 -1.080148 2.092186
O 1.687584 -0.050631 -1.077090
H 2.095636 -0.871035 -1.419454
H 1.973354 0.659416 -1.687083
O -0.284422 1.943051 0.450862
H -0.095332 2.276461 1.351535
H -1.062187 2.453319 0.144785
O -1.604022 -0.661074 -1.045346
H -2.418890 -1.009333 -0.631085
H -1.536519 -1.108847 -1.912893
Mg -0.0191170.020856 -0.043266
13

O 1.961604 -0.258524 -0.422320
H 2.324632 -0.051755 -1.307171
H 2.489768 -1.015503 -0.094730
O -0.665428 -1.507008 1.210186
H -1.260135 -2.215713 0.891006
H -0.870855 -1.398864 2.161021
O -0.139632 1.641523 1.116751
H -0.982897 1.970085 1.488114
H 0.381591 2.443494 0.908785
O -0.977209 -0.005825 -1.682600
H -0.521503 0.077135 -2.545359
H -1.818493 0.482454 -1.788436
Mg 0.030125 -0.042955 0.048534
13

O 1.690354 0.830423 -0.532930
H 2.566580 0.488851 -0.263071
H 1.821078 1.199396 -1.430347
O -0.008458 -1.972261 -0.246271
H -0.161815 -2.628196 0.463931
H 0.570331 -2.418191 -0.897334
O -1.518056 0.728034 -1.083174
H -1.823965 0.341241 -1.927924
H -1.834356 1.653213 -1.082052
O -0.419054 0.589167 1.911163
H -1.150958 0.238873 2.457489
H 0.277196 0.856507 2.545001
Mg -0.0383750.003677 0.042349

Mg – 8 water molecules

25

O 1.358843 -1.560724 -0.463652
H 2.213533 -1.129199 -0.708564
H 1.287582 -2.361196 -1.004270
O -0.520322 -0.080117 -2.315468
H -0.141989 -0.729031 -2.929191
H -0.405802 0.777041 -2.755011
O 3.357951 0.149698 -0.958143
H 3.689938 0.298999 -1.859032
H 4.143893 0.198124 -0.390172
O 1.092956 1.281906 -0.124880
H 0.836126 2.138730 -0.497752
H 2.000376 1.088282 -0.466889
O -0.200508 -0.590985 1.807673
H -0.746387 0.042673 2.333375
H 0.673918 -0.597203 2.225236
O -1.503201 -1.955155 -0.413315
H -2.266923 -1.976226 -1.010488
H -1.807184 -2.372015 0.408375
O -1.935826 1.248635 2.693110

H	-1.683042	2.096360	3.093905
H	-2.759289	0.991905	3.139186
O	-1.763814	1.108305	0.013827
H	-2.602653	1.007652	-0.461340
H	-2.005943	1.261327	0.961416
Mg	-0.259220	-0.288788	-0.251305

25

O	1.387104	1.022008	-2.499957
H	0.886988	0.767460	-3.292404
H	2.224160	1.376809	-2.842073
O	0.200904	2.129247	-0.402207
H	-0.448748	2.835478	-0.533948
H	0.610840	1.949088	-1.285174
O	-1.466364	-0.278658	-1.020693
H	-1.690699	-1.216224	-1.122288
H	-1.367730	0.058429	-1.923969
O	-2.055041	1.261359	1.316422
H	-2.050001	1.990942	1.954429
H	-2.800804	1.432538	0.720453
O	0.614723	1.203685	2.291209
H	1.224250	1.936625	2.108830
H	1.083444	0.630014	2.917344
O	1.393694	-0.467468	-0.216202
H	1.548192	-0.130571	-1.127499
H	1.328582	-1.448288	-0.277037
O	-0.692333	-1.382396	1.576630
H	-0.307611	-2.179491	1.135135
H	-1.575940	-1.625513	1.889552
O	0.725356	-3.066793	0.070635
H	1.340263	-3.674565	0.513121
H	0.313456	-3.594983	-0.632222
Mg	-0.312293	0.395897	0.602326

25

O	2.042584	-0.081298	0.066367
H	2.512470	-0.166976	-0.798625
H	2.615807	0.435806	0.650395
O	0.067271	-0.593832	-1.975129
H	0.981955	-0.598574	-2.350899
H	-0.308926	-1.457922	-2.203573
O	2.722212	-0.436879	-2.492452
H	3.092578	0.246685	-3.073890
H	3.162713	-1.259845	-2.762348
O	-0.015317	1.998433	-0.552264
H	0.791389	2.395611	-0.916192
H	-0.726041	2.306899	-1.136594
O	-0.129188	-2.010248	0.673907
H	0.675125	-2.527316	0.834043
H	-0.792251	-2.641055	0.355371
O	-2.084109	-0.062915	0.010571
H	-2.613531	0.432087	-0.632003
H	-2.503051	0.103472	0.891624
O	-2.674928	0.399447	2.591291
H	-3.098624	1.231008	2.862195
H	-3.041925	-0.273481	3.187294
O	-0.029289	0.555661	2.054720
H	0.313233	1.440705	2.254498
H	-0.940842	0.540199	2.439367
Mg	-0.017095	-0.024680	0.036664

25

O	0.477016	-2.416881	-0.850093
H	0.896443	-2.716869	-1.671422
H	0.935095	-2.891511	-0.138680
O	-0.500358	-0.268653	-2.431496
H	-0.888741	0.578352	-2.703393
H	-1.007170	-0.943337	-2.909718
O	1.980737	0.134766	-0.758829
H	2.169124	1.104998	-0.759987
H	2.445966	-0.231016	-1.526272
O	1.954694	2.825926	-0.497981
H	2.115330	3.390828	-1.271668
H	2.458729	3.237920	0.222588
O	0.462591	-0.917892	1.551353
H	-0.273861	-0.864206	2.205554
H	1.250999	-0.561907	1.986782
O	-1.961069	-0.884603	0.103351
H	-2.182389	-0.844503	1.066500
H	-2.707144	-0.488158	-0.369375
O	-1.952467	-0.829405	2.779108
H	-2.266696	-0.068936	3.294692
H	-2.270598	-1.608746	3.263364
O	-0.398275	1.583761	-0.205315
H	0.351693	2.226735	-0.220161
H	-1.088534	1.966204	0.354696
Mg	0.005250	-0.434065	-0.415028

25

O	1.482881	0.624078	-1.851870
H	0.960330	1.168214	-2.461345
H	1.990956	0.021500	-2.418549

O	0.073007	-0.736082	1.798526
H	-0.557493	-0.094124	2.211615
H	0.695059	-1.006104	2.489439
O	-0.989040	1.052437	-0.328392
H	-1.416168	1.242294	0.538712
H	-1.677896	0.648945	-0.906750
O	-0.222354	-1.712337	-1.043642
H	-1.075934	-1.448317	-1.469982
H	-0.433524	-2.500347	-0.519786
O	2.386919	-1.321400	0.096070
H	3.163829	-1.188510	0.658778
H	2.419318	-2.246345	-0.192494
O	-1.658875	1.201569	2.303962
H	-1.380454	2.010102	2.764543
H	-2.556844	1.024713	2.628152
O	1.707965	1.521751	0.774075
H	2.282785	1.961822	0.126641
H	2.237610	1.463962	1.584300
O	-2.445225	-0.489575	-2.002856
H	-3.328344	-0.798949	-1.743258
H	-2.525149	-0.267891	-2.945168
Mg	0.708997	-0.120095	-0.067454

25

O	1.352096	-1.540748	-0.574183
H	2.231136	-1.083168	-0.726280
H	1.327077	-2.286394	-1.203830
O	-0.669716	-0.102788	-2.415718
H	-0.435779	-0.844995	-3.008396
H	-0.215973	0.669781	-2.810488
O	3.383894	0.150850	-0.811881
H	3.873188	0.265905	-1.652279
H	4.071854	0.187964	-0.115909
O	1.026438	1.339206	-0.552193
H	0.973254	2.144670	-0.003940
H	1.998725	1.102565	-0.611950
O	-0.153765	-0.531862	1.715448
H	-0.698316	0.100482	2.269549
H	0.703731	-0.628745	2.171288
O	-1.540446	-1.959215	-0.383659
H	-2.445521	-1.894287	-0.748856
H	-1.667888	-2.332735	0.512149
O	-1.895328	1.242743	2.637598
H	-1.640753	2.078252	3.080439
H	-2.674180	0.923648	3.138487
O	-1.831781	1.101099	-0.011531
H	-2.698712	0.951060	-0.435543
H	-2.033199	1.263694	0.958422
Mg	-0.287021	-0.267984	-0.350114

25

O	2.107890	1.293173	-1.981976
H	2.275678	1.388598	-2.941860
H	2.932275	1.604648	-1.556539
O	-0.261880	1.986217	-1.003657
H	-0.377037	2.896683	-0.670748
H	0.649619	1.952144	-1.422454
O	-2.303295	-0.216181	-0.935210
H	-2.986934	-0.818624	-0.579754
H	-2.021236	-0.647766	-1.767431
O	-1.992904	1.495714	1.357129
H	-1.770329	1.710416	2.284408
H	-2.959408	1.351713	1.353050
O	0.835232	1.039015	1.567085
H	1.597931	1.585048	1.294994
H	1.191297	0.423480	2.237792
O	0.589528	-0.713286	-1.049007
H	1.344349	-0.182657	-1.423699
H	0.956456	-1.560525	-0.674486
O	-0.758045	-1.309285	1.499041
H	-0.180405	-2.068017	1.179671
H	-1.612581	-1.715630	1.740034
O	0.987323	-2.954075	0.366217
H	1.813193	-3.173766	0.843682
H	0.700552	-3.799624	-0.035392
Mg	-0.642877	0.357213	0.239519

25

O	2.148839	-0.025345	0.046394
H	2.525236	-0.287079	-0.846854
H	2.544225	0.849743	0.228327
O	0.031213	-0.552732	-2.038730
H	0.961486	-0.684606	-2.395110
H	-0.422615	-0.004126	-2.707174
O	2.638013	-0.795356	-2.455996
H	3.087670	-0.178993	-3.070135
H	3.049734	-1.666625	-2.630671
O	-0.019632	1.971284	-0.478649
H	-0.319855	2.617446	0.190756
H	-0.408340	2.290782	-1.316756
O	0.237142	-2.145401	0.397309
H	0.655988	-2.382410	1.249183

H -0.638109 -2.582461 0.431692
O -2.016962 -0.371801 0.080855
H -2.605793 -0.122722 -0.656844
H -2.450558 -0.010289 0.909243
O -2.610683 0.613072 2.475581
H -3.062165 1.476023 2.576643
H -3.029954 0.032348 3.143733
O -0.012417 0.396746 2.022269
H 0.593609 1.018912 2.466711
H -0.925940 0.576784 2.394848
Mg 0.052092 -0.082206 -0.002289
25

O 0.306093 -2.392637 -0.725776
H 0.800419 -2.738208 -1.495409
H 0.779092 -2.756640 0.050586
O -0.539914 -0.233354 -2.480373
H -0.937638 0.629267 -2.717175
H -1.119019 -0.893761 -2.909639
O 1.980714 0.105545 -0.814755
H 2.210356 1.079856 -0.749005
H 2.365799 -0.190398 -1.662419
O 2.069448 2.737714 -0.438231
H 2.282963 3.355398 -1.167679
H 2.538110 3.101531 0.340782
O 0.461224 -0.691604 1.548853
H -0.305645 -0.769582 2.189793
H 1.168280 -0.209674 2.017504
O -2.039516 -0.621924 0.090455
H -2.190204 -0.798921 1.066439
H -2.556610 -1.306346 -0.376621
O -1.895023 -0.971916 2.723869
H -2.264421 -0.309778 3.343536
H -2.114858 -1.838068 3.124215
O -0.372387 1.721360 -0.362900
H 0.444599 2.298812 -0.300347
H -1.030548 2.105912 0.246785
Mg -0.034949 -0.333780 -0.443919
25

O 1.540272 0.471070 -1.931139
H 1.078339 1.178518 -2.423145
H 1.788471 -0.184160 -2.613127
O 0.222413 -0.529693 1.908888
H -0.567469 0.025267 2.186606
H 0.018758 -1.439088 2.200357
O -0.801002 1.164053 -0.340948
H -1.260516 1.350388 0.527783
H -1.509078 0.737702 -0.902871
O -0.241228 -1.733169 -0.937907
H -1.130322 -1.433994 -1.298993
H -0.429931 -2.544154 -0.427669
O 2.428880 -1.467154 0.159751
H 3.243457 -1.007689 0.448332
H 2.720149 -2.040233 -0.577036
O -1.758657 1.211084 2.172150
H -1.660703 1.992346 2.754726
H -2.676779 0.905968 2.322665
O 2.062740 1.313731 0.757611
H 2.283091 2.123899 0.257682
H 1.974163 1.603713 1.686330
O -2.417310 -0.463204 -1.753845
H -3.283111 -0.724589 -1.378565
H -2.590641 -0.344589 -2.710536
Mg 0.808370 -0.154710 -0.063835

Mg – 12 water molecules

37

O 1.072029 -0.664835 -2.515511
H 1.041415 0.157449 -3.060473
H 1.965943 -1.017305 -2.643598
O -0.852273 2.738970 0.870536
H -1.629346 2.728779 0.262974
H -0.838708 3.616940 1.280544
O 2.561146 -0.682764 0.053331
H 3.063678 0.114430 0.280072
H 2.610888 -1.274156 0.845685
O 0.272490 -2.307446 -0.000890
H 0.818671 -2.586785 0.770377
H -0.667565 -2.515203 0.204372
O 0.052802 0.284170 1.433463
H -0.343674 1.178202 1.521959
H 0.170469 -0.113581 2.324051
O 2.077853 -2.435315 2.025161
H 1.613151 -2.019415 2.790692
H 2.632600 -3.140570 2.390541
O -2.430677 -2.361036 0.174578
H -2.921247 -3.019743 -0.343065

H	-2.945380	-2.254238	0.990452
O	-1.426368	-0.195271	-1.129713
H	-1.933873	0.649035	-1.125402
H	-1.990561	-0.873421	-0.693215
O	-2.699937	2.226396	-1.050742
H	-2.701313	2.735004	-1.878097
H	-3.639612	2.138959	-0.819683
O	0.904299	1.861003	-3.576382
H	0.161523	2.129590	-4.140669
H	1.685952	2.262189	-3.990230
O	0.921523	1.695296	-0.881555
H	0.363937	2.294314	-0.329258
H	0.848425	1.984421	-1.818983
O	0.553585	-1.021432	3.752369
H	0.981385	-0.466407	4.424949
H	-0.193744	-1.435994	4.213769
Mg	0.550777	-0.306066	-0.484422
37			
O	2.028485	2.367003	-1.579200
H	1.556173	2.275524	-2.441352
H	2.713378	3.041463	-1.701919
O	0.012495	2.306899	0.125280
H	-0.781135	2.790062	-0.148651
H	0.738413	2.576070	-0.494972
O	-0.037029	0.343186	2.302931
H	0.361176	1.128062	2.707654
H	0.428079	-0.443628	2.690302
O	0.312271	1.806875	-3.597239
H	0.637503	1.398462	-4.416492
H	-0.327651	2.475110	-3.892225
O	-2.760140	-2.850937	0.315237
H	-3.344541	-2.709961	1.078228
H	-2.828638	-3.802295	0.131256
O	-0.205283	-1.872400	0.499760
H	0.291938	-2.147321	1.299510
H	-1.088162	-2.309185	0.546015
O	1.894499	0.115689	-0.110469
H	2.492142	0.107668	0.674656
H	2.186528	0.870744	-0.672910
O	-0.506217	-0.061069	-1.800125
H	-0.287503	0.598614	-2.499465
H	-1.401234	-0.410319	-2.008176
O	-3.026679	-1.002609	-1.662019
H	-3.884324	-0.905432	-2.102499
H	-3.089621	-1.801950	-1.086277

O	1.370706	-1.870876	2.761296
H	2.215660	-1.369570	2.679276
H	1.383077	-2.283300	3.638625
O	3.316432	-0.051680	2.178880
H	3.333326	0.724071	2.762939
H	4.248354	-0.307184	2.080249
O	-2.221334	0.490459	0.397492
H	-2.730991	0.035006	-0.320335
H	-2.658639	0.271543	1.233526
Mg	-0.156876	0.210187	0.221519
37			
O	0.014255	1.539700	1.337232
H	0.149050	1.333055	2.292433
H	-0.659553	2.257866	1.303439
O	-1.972432	3.345364	0.864353
H	-1.706588	4.277912	0.823811
H	-2.734184	3.324527	1.465846
O	1.134843	-1.138672	0.745949
H	1.519245	-1.919792	0.284592
H	0.762951	-1.471497	1.597466
O	1.459442	1.059374	-1.150244
H	2.096234	1.438579	-0.526064
H	1.955514	0.375682	-1.661353
O	-1.602569	1.457124	-1.004319
H	-1.655622	1.582803	-1.974366
H	-1.867811	2.276692	-0.536474
O	-1.484602	0.950411	-3.655464
H	-0.880982	1.334801	-4.310675
H	-2.288743	0.735863	-4.155471
O	0.286512	0.875182	3.937312
H	1.161733	1.048256	4.323546
H	-0.337324	1.313574	4.538257
O	-0.332603	-1.582497	2.970799
H	-0.214855	-2.351646	3.548951
H	-0.092379	-0.790974	3.509102
O	-0.441956	-0.961446	-1.957537
H	0.459566	-1.163369	-2.312315
H	-0.857713	-0.406034	-2.658964
O	-1.773767	-0.855087	0.797606
H	-2.130140	-1.602473	0.293308
H	-1.437423	-1.252506	1.637866
O	2.145979	-3.189158	-0.748569
H	2.978297	-3.604643	-0.467970
H	1.569539	-3.930984	-0.993969
O	2.188182	-1.157120	-2.481907

H	2.539125	-1.318120	-3.371110
H	2.356635	-1.978203	-1.958749
Mg	-0.206409	0.167755	-0.191897
37			
O	1.525898	-0.191937	2.044771
H	1.204771	0.455668	2.723767
H	2.491929	-0.119762	2.045095
O	0.033535	0.238860	-3.943695
H	-0.533846	-0.270973	-4.545528
H	0.146475	1.099356	-4.381015
O	0.999838	-1.844254	-0.556847
H	0.173551	-2.322880	-0.794046
H	1.482205	-1.713917	-1.408211
O	-2.212810	2.458307	-0.708031
H	-3.132533	2.418016	-0.398788
H	-2.166922	3.249198	-1.269520
O	-1.203934	-0.840460	1.216400
H	-1.076098	-1.140947	2.147169
H	-1.570483	-1.590933	0.702367
O	2.086020	0.820381	-0.705431
H	2.344587	0.305468	-1.513453
H	2.906178	1.000325	-0.223373
O	0.095853	1.403528	3.619359
H	0.496147	1.853941	4.378891
H	-0.304855	0.573881	3.967188
O	-0.581445	-1.215863	3.834515
H	0.307528	-1.608566	3.809116
H	-1.081435	-1.765207	4.458979
O	2.182305	-0.844711	-2.779247
H	1.491572	-0.496618	-3.393689
H	2.939232	-1.095761	-3.330298
O	-0.895470	0.263645	-1.400899
H	-1.495979	1.040658	-1.265998
H	-0.585743	0.322581	-2.338823
O	-0.107625	1.927113	0.944799
H	-0.216994	1.965743	1.919558
H	-0.923832	2.288996	0.534192
O	-1.642950	-2.350378	-0.948142
H	-2.274171	-2.900790	-1.434834
H	-1.684716	-1.453826	-1.344675
Mg	0.424426	0.025191	0.261740
37			
O	0.468485	-1.243998	-1.418441
H	1.309224	-1.418800	-0.937478
H	-0.095151	-2.037279	-1.259644
O	0.302532	-0.168315	1.277101
H	-0.212473	-0.505106	2.044909
H	1.095076	-0.741623	1.172015
O	-1.421059	2.090445	0.300734
H	-2.045425	1.775737	1.001724
H	-0.857047	2.755153	0.723093
O	3.229486	1.269139	0.983780
H	2.932495	1.516666	1.874965
H	4.079061	1.724875	0.867072
O	-1.441815	-3.097731	-0.762912
H	-1.801726	-3.633772	-1.488456
H	-1.221852	-3.741335	-0.070183
O	-1.339215	-0.925695	3.320866
H	-1.581258	-1.861916	3.410357
H	-1.027066	-0.665450	4.203131
O	-0.923819	1.007098	-2.567642
H	-1.482969	1.786518	-2.703735
H	-0.103397	1.172891	-3.090376
O	-2.976882	0.670746	1.911646
H	-2.502101	0.123587	2.583400
H	-3.886427	0.771625	2.230940
O	2.574687	-1.303260	0.349851
H	3.082756	-1.991449	0.805266
H	3.017175	-0.451131	0.572494
O	-2.246835	-0.537573	-0.382764
H	-2.702834	-0.287202	0.455586
H	-2.167623	-1.517012	-0.413464
O	1.278508	1.607009	-0.829086
H	2.034417	1.576487	-0.196467
H	1.642501	1.575799	-1.742284
O	1.619750	1.378318	-3.509916
H	1.899832	2.152977	-4.023662
H	2.099684	0.631857	-3.902936
Mg	-0.426848	0.467222	-0.578215
37			
O	1.201587	-0.740095	-2.423564
H	1.187598	0.095034	-2.978207
H	2.147489	-0.982063	-2.370312
O	-0.750039	2.852823	0.836461
H	-1.607882	2.759755	0.326577
H	-0.775473	3.724493	1.275899
O	2.456007	-0.651547	0.206788
H	2.921714	0.117525	0.587479
H	2.461779	-1.362608	0.921769

O	0.189475	-2.336583	-0.085573
H	0.672682	-2.632758	0.736091
H	-0.774435	-2.561111	0.029023
O	-0.288736	0.276618	1.391357
H	-0.455670	1.258722	1.444728
H	0.105141	0.000721	2.264543
O	1.884859	-2.520905	1.967753
H	1.565252	-1.971764	2.744938
H	2.445399	-3.230854	2.336921
O	-2.488855	-2.405489	-0.196126
H	-2.933049	-3.055575	-0.778033
H	-3.067500	-2.344108	0.590861
O	-1.438384	-0.180386	-1.314153
H	-1.983351	0.634645	-1.124142
H	-1.977507	-0.940148	-0.953970
O	-2.785030	2.105181	-0.701813
H	-3.012846	2.653222	-1.481270
H	-3.645462	1.960636	-0.256086
O	1.014427	1.711442	-3.502684
H	0.259739	1.887746	-4.100619
H	1.785397	2.100567	-3.963795
O	0.963022	1.708416	-0.815176
H	0.395291	2.346960	-0.290268
H	0.913010	1.964231	-1.775061
O	0.880331	-0.712534	3.626601
H	1.516161	-0.135596	4.097938
H	0.249242	-0.994897	4.320519
Mg	0.478877	-0.295553	-0.467409
37			
O	1.993851	2.606365	-1.511051
H	1.547468	2.377525	-2.380544
H	2.485302	3.437399	-1.660586
O	-0.128575	2.429294	0.023905
H	-0.919899	2.851046	-0.362454
H	0.647365	2.695798	-0.566006
O	-0.076325	0.667192	2.341330
H	0.416239	1.466494	2.609403
H	0.373086	-0.107279	2.808752
O	0.454486	1.677750	-3.478385
H	0.886062	1.263485	-4.254142
H	-0.169536	2.323012	-3.870756
O	-2.410894	-3.058009	0.004725
H	-3.012249	-3.314018	0.734641
H	-2.215146	-3.904153	-0.448951
O	-0.169779	-1.708817	0.694423
H	0.174852	-1.920786	1.602738
H	-0.972754	-2.281598	0.539263
O	1.823601	0.302636	-0.124125
H	2.469470	0.036733	0.589285
H	2.175107	1.128406	-0.549448
O	-0.595225	-0.116819	-1.748485
H	-0.305561	0.520402	-2.460625
H	-1.535321	-0.373699	-1.944184
O	-3.132253	-0.970340	-1.481455
H	-4.018513	-0.968928	-1.892053
H	-3.025152	-1.860330	-1.030370
O	1.105502	-1.557253	3.053756
H	2.044033	-1.331484	2.778560
H	1.158685	-1.931580	3.954383
O	3.330053	-0.631941	1.918051
H	3.845231	0.027892	2.427079
H	4.002479	-1.279879	1.621110
O	-2.316501	0.563980	0.473708
H	-2.818491	0.026839	-0.220044
H	-2.694622	0.310497	1.337431
Mg	-0.231435	0.337148	0.261428
37			
O	0.161894	1.519895	1.452639
H	-0.036141	1.256850	2.395853
H	-0.279997	2.401116	1.305321
O	-1.074489	3.730810	0.510269
H	-0.515765	4.461031	0.174883
H	-1.805405	4.178411	0.982679
O	1.132107	-1.177345	0.802495
H	1.668681	-1.841640	0.286692
H	0.744671	-1.666662	1.577956
O	1.367985	1.046737	-1.185664
H	2.110377	1.360707	-0.633935
H	1.770915	0.376624	-1.817745
O	-1.646472	1.489216	-0.840464
H	-1.785502	1.460659	-1.823797
H	-1.526856	2.435775	-0.557085
O	-1.918722	0.647979	-3.368585
H	-1.448917	0.985177	-4.158010
H	-2.820706	0.444663	-3.689753
O	-0.292073	0.526142	3.933169
H	0.428039	0.735021	4.563804
H	-1.102803	0.844682	4.381143
O	-0.379541	-1.915233	2.882703
H	-0.669245	-2.662267	3.441292

H	-0.348978	-1.104269	3.473870
O	-0.564440	-1.069893	-1.776162
H	0.309334	-1.206795	-2.250765
H	-1.116984	-0.575614	-2.447622
O	-1.788571	-0.809813	0.957827
H	-2.227365	-1.466509	0.381660
H	-1.405883	-1.357783	1.715216
O	2.685188	-2.741391	-0.763947
H	3.616786	-2.758976	-0.461858
H	2.447747	-3.685060	-0.877567
O	1.950326	-1.058879	-2.665802
H	2.294315	-1.187027	-3.571123
H	2.378898	-1.760804	-2.088541
Mg	-0.212960	0.164764	-0.086595

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O	1.686289	-0.341454	1.776232
H	1.384404	0.214015	2.562384
H	2.643177	-0.164842	1.696188
O	0.103520	0.625491	-4.000000
H	-0.484437	0.201400	-4.658727
H	0.315763	1.498277	-4.390517
O	1.009637	-1.757105	-0.767524
H	0.235178	-2.381362	-0.831328
H	1.381594	-1.637053	-1.685106
O	-2.171771	2.616137	-0.352654
H	-3.074503	2.497813	0.006009
H	-2.189653	3.497047	-0.778512
O	-1.172390	-0.851986	1.039625
H	-1.229912	-0.971468	2.028014
H	-1.352080	-1.745836	0.636201
O	2.065356	0.945907	-0.969817
H	2.290618	0.375719	-1.770582
H	2.914484	1.074310	-0.505676
O	0.414820	1.165084	3.531024
H	0.774691	1.559347	4.348896
H	-0.265789	0.483039	3.813764
O	-1.295215	-0.845521	3.747104
H	-0.981876	-1.627356	4.247158
H	-2.203414	-0.693467	4.080766
O	2.117407	-0.758825	-2.981386
H	1.435692	-0.299875	-3.558636
H	2.865297	-0.997047	-3.562871
O	-0.863945	0.524054	-1.466576
H	-1.435125	1.307332	-1.233998
H	-0.559225	0.666853	-2.405237
O	0.043634	1.926043	0.997794
H	0.032114	1.868720	1.992932
H	-0.832003	2.297808	0.701229
O	-1.262017	-3.138473	-0.398457
H	-1.207780	-4.015838	0.031598
H	-1.942816	-3.247631	-1.093155
Mg	0.450487	0.073816	0.097202

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O	0.739637	-1.334868	-1.174619
H	1.457853	-1.549153	-0.507859
H	0.137740	-2.130531	-1.134415
O	0.291065	-0.054266	1.469617
H	-0.337267	-0.302036	2.203406
H	1.046637	-0.707798	1.497237
O	-1.521455	1.968609	0.193750
H	-2.257943	1.623268	0.786540
H	-1.040880	2.627415	0.731373
O	3.689650	0.729305	0.343695
H	4.054793	1.257376	1.083601
H	4.416312	0.696730	-0.312504
O	-1.172093	-3.227947	-0.787131
H	-1.527794	-3.743944	-1.539174
H	-1.022021	-3.893229	-0.084851
O	-1.593626	-0.512787	3.355698
H	-1.771167	-1.431082	3.646366
H	-1.424334	-0.025332	4.188442
O	-0.809446	0.839032	-2.501163
H	-1.630675	1.364332	-2.567068
H	-0.111311	1.399061	-2.952410
O	-3.259389	0.527220	1.575264
H	-2.787054	0.165804	2.383896
H	-4.183842	0.696419	1.841753
O	2.418650	-1.534570	0.889714
H	2.911613	-2.287824	1.268393
H	3.074574	-0.784091	0.773334
O	-2.101015	-0.740218	-0.443804
H	-2.706063	-0.494012	0.312173
H	-1.968930	-1.727096	-0.443017
O	1.333020	1.628008	-0.670009
H	2.214923	1.356287	-0.287997
H	1.519075	1.905214	-1.608346
O	1.320290	2.242299	-3.290234
H	1.232303	3.177995	-3.564234
H	1.892871	1.836439	-3.972672
Mg	-0.322855	0.365474	-0.491474

Mg – 16 water molecules

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O	0.818757	-0.302718	3.610897
H	0.970384	-1.166125	3.137109
H	0.906198	-0.521657	4.553221
O	-2.925626	-1.327361	1.550678
H	-3.435320	-1.966383	2.071115
H	-2.588889	-0.647304	2.186914
O	1.339285	-2.414901	2.046095
H	2.176055	-2.090822	1.620456
H	1.508553	-3.318470	2.354760
O	-0.478518	1.419191	-2.385424
H	0.415553	1.822579	-2.438818
H	-0.722934	1.125996	-3.290940
O	1.539092	-0.343436	-1.128241
H	2.168917	-0.609527	-0.412387
H	1.917799	0.489444	-1.504149
O	3.224400	-1.007737	0.850168
H	3.313804	-0.283463	1.525494
H	4.124840	-1.283569	0.618599
O	-1.605986	0.605617	2.849655
H	-1.958809	1.274387	3.456693
H	-0.769567	0.268964	3.266080
O	1.935806	2.525738	0.787206
H	2.420802	2.026560	1.496816
H	1.840894	3.428435	1.130545
O	2.110636	2.146978	-1.892336
H	2.196398	2.427758	-0.947966
H	2.910016	2.454360	-2.345224
O	-2.611704	-0.041679	-0.829534
H	-3.186219	-0.158642	-1.622304
H	-3.009197	-0.552494	-0.092607
O	-1.558914	0.079149	-4.469298
H	-1.537782	-0.020743	-5.432710
H	-2.507113	0.022994	-4.198417
O	-0.622335	-1.532155	-2.570928
H	-0.892302	-1.089403	-3.414815
H	0.289201	-1.828137	-2.719874
O	2.973462	0.932415	2.646818
H	3.646086	1.160844	3.306986
H	2.193947	0.565707	3.145990
O	-3.942659	-0.165611	-3.169485
H	-4.442349	-0.975019	-3.368029
H	-4.591727	0.550227	-3.270021
O	-0.621536	-1.797962	0.320954
H	-1.454226	-1.804065	0.855202
H	0.098062	-2.092108	0.931308
O	-0.447001	1.315288	0.521567
H	0.398081	1.802352	0.686587
H	-0.877679	1.158237	1.396495
Mg	-0.529201	-0.151105	-0.942390

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O	0.822909	-0.350801	3.893731
H	0.960958	-1.212797	3.413680
H	0.924657	-0.554201	4.837389
O	-2.946010	-0.960661	1.583226
H	-3.505878	-1.555663	2.104558
H	-2.521248	-0.341793	2.229883
O	1.247177	-2.393515	2.236523
H	2.062849	-2.033191	1.798270
H	1.452902	-3.303213	2.503265
O	-0.427918	1.140954	-2.442483
H	0.413606	1.601369	-2.629918
H	-1.043310	1.236565	-3.202985
O	1.590109	-0.478664	-1.134432
H	2.161868	-0.668407	-0.348366
H	1.953903	0.351836	-1.530614
O	3.100501	-0.929501	1.014415
H	3.126124	-0.160352	1.644798
H	4.020719	-1.206411	0.882589
O	-1.405489	0.720956	2.961050
H	-1.690300	1.496690	3.467963
H	-0.628795	0.331640	3.445663
O	1.881220	2.561593	0.619242
H	2.279581	2.111476	1.408801
H	1.705680	3.471350	0.907652
O	2.126952	1.986729	-2.033417
H	2.177489	2.330940	-1.109081
H	2.965139	2.231188	-2.453945
O	-2.567806	-0.197407	-1.007251
H	-2.994189	-0.688070	-1.744019
H	-2.969886	-0.510413	-0.167401
O	-2.340059	1.129063	-4.399742
H	-1.989741	1.215608	-5.301599
H	-2.983741	1.851655	-4.316130
O	-0.604110	-1.845506	-2.485652

H	-1.461750	-1.784338	-2.980445
H	0.090677	-1.785727	-3.157990
O	2.722601	1.100440	2.701622
H	3.434695	1.362101	3.306274
H	2.032895	0.655470	3.265036
O	-3.016307	-1.286637	-3.435148
H	-3.604178	-1.857247	-3.952564
H	-2.900570	-0.452901	-3.952872
O	-0.679915	-1.857018	0.446233
H	-1.499402	-1.696139	0.974516
H	0.022401	-2.119639	1.090664
O	-0.399277	1.140592	0.475851
H	0.402451	1.713677	0.552282
H	-0.774914	1.046179	1.384122
Mg	-0.472114	-0.343488	-0.982083

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O	0.634890	-1.565835	3.600615
H	0.543480	-0.610907	3.376967
H	0.409417	-1.640504	4.541025
O	-3.695918	-1.012785	1.540574
H	-3.973947	-1.089863	0.594300
H	-4.502719	-0.863325	2.055367
O	3.017597	-1.597539	2.320798
H	2.274979	-1.756230	2.955395
H	3.633987	-2.338718	2.422170
O	-0.877371	1.903810	-2.919168
H	-0.656874	2.646421	-3.502689
H	-0.494570	1.096211	-3.347315
O	1.439806	-1.201726	0.163242
H	2.089197	-1.444281	0.863597
H	1.924684	-1.137801	-0.694554
O	2.576090	-0.648509	-2.199509
H	2.972389	0.156475	-1.779156
H	3.322128	-1.186746	-2.506686
O	-1.080703	-1.702796	1.501539
H	-0.612359	-1.854948	2.353009
H	-2.036379	-1.621377	1.715614
O	3.184720	1.470946	-0.665361
H	3.334180	1.324380	0.304300
H	3.683023	2.269243	-0.897694
O	0.469535	1.558100	-0.594601
H	1.450070	1.649232	-0.680609
H	0.069848	1.802406	-1.464633
O	-1.118312	-0.949020	-1.269293
H	-0.726552	-0.861332	-2.170566
H	-2.093819	-1.063774	-1.356375
O	-3.169131	1.627207	-1.485955
H	-2.409926	1.769675	-2.108356
H	-3.757103	2.388497	-1.608548
O	0.237358	-0.442036	-3.538763
H	0.192340	-1.009245	-4.323467
H	1.162159	-0.516225	-3.189318
O	3.176994	1.012493	1.981104
H	3.346350	0.061268	2.206698
H	3.676101	1.541947	2.621856
O	-2.024147	1.011103	0.896482
H	-2.715962	0.404800	1.258969
H	-2.450144	1.402008	0.092646
O	-3.817419	-0.947939	-1.150680
H	-3.786983	0.010034	-1.403676
H	-4.368079	-1.386512	-1.816971
O	0.541976	0.750192	2.183003
H	1.503877	1.014966	2.157190
H	0.044490	1.535585	2.459331
Mg	-0.286263	-0.093793	0.407896

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O	0.658917	-0.185508	3.582252
H	0.837448	-1.055368	3.127832
H	0.630281	-0.407609	4.527679
O	-2.923850	-1.411474	1.191105
H	-3.507140	-2.052201	1.625123
H	-2.656237	-0.758084	1.884547
O	1.267063	-2.324499	2.097837
H	2.129113	-2.024395	1.703751
H	1.421023	-3.204629	2.475481
O	-0.186777	1.152610	-2.586807
H	0.458934	1.848957	-2.344902
H	-1.048494	1.571880	-2.815383
O	1.722928	-0.313740	-1.107881
H	2.298757	-0.580684	-0.348984
H	2.026228	0.595824	-1.353428
O	3.243338	-0.987636	0.980595
H	3.337958	-0.295494	1.687530
H	4.134173	-1.333376	0.813636
O	-1.787432	0.494169	2.675065
H	-2.192787	1.197216	3.205548
H	-0.945528	0.242234	3.138128
O	1.748378	2.437268	1.114542
H	2.320631	1.982770	1.786980
H	1.522695	3.296843	1.503814

O	2.055502	2.301472	-1.537291
H	2.075444	2.498908	-0.567698
H	2.868154	2.676629	-1.908284
O	-2.440018	-0.357989	-1.235063
H	-2.875079	0.402035	-1.672682
H	-2.918910	-0.598612	-0.413693
O	-2.399639	-0.863496	-4.423795
H	-2.118480	-0.852544	-5.353802
H	-3.156268	-1.472424	-4.408754
O	-0.352362	-1.707785	-2.781049
H	-1.088469	-1.484394	-3.401594
H	-0.538943	-2.609697	-2.478782
O	3.007140	0.880630	2.859586
H	3.636105	1.091309	3.566776
H	2.174553	0.560586	3.299206
O	-2.790210	1.494721	-3.120010
H	-2.769249	0.730905	-3.746188
H	-3.312781	2.183661	-3.557090
O	-0.521470	-1.959168	0.136784
H	-1.399793	-1.936079	0.592931
H	0.142224	-2.166914	0.841369
O	-0.502752	1.121695	0.379071
H	0.317924	1.576132	0.691950
H	-1.034505	0.969886	1.197725
Mg	-0.351365	-0.335828	-1.130390

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O	-0.561247	-2.879846	-3.286149
H	-1.539092	-2.999252	-3.372826
H	-0.228877	-2.860384	-4.197838
O	-0.642130	-0.449537	-2.204658
H	-0.574358	-1.322169	-2.672439
H	-0.160343	0.187497	-2.752285
O	2.561800	0.483781	3.054388
H	2.778494	0.018860	3.877101
H	2.299692	1.406591	3.303227
O	-2.280451	2.747941	0.189332
H	-1.954392	2.799317	1.121200
H	-2.769501	3.566570	0.020724
O	-3.291107	-2.773700	-3.281484
H	-3.642251	-2.063396	-3.842790
H	-3.807390	-3.559462	-3.525774
O	1.827960	-0.665673	-0.640655
H	2.619328	-0.312469	-0.168048
H	1.977853	-1.606681	-0.874243
O	1.388014	-3.249289	-1.352075
H	0.790055	-3.299558	-2.131638
H	1.794806	-4.125229	-1.269824
O	0.123488	1.797832	-0.718376
H	-0.680551	2.324583	-0.501215
H	0.890403	2.289866	-0.330400
O	3.701369	0.713780	0.690919
H	3.493796	0.538004	1.644671
H	4.665723	0.666763	0.601379
O	-3.159109	-2.245086	-0.605347
H	-3.816182	-2.761372	-0.114662
H	-3.320765	-2.439389	-1.560483
O	-2.143732	0.099984	0.268383
H	-2.512785	0.991651	0.096347
H	-2.733741	-0.582541	-0.122486
O	1.511613	2.966151	3.071663
H	1.865384	3.700441	3.597254
H	1.825158	3.127318	2.141990
O	2.239367	2.951135	0.486795
H	2.674684	3.709573	0.065899
H	2.912129	2.218243	0.476824
O	-0.567717	-2.225465	0.193921
H	-1.478391	-2.453560	-0.112043
H	0.064046	-2.813718	-0.282178
O	0.189500	0.100540	1.832962
H	-0.342115	0.856258	2.182102
H	1.057111	0.129808	2.301556
O	-1.086476	2.377764	2.588976
H	-1.600086	2.291941	3.407299
H	-0.216208	2.766028	2.863538
Mg	-0.137076	-0.209291	-0.180784

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O	0.942632	-0.273528	3.751394
H	1.040747	-1.161064	3.256503
H	1.089214	-0.483459	4.696205
O	-2.920588	-1.241254	1.517678
H	-3.436813	-1.902673	2.017634
H	-2.489352	-0.639538	2.199610
O	1.208052	-2.304512	2.146989
H	2.052295	-2.015705	1.661183
H	1.367817	-3.217460	2.459206
O	-0.458871	1.465739	-2.294144
H	0.465277	1.830525	-2.362343
H	-0.734970	1.205972	-3.214342
O	1.562236	-0.412249	-1.225930
H	2.171508	-0.716861	-0.489605

H	1.932649	0.479152	-1.509031
O	3.109947	-1.105474	0.846470
H	3.192407	-0.294794	1.450785
H	4.016181	-1.453383	0.727094
O	-1.450830	0.459400	2.922512
H	-1.815570	1.185703	3.466395
H	-0.591327	0.175743	3.377016
O	1.832065	2.651049	0.735934
H	2.315027	2.108107	1.441581
H	1.733127	3.549534	1.108730
O	2.113251	2.110338	-1.833782
H	2.149544	2.457261	-0.889201
H	2.934261	2.404214	-2.273311
O	-2.608064	-0.023499	-0.869565
H	-3.171687	-0.228804	-1.665416
H	-2.998107	-0.505160	-0.092824
O	-1.553603	0.235987	-4.417897
H	-1.506004	0.151855	-5.390057
H	-2.513348	0.083594	-4.163140
O	-0.653816	-1.503417	-2.647399
H	-0.928793	-0.976504	-3.460629
H	0.281634	-1.734721	-2.818349
O	2.879739	0.964051	2.450524
H	3.628031	1.221434	3.025912
H	2.169066	0.584472	3.070067
O	-3.886657	-0.285088	-3.245309
H	-4.296365	-1.142575	-3.481759
H	-4.613016	0.364011	-3.348306
O	-0.656550	-1.873823	0.275044
H	-1.511386	-1.804423	0.799569
H	0.043441	-2.091419	0.960480
O	-0.405457	1.199141	0.577216
H	0.393429	1.792339	0.699461
H	-0.787008	1.008143	1.484094
Mg	-0.515961	-0.185754	-0.954433

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O	0.919276	-0.221763	3.766150
H	1.034856	-1.111855	3.281020
H	1.067665	-0.418800	4.713463
O	-2.898158	-1.272174	1.546811
H	-3.450606	-1.902483	2.048140
H	-2.483050	-0.650697	2.222068
O	1.229718	-2.270545	2.182558
H	2.069797	-1.956149	1.705261
H	1.421640	-3.171175	2.512047
O	-0.488482	1.352583	-2.333150
H	0.413349	1.758781	-2.428997
H	-0.868182	1.238478	-3.247713
O	1.552332	-0.388654	-1.175045
H	2.159402	-0.655234	-0.423136
H	1.906056	0.498732	-1.488179
O	3.113536	-1.015043	0.908617
H	3.178623	-0.198303	1.506736
H	4.027090	-1.340636	0.782916
O	-1.476146	0.478430	2.925618
H	-1.857889	1.200308	3.463688
H	-0.615721	0.209939	3.388020
O	1.759317	2.685211	0.691551
H	2.243670	2.170508	1.416373
H	1.630487	3.587606	1.045315
O	2.056516	2.122000	-1.878254
H	2.082272	2.481677	-0.938728
H	2.893290	2.392205	-2.303013
O	-2.643509	-0.065413	-0.845002
H	-3.083103	-0.470699	-1.639838
H	-2.997426	-0.542917	-0.046061
O	-1.884255	0.918960	-4.615295
H	-1.397657	0.647394	-5.420635
H	-2.376874	1.719465	-4.890618
O	-0.736307	-1.654898	-2.530027
H	-1.668139	-1.594223	-2.907775
H	-0.729661	-2.507885	-2.049999
O	2.823331	1.072471	2.473123
H	3.555566	1.364921	3.052294
H	2.121645	0.672612	3.089852
O	-3.179921	-1.006168	-3.307598
H	-3.777947	-1.581594	-3.822995
H	-2.849653	-0.298126	-3.938525
O	-0.638882	-1.908351	0.304674
H	-1.492078	-1.843570	0.833038
H	0.065751	-2.114581	0.989836
O	-0.458689	1.199330	0.561714
H	0.332862	1.805675	0.667711
H	-0.828748	1.017009	1.474988
Mg	-0.523806	-0.217988	-0.941835

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O	0.663491	-1.515523	3.674735
H	0.591490	-0.557352	3.384232
H	0.543203	-1.509771	4.645330
O	-3.666929	-1.077610	1.396150

H	-3.911470	-1.102997	0.420816
H	-4.506332	-0.985561	1.886952
O	2.944364	-1.575152	2.321929
H	2.198406	-1.698114	2.990486
H	3.585967	-2.295361	2.479546
O	-0.874856	1.903887	-2.866499
H	-0.623544	2.649827	-3.445962
H	-0.468284	1.071073	-3.273129
O	1.405877	-1.355234	0.140204
H	2.066296	-1.544715	0.867034
H	1.924575	-1.211602	-0.705514
O	2.544676	-0.619698	-2.162065
H	2.903097	0.227328	-1.742995
H	3.318276	-1.086474	-2.535498
O	-1.072675	-1.764353	1.619668
H	-0.643524	-1.831032	2.514785
H	-2.052452	-1.673534	1.765749
O	3.069351	1.526836	-0.756593
H	3.271542	1.355465	0.217265
H	3.568837	2.328423	-1.008240
O	0.403087	1.496164	-0.571395
H	1.389525	1.635989	-0.679435
H	-0.016598	1.760516	-1.443902
O	-1.122145	-1.128454	-1.226313
H	-0.698100	-0.959127	-2.117737
H	-2.115739	-1.106931	-1.359295
O	-3.084129	1.693407	-1.427714
H	-2.327666	1.834104	-2.081583
H	-3.680599	2.460648	-1.532328
O	0.227280	-0.396800	-3.420728
H	0.198782	-0.885773	-4.266213
H	1.175783	-0.473525	-3.076136
O	3.154758	0.987246	1.835590
H	3.304501	0.016250	2.078727
H	3.680950	1.508853	2.474442
O	-2.000403	0.952500	0.926260
H	-2.719931	0.321458	1.231062
H	-2.403002	1.379832	0.112672
O	-3.777666	-0.829465	-1.243718
H	-3.693110	0.159878	-1.433628
H	-4.348608	-1.198798	-1.945772
O	0.585235	0.692302	2.218672
H	1.555861	0.982637	2.119612
H	0.077985	1.491629	2.464979
Mg	-0.288447	-0.190064	0.435235
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O	0.728829	-0.352818	3.761950
H	0.887257	-1.232059	3.270373
H	0.807528	-0.566049	4.714184
O	-2.886471	-1.337171	1.253679
H	-3.501077	-1.954710	1.695050
H	-2.529990	-0.725440	1.969306
O	1.195254	-2.366928	2.165829
H	2.065528	-2.019433	1.774458
H	1.385859	-3.266439	2.499306
O	-0.174035	1.088393	-2.578313
H	0.534173	1.751096	-2.357413
H	-1.036324	1.564405	-2.727015
O	1.756109	-0.425244	-1.133149
H	2.306714	-0.686813	-0.336837
H	2.058596	0.504520	-1.362826
O	3.146662	-1.043902	1.064841
H	3.141304	-0.231767	1.671679
H	4.076185	-1.343266	1.010721
O	-1.581700	0.383553	2.745687
H	-1.979616	1.128059	3.239008
H	-0.756356	0.108088	3.265183
O	1.583639	2.643978	0.876584
H	2.068752	2.116173	1.593830
H	1.381998	3.515953	1.269940
O	2.085991	2.175913	-1.659491
H	2.030632	2.517453	-0.714407
H	2.886377	2.573026	-2.053788
O	-2.446515	-0.466734	-1.233171
H	-2.820811	0.351127	-1.658050
H	-2.880779	-0.606934	-0.350452
O	-2.186026	-0.640792	-4.473151
H	-1.788086	-0.487910	-5.355332
H	-2.943820	-1.232031	-4.663439
O	-0.364030	-1.756305	-2.780711
H	-1.042433	-1.416294	-3.436483
H	-0.710151	-2.627999	-2.506187
O	2.666717	1.019846	2.622399
H	3.345694	1.330781	3.254496
H	1.937311	0.588755	3.183618
O	-2.759093	1.518909	-2.967457
H	-2.708256	0.826637	-3.688402
H	-3.386294	2.198432	-3.281817
O	-0.549156	-2.057819	0.158682
H	-1.430727	-1.949507	0.630032
H	0.106971	-2.238550	0.896969

O -0.498575 1.042511 0.381377
H 0.248808 1.681312 0.584073
H -0.919116 0.842464 1.269703
Mg -0.337073-0.409758 -1.111772
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O -0.274041 -2.577664 -3.419914
H -1.214973 -2.932374 -3.456149
H 0.040496 -2.560475 -4.345769
O -0.840673 -0.288902 -2.178217
H -0.564452 -1.079284 -2.734954
H -0.353430 0.474604 -2.547456
O 2.478382 0.548280 3.010734
H 2.778218 0.186274 3.867745
H 2.257464 1.521548 3.169460
O -2.150984 2.836164 0.450621
H -1.798308 2.838472 1.394561
H -2.526309 3.723542 0.292090
O -2.848505 -3.230142 -3.217360
H -3.399223 -2.894226 -3.955408
H -3.054668 -4.187875 -3.184181
O 1.652897 -0.734037 -0.623236
H 2.469964 -0.394063 -0.154466
H 1.767368 -1.702794 -0.815542
O 1.161968 -3.287487 -1.322901
H 0.726968 -3.189642 -2.224166
H 1.503503 -4.200999 -1.275176
O 0.039001 1.800517 -0.631473
H -0.727308 2.360703 -0.301904
H 0.875514 2.256036 -0.318687
O 3.572784 0.581126 0.647949
H 3.354128 0.474075 1.630371
H 4.539105 0.459983 0.560207
O -3.282288 -2.067626 -0.822637
H -3.947093 -2.594545 -0.336627
H -3.242379 -2.475989 -1.737140
O -2.306976 0.170626 0.356333
H -2.589814 1.114041 0.235192
H -2.878335 -0.418271 -0.202217
O 1.607287 3.038913 2.895026
H 1.984415 3.795725 3.386227
H 1.913061 3.146191 1.933103
O 2.289940 2.861671 0.368867
H 2.749818 3.571460 -0.122662
H 2.927163 2.072667 0.385981
O -0.783526 -2.231360 0.144955
H -1.707024 -2.360742 -0.225510
H -0.158825 -2.818087 -0.375213
O 0.060915 0.022511 1.940139
H -0.415468 0.824194 2.311837
H 0.969687 0.078767 2.355316
O -0.946573 2.390514 2.757189
H -1.390340 2.431881 3.627494
H -0.025707 2.783948 2.897741
Mg -0.287122-0.206695 -0.112424

Mg – 20 water molecules

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O -0.232118 -3.525503 1.260044
H -0.396404 -3.339374 2.220241
H -0.899904 -4.182060 1.008176
O -3.451213 0.121698 0.962758
H -3.449224 -0.163468 1.911217
H -4.169008 -0.378070 0.544277
O -0.767357 3.922780 -0.708252
H -1.671675 3.565063 -0.538786
H -0.775676 4.834583 -0.377943
O -0.933946 1.204409 3.338180
H -0.145395 0.614473 3.487261
H -0.904465 1.854348 4.057967
O 1.868531 -0.273988 0.979343
H 2.688499 -0.758605 0.696435
H 1.669412 -0.491256 1.918180
O 1.585692 1.410392 -1.416540
H 2.407578 1.010513 -1.785815
H 1.259085 2.073786 -2.067844
O -0.584129 0.941179 -4.020243
H -1.201511 0.990907 -4.766185
H -0.268320 1.866046 -3.857853
O 3.644965 -0.079472 -2.370206
H 3.016761 -0.366883 -3.077411
H 4.395322 0.319786 -2.837234
O 0.387923 3.209465 -3.036631
H -0.091148 3.606602 -2.263616
H 0.945032 3.910164 -3.408060
O -0.914278 -0.898573 0.938373
H -1.867303 -0.696526 0.812623
H -0.792402 -1.873686 0.917717

O	1.911461	-3.420353	-0.390087
H	1.936825	-4.246576	-0.897171
H	1.227603	-3.559330	0.313056
O	3.911672	-1.570895	-0.063115
H	3.896572	-1.107467	-0.931622
H	3.329703	-2.351496	-0.197303
O	-2.815945	-0.709625	3.447553
H	-2.175698	0.053648	3.492708
H	-3.384669	-0.610452	4.227465
O	-1.361421	0.686673	-1.444283
H	-1.224534	0.770526	-2.416426
H	-1.985052	1.391471	-1.161368
O	-3.007971	2.480753	-0.238957
H	-3.227505	1.713440	0.349898
H	-3.822365	2.661160	-0.733175
O	-0.778864	-2.555615	3.690960
H	-1.593789	-1.991102	3.642609
H	-0.851469	-3.063766	4.514035
O	1.056530	-0.592372	3.538362
H	1.664510	-0.583342	4.293743
H	0.475496	-1.387935	3.662278
O	1.561246	-0.702452	-3.931260
H	0.810340	-0.080652	-4.118264
H	1.514904	-1.388832	-4.614684
O	0.547818	-1.408194	-1.526398
H	0.910571	-1.233143	-2.427205
H	1.059956	-2.179570	-1.177456
O	0.042750	1.903349	0.922352
H	-0.213623	2.741067	0.479198
H	-0.449406	1.807918	1.770281
Mg	0.318903	0.234401	-0.269330
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O	-1.253556	-3.260044	1.458936
H	-2.146245	-2.990698	1.779758
H	-1.393629	-3.704744	0.609378
O	-3.402715	0.771249	1.297784
H	-2.901965	1.244377	2.007056
H	-3.692365	-0.077950	1.701362
O	-1.213503	3.718986	-1.164866
H	-2.061254	3.208314	-1.217420
H	-1.465630	4.643873	-1.019599
O	-1.578258	1.769343	3.040823
H	-1.430228	0.896004	3.490822
H	-1.745325	2.413437	3.745270
O	1.788013	0.062769	1.501670
H	2.696061	-0.197792	1.209764
H	1.472462	-0.688198	2.058531
O	1.737738	1.389389	-1.243471
H	2.545455	0.952988	-1.604710
H	1.400479	2.011568	-1.934156
O	-0.089048	0.585870	-4.083829
H	-0.678365	0.564742	-4.853427
H	0.146979	1.535479	-3.930508
O	3.803160	-0.166353	-2.084376
H	3.193110	-0.667469	-2.683437
H	4.487129	0.214962	-2.656344
O	0.528787	2.971679	-3.065754
H	-0.151435	3.365319	-2.457986
H	1.028508	3.712498	-3.441130
O	-0.987284	-0.574908	1.096223
H	-1.885316	-0.187515	1.030938
H	-1.083539	-1.549288	1.025371
O	2.814382	-3.206719	0.202205
H	3.440629	-2.475395	0.420016
H	3.247306	-3.674073	-0.529224
O	4.114236	-0.875269	0.503382
H	4.137276	-0.622353	-0.454031
H	4.991501	-0.665945	0.859460
O	-1.428817	-0.735682	4.013038
H	-1.482713	-0.883230	4.970571
H	-0.601111	-1.196741	3.716764
O	-1.050499	0.357387	-1.595607
H	-0.799687	0.408351	-2.548917
H	-1.874391	0.887479	-1.487712
O	-3.196907	1.956305	-1.135632
H	-3.443020	1.550761	-0.266419
H	-3.960556	1.835204	-1.720368
O	-3.380412	-1.759445	2.446363
H	-2.733370	-1.421225	3.119977
H	-4.094877	-2.156719	2.968293
O	0.725110	-2.033510	2.958475
H	1.273598	-2.607866	3.515422
H	0.194126	-2.638954	2.393389
O	1.752516	-1.297036	-3.415725
H	1.130594	-0.633987	-3.807929
H	1.774643	-2.043125	-4.034488
O	0.946653	-1.581627	-0.816502
H	1.169815	-1.594755	-1.776473
H	1.585894	-2.218699	-0.399040
O	-0.173993	2.132995	0.759645
H	-0.563750	2.829377	0.182039

H	-0.675749	2.108170	1.607763
Mg	0.411662	0.316688	-0.088412
61			
O	-0.521843	-2.794781	2.923638
H	-1.504523	-2.793968	3.115109
H	-0.318886	-3.694402	2.622937
O	-3.211596	-0.016779	1.286430
H	-3.233268	0.121947	2.273120
H	-3.899186	-0.681802	1.119992
O	-1.091143	3.573601	-0.256226
H	-1.992558	3.162553	-0.289003
H	-1.209918	4.450751	0.140165
O	-0.487450	0.920648	3.670243
H	0.249296	0.253741	3.682593
H	-0.187181	1.642456	4.245253
O	2.120601	-0.524434	0.725717
H	2.845045	-1.042323	0.305050
H	2.024411	-0.792274	1.667230
O	1.612119	1.364487	-1.418320
H	2.458510	1.121385	-1.856864
H	1.203840	2.106098	-1.921108
O	-0.463023	1.145239	-4.051652
H	-1.102580	1.244244	-4.773542
H	-0.278018	2.058499	-3.713240
O	3.756150	0.260632	-2.657960
H	3.104652	-0.011713	-3.355032
H	4.449508	0.764204	-3.111606
O	0.121835	3.299443	-2.624527
H	-0.383580	3.503868	-1.792529
H	0.559017	4.124748	-2.883752
O	-0.825672	-1.209389	0.754860
H	-1.704857	-0.801229	0.950894
H	-0.634898	-1.816160	1.507801
O	2.207729	-3.633683	-1.376046
H	2.372067	-3.998411	-2.259170
H	2.981913	-3.042750	-1.205401
O	3.980680	-1.712557	-0.847040
H	4.027564	-1.007822	-1.544912
H	4.884927	-1.821496	-0.514899
O	-3.008804	0.014329	3.922069
H	-2.084187	0.372729	3.987536
H	-3.572442	0.598956	4.451107
O	-1.202479	0.581039	-1.493280
H	-1.067814	0.714685	-2.458832
H	-1.972682	1.132200	-1.222727
O	-3.216194	2.015664	-0.453833
H	-3.361439	1.324857	0.245453
H	-4.041854	2.088582	-0.956235
O	-3.177596	-2.599166	3.191508
H	-3.229304	-1.702982	3.596574
H	-3.539390	-3.188778	3.870815
O	1.416825	-0.957899	3.337600
H	2.035227	-1.136416	4.063033
H	0.789289	-1.722383	3.325918
O	1.653773	-0.488150	-4.083896
H	0.917575	0.167479	-4.212733
H	1.655704	-1.050235	-4.873574
O	0.680462	-1.474127	-1.762117
H	1.021690	-1.182529	-2.641001
H	1.166849	-2.320858	-1.579166
O	0.146285	1.548053	1.053288
H	-0.298907	2.359580	0.712472
H	-0.197356	1.380161	1.959864
Mg	0.434785	0.022224	-0.337243
61			
O	1.161067	-3.783086	-0.759599
H	1.218104	-4.627649	-1.232015
H	2.072771	-3.394014	-0.779188
O	-3.131284	0.483745	1.669374
H	-2.937096	0.685002	2.623087
H	-4.020867	0.097046	1.667543
O	-0.614801	3.747989	-0.684800
H	-1.539598	3.451651	-0.492756
H	-0.558821	4.652954	-0.341043
O	0.159348	1.520377	3.597374
H	0.654192	0.657121	3.641000
H	0.725228	2.180043	4.027227
O	1.666091	-0.675580	0.688176
H	2.315325	-1.317686	0.319633
H	1.525417	-0.897329	1.640702
O	1.288121	1.156626	-1.490172
H	2.148648	0.784467	-1.789824
H	1.019958	1.842630	-2.142370
O	-0.822157	0.824555	-4.096388
H	-1.401682	0.884723	-4.871353
H	-0.481909	1.739836	-3.935240
O	3.398320	-0.244950	-2.453118
H	2.794694	-0.431918	-3.216206
H	4.198792	0.155274	-2.826650
O	0.262774	3.058626	-3.141006

H	-0.105602	3.475372	-2.318073
H	0.907171	3.687784	-3.499823
O	-1.234540	-1.266621	0.740590
H	-1.915156	-0.771626	1.248932
H	-0.822636	-1.975053	1.300264
O	0.157300	-3.314814	1.758744
H	-0.491226	-3.992474	2.000071
H	0.514514	-3.614193	0.891215
O	3.341980	-2.272227	-0.703103
H	3.490286	-1.578876	-1.399393
H	4.209526	-2.452538	-0.309737
O	-2.315759	0.762115	4.177196
H	-1.423622	1.192836	4.107188
H	-2.785597	1.200989	4.902331
O	-1.659272	0.563699	-1.508687
H	-1.515746	0.675701	-2.475439
H	-2.184143	1.326670	-1.172130
O	-2.929634	2.480197	-0.141518
H	-3.006328	1.818642	0.598812
H	-3.836004	2.683614	-0.417560
O	-1.382739	-1.773307	3.730697
H	-1.816292	-0.945303	4.040754
H	-1.464961	-2.383656	4.479033
O	1.124125	-0.939456	3.340757
H	1.740049	-1.391539	3.937209
H	0.243106	-1.397941	3.460334
O	1.371745	-0.752285	-4.084687
H	0.607672	-0.137610	-4.241188
H	1.388900	-1.361483	-4.838503
O	0.112573	-1.587552	-1.822523
H	0.592041	-1.396566	-2.661272
H	0.430386	-2.471973	-1.514023
O	-0.233483	1.539615	0.902646
H	-0.169913	2.430036	0.499837
H	-0.072975	1.625120	1.870063
Mg	-0.004169	-0.060071	-0.399419
61			
O	0.712632	-3.906678	2.096453
H	0.498410	-4.851737	2.135538
H	1.011149	-3.768653	1.165035
O	-3.741201	0.654307	1.095834
H	-3.516223	0.860807	2.054171
H	-4.586569	0.179527	1.124414
O	-1.148259	3.683035	-0.533587
H	-2.024185	3.300003	-0.791266
H	-1.346177	4.519332	-0.084350
O	-0.397460	1.633660	3.546456
H	0.077335	0.793103	3.779913
H	0.062913	2.344897	4.018249
O	1.209116	-1.053804	1.092843
H	2.137800	-1.216390	0.822954
H	1.170333	-0.988540	2.072742
O	1.702453	0.793810	-1.092889
H	2.401886	0.395186	-1.658620
H	1.626422	1.740640	-1.353057
O	0.377853	1.577940	-3.920710
H	-0.073252	2.018839	-4.657388
H	0.744694	2.304927	-3.357268
O	3.515230	-0.561635	-2.602022
H	2.834718	-0.819479	-3.276136
H	4.203706	-0.072261	-3.077609
O	1.127566	3.289540	-1.979776
H	0.302023	3.560057	-1.504418
H	1.699711	4.071172	-2.006158
O	-1.697343	-1.002340	0.536577
H	-2.474295	-0.412699	0.705175
H	-1.585999	-1.520698	1.372431
O	1.621643	-3.639414	-0.499698
H	1.889571	-4.442229	-0.972585
H	2.439076	-3.079448	-0.419823
O	3.524949	-1.793859	-0.210737
H	3.668297	-1.374457	-1.094907
H	4.403011	-2.044078	0.114186
O	-3.063503	1.017419	3.614523
H	-2.117992	1.301968	3.652710
H	-3.547966	1.765623	3.996780
O	-1.182999	0.730363	-1.810353
H	-0.750350	1.058909	-2.629873
H	-2.004479	1.257786	-1.662409
O	-3.310379	2.162552	-1.069619
H	-3.589402	1.683888	-0.244441
H	-4.101280	2.258329	-1.621152
O	-1.271467	-2.358480	2.806121
H	-0.582384	-3.034854	2.520854
H	-1.972399	-2.849835	3.260861
O	0.621912	-0.814604	3.777647
H	1.161087	-1.239860	4.461956
H	-0.159108	-1.411135	3.624625
O	1.291489	-0.975498	-3.972213
H	0.974016	-0.043952	-4.088143
H	1.072823	-1.439976	-4.794797

O	0.151617	-1.714895	-1.607415
H	0.520721	-1.518259	-2.500198
H	0.645069	-2.502399	-1.267754
O	-0.195312	1.595059	0.864142
H	-0.573817	2.416235	0.471300
H	-0.272136	1.662856	1.846393
Mg	-0.017484	-0.106509	-0.298267
61			
O	-0.737227	-3.479415	1.214133
H	-0.921778	-3.288978	2.187352
H	-1.486642	-4.022839	0.900444
O	-3.452001	0.102298	1.101081
H	-3.319478	-0.007216	2.099993
H	-4.159255	-0.528440	0.859407
O	-1.144372	3.770713	-0.620267
H	-2.021765	3.273945	-0.609049
H	-1.340145	4.668316	-0.286845
O	-0.532930	1.162462	3.379950
H	0.155920	0.414376	3.448529
H	-0.328061	1.770221	4.118920
O	1.993954	-0.311494	0.980158
H	2.770193	-0.809090	0.570378
H	1.754453	-0.726710	1.851205
O	1.793901	1.376160	-1.358372
H	2.502030	0.924236	-1.905466
H	1.429494	2.133170	-1.897596
O	-0.284777	1.171128	-4.053355
H	-0.915099	1.342997	-4.780514
H	0.001219	2.077103	-3.708346
O	3.531615	-0.138601	-2.691098
H	2.813059	-0.478184	-3.317779
H	4.211945	0.275113	-3.257504
O	0.448566	3.291457	-2.698070
H	-0.199836	3.578406	-1.976918
H	0.875131	4.106705	-3.026214
O	-0.912466	-0.819912	0.938948
H	-1.869549	-0.550950	0.861636
H	-0.904833	-1.818504	0.884800
O	1.686220	-3.502583	0.020141
H	1.744699	-4.311487	-0.525371
H	0.818332	-3.616735	0.504443
O	4.111444	-1.283801	-0.297929
H	3.928466	-0.947824	-1.222474
H	4.792061	-0.658263	0.022205
O	-2.652941	-0.349132	3.562745
H	-1.879916	0.320794	3.578318
H	-3.188481	-0.154149	4.358258
O	-1.183400	0.583453	-1.594878
H	-0.983744	0.782784	-2.553873
H	-1.954795	1.160017	-1.330972
O	-3.173394	2.105767	-0.587267
H	-3.377765	1.443108	0.147370
H	-3.979142	2.157238	-1.138071
O	-1.085500	-2.501240	3.632164
H	-1.779984	-1.761936	3.641853
H	-1.208920	-2.996708	4.466268
O	1.055446	-0.946868	3.428316
H	1.637538	-1.045776	4.207751
H	0.316169	-1.626355	3.556072
O	1.382583	-0.893937	-3.959737
H	0.777955	-0.102861	-4.127439
H	1.328763	-1.457551	-4.755967
O	0.683327	-1.532449	-1.421218
H	0.976687	-1.471522	-2.369114
H	1.168223	-2.296749	-0.969300
O	0.115357	1.922347	0.872554
H	-0.379932	2.688014	0.467769
H	-0.236928	1.761717	1.792461
Mg	0.428183	0.204181	-0.288053
61			
O	-1.427519	-3.082140	2.025709
H	-2.282090	-2.738058	2.438324
H	-1.623066	-3.961982	1.649601
O	-3.452487	0.500445	1.314672
H	-2.925935	1.104544	1.926904
H	-3.675818	-0.282551	1.897246
O	-1.461025	3.460120	-1.177148
H	-2.249533	2.833377	-1.224913
H	-1.818408	4.324296	-0.892925
O	-1.722507	1.800094	2.835566
H	-1.507490	1.056468	3.488902
H	-1.934516	2.588387	3.372958
O	1.667141	-0.263442	1.320984
H	2.571039	-0.578149	1.031154
H	1.348010	-0.904542	2.018280
O	1.892160	1.323757	-1.115957
H	2.707912	0.938211	-1.546510
H	1.574515	2.068481	-1.700777
O	0.366533	1.040490	-4.212286
H	-0.106550	1.188295	-5.054271

H	0.535906	1.954759	-3.814117
O	3.926681	-0.059356	-2.148454
H	3.327786	-0.465662	-2.857580
H	4.665216	0.371425	-2.621406
O	0.696546	3.151049	-2.709332
H	-0.160652	3.358079	-2.219464
H	1.088265	4.012569	-2.952767
O	-1.215425	-0.860293	0.565090
H	-2.045319	-0.368210	0.823863
H	-1.263519	-1.760547	0.993863
O	2.644807	-3.370252	-0.148479
H	3.301029	-2.642812	0.069556
H	3.084966	-3.867774	-0.866352
O	4.004823	-1.133581	0.276749
H	4.096624	-0.746257	-0.649757
H	4.870061	-1.004551	0.712287
O	-1.359192	-0.369851	4.264514
H	-1.309575	-0.316693	5.240206
H	-0.546201	-0.907095	3.973216
O	-0.896592	0.362569	-1.944779
H	-0.589973	0.631977	-2.853848
H	-1.808344	0.737401	-1.797526
O	-3.221335	1.484575	-1.167230
H	-3.424166	1.067227	-0.275855
H	-4.045490	1.421514	-1.688704
O	-3.366570	-1.594162	3.025145
H	-2.705553	-1.151330	3.649066
H	-4.087590	-1.917010	3.601962
O	0.558304	-1.841118	3.216218
H	1.111250	-2.357589	3.836307
H	-0.081543	-2.502443	2.804142
O	2.011537	-0.959259	-3.675376
H	1.441113	-0.190194	-4.000901
H	2.097937	-1.572906	-4.431312
O	0.962213	-1.653814	-1.269511
H	1.304267	-1.507604	-2.195587
H	1.578595	-2.342248	-0.857785
O	-0.200949	1.919377	0.634022
H	-0.664205	2.581619	0.045679
H	-0.721633	1.905518	1.487735
Mg	0.383847	0.115102	-0.296010
61			
O	-0.585059	-2.852253	2.637058
H	-1.408597	-2.820624	3.260190
H	-0.384052	-3.798940	2.496486
O	-3.366324	-0.029766	1.097260
H	-3.249763	0.088403	2.101078
H	-4.188041	-0.550538	0.994581
O	-1.185908	3.620353	-0.331203
H	-2.066633	3.131833	-0.428307
H	-1.393403	4.470652	0.103426
O	-0.373638	0.896123	3.532531
H	0.296908	0.130065	3.585960
H	-0.068537	1.561301	4.181766
O	1.837079	-0.645187	0.800144
H	2.679974	-1.016536	0.415847
H	1.766739	-0.910437	1.758909
O	1.617369	1.311187	-1.268097
H	2.405821	0.995254	-1.793393
H	1.269609	2.125138	-1.730885
O	-0.283851	1.439264	-4.056825
H	-0.860864	1.685896	-4.806386
H	-0.035985	2.303842	-3.595639
O	3.599127	0.126488	-2.643204
H	2.951414	-0.120857	-3.379396
H	4.314639	0.639068	-3.068020
O	0.375884	3.391585	-2.444351
H	-0.262341	3.604522	-1.685687
H	0.871766	4.212609	-2.629621
O	-1.121584	-1.396723	0.432399
H	-1.973428	-0.930711	0.677301
H	-0.911722	-1.979431	1.218864
O	2.304719	-3.567701	-1.223840
H	2.640566	-3.973197	-2.047970
H	3.037312	-2.932077	-0.963082
O	3.920383	-1.556177	-0.621577
H	3.915575	-0.944599	-1.425590
H	4.844405	-1.582109	-0.304870
O	-2.831227	0.044207	3.662053
H	-1.888038	0.432209	3.700037
H	-3.378620	0.618449	4.234640
O	-1.287960	0.451100	-1.759529
H	-1.034237	0.804542	-2.658616
H	-2.035445	1.029373	-1.433256
O	-3.183951	1.965183	-0.596342
H	-3.345916	1.274676	0.130432
H	-4.037940	2.090350	-1.054370
O	-2.660183	-2.571422	4.144141
H	-2.780132	-1.573961	4.068268
H	-2.376572	-2.705334	5.070598
O	1.224897	-1.161839	3.351148

H	1.825462	-1.459197	4.062989
H	0.582796	-1.934470	3.168306
O	1.564456	-0.444373	-4.178514
H	0.897281	0.312111	-4.265182
H	1.526022	-0.943008	-5.017936
O	0.703074	-1.557738	-1.865464
H	0.997376	-1.245617	-2.766373
H	1.288508	-2.352873	-1.645700
O	-0.249670	1.423992	0.903271
H	-0.548056	2.330473	0.620686
H	-0.312403	1.348887	1.896411
Mg	0.268620	-0.081854	-0.436745

61

O	1.468091	-3.740718	-0.543607
H	1.625812	-4.572343	-1.031563
H	2.347858	-3.242566	-0.548499
O	-3.164414	0.493146	1.676713
H	-2.812566	0.789856	2.577637
H	-4.048684	0.120115	1.864381
O	-0.996074	3.745083	-0.606378
H	-1.908194	3.319312	-0.508283
H	-1.073285	4.641926	-0.226630
O	0.420457	1.459557	3.388233
H	0.777633	0.507915	3.460875
H	1.052362	2.034238	3.862826
O	1.634338	-0.660704	0.815560
H	2.388523	-1.190266	0.435094
H	1.445221	-0.999103	1.737135
O	1.489549	1.101464	-1.397215
H	2.225069	0.643404	-1.895921
H	1.203591	1.887833	-1.943524
O	-0.563907	1.110357	-4.100231
H	-1.144397	1.339107	-4.852768
H	-0.203611	1.987984	-3.749577
O	3.261393	-0.454126	-2.679572
H	2.565063	-0.677778	-3.378730
H	4.020057	-0.072835	-3.163703
O	0.386296	3.140600	-2.762981
H	-0.186473	3.492946	-2.005046
H	0.929144	3.890436	-3.074872
O	-1.300269	-1.218218	0.689936
H	-1.980586	-0.715046	1.214705
H	-0.962942	-2.025012	1.190777
O	-0.220044	-3.480779	1.583636
H	-0.929644	-4.129669	1.406911
H	0.414535	-3.632899	0.825258
O	3.465859	-2.056732	-0.581091
H	3.501880	-1.515055	-1.433817
H	4.391624	-2.200047	-0.303529
O	-2.052551	0.920424	4.019256
H	-1.108923	1.275718	3.903916
H	-2.441988	1.397550	4.778160
O	-1.542247	0.497837	-1.661309
H	-1.329395	0.743959	-2.604844
H	-2.186972	1.172481	-1.301669
O	-3.109170	2.218348	-0.331522
H	-3.165506	1.629885	0.495108
H	-4.028399	2.378228	-0.621076
O	-1.465611	-1.699818	3.984354
H	-1.774949	-0.753461	4.113655
H	-1.414329	-2.048491	4.896821
O	0.986756	-1.085049	3.355131
H	1.580558	-1.467095	4.030698
H	0.048365	-1.450884	3.560882
O	1.136724	-0.910676	-4.127934
H	0.519636	-0.116536	-4.251979
H	1.036622	-1.468020	-4.924170
O	0.218011	-1.706158	-1.720871
H	0.555288	-1.544599	-2.646226
H	0.657766	-2.541903	-1.385281
O	-0.339091	1.563236	0.824583
H	-0.408305	2.475342	0.434742
H	0.026830	1.648797	1.748420
Mg	0.043825	-0.074820	-0.409004

61

O	0.342306	-4.408960	1.681001
H	-0.390746	-4.891777	1.249351
H	0.908008	-4.109002	0.902019
O	-3.610315	0.663884	1.086467
H	-3.615977	0.892288	2.094536
H	-4.464209	0.215549	0.923228
O	-0.811398	3.770732	-0.462239
H	-1.755079	3.417167	-0.566400
H	-0.891295	4.656064	-0.056446
O	-0.863247	1.462192	3.547454
H	-0.229058	0.687617	3.737800
H	-0.506882	2.216124	4.059030
O	1.352938	-1.006178	1.083765
H	2.282140	-1.224854	0.804029
H	1.358365	-0.779364	2.052720

O	1.682826	0.991602	-1.060141
H	2.425502	0.536393	-1.551082
H	1.489155	1.833756	-1.563137
O	-0.053268	1.271595	-3.969997
H	-0.553202	1.565450	-4.756644
H	0.313151	2.108008	-3.535731
O	3.511023	-0.482170	-2.353705
H	2.841001	-0.704171	-3.079889
H	4.261609	-0.036658	-2.793026
O	0.850943	3.165296	-2.412384
H	0.191593	3.526341	-1.732940
H	1.460446	3.898564	-2.625814
O	-1.566102	-1.041233	0.663274
H	-2.346215	-0.442214	0.857122
H	-1.380492	-1.553445	1.504495
O	1.746853	-3.695038	-0.482362
H	2.039163	-4.453283	-1.026201
H	2.576426	-3.136439	-0.320022
O	3.594465	-1.884238	-0.115456
H	3.697459	-1.401287	-0.995443
H	4.496428	-2.016826	0.236239
O	-3.494694	1.171900	3.615316
H	-2.493156	1.273525	3.693486
H	-3.823239	2.086658	3.726095
O	-1.315884	0.607899	-1.692360
H	-0.966721	0.844131	-2.598736
H	-1.990215	1.307767	-1.453674
O	-3.028079	2.434513	-0.734533
H	-3.340969	1.830703	0.025696
H	-3.826042	2.690483	-1.236853
O	-0.853797	-2.432138	2.839058
H	-0.355157	-3.221315	2.396411
H	-1.538297	-2.832718	3.410566
O	0.750356	-0.584055	3.669173
H	1.275825	-0.817560	4.459882
H	0.130332	-1.376775	3.499240
O	1.437202	-0.904513	-3.876328
H	0.921711	-0.050416	-4.046226
H	1.369532	-1.436822	-4.693106
O	0.296050	-1.720037	-1.561814
H	0.683413	-1.515796	-2.459616
H	0.814772	-2.505501	-1.216214
O	-0.139363	1.600390	0.972133
H	-0.356262	2.482115	0.557564
H	-0.494624	1.614664	1.906975
Mg	0.050804	-0.085473	-0.254361

Ca – 1 water molecule

4

O	-0.158105	-0.052760	-0.082185
H	-1.005755	-0.302343	0.327688
H	-0.192859	-0.397777	-0.993351
Ca	1.578291	0.877548	0.871216

4

O	-0.044955	0.054403	-0.166795
H	-0.663789	-0.406605	-0.762216
H	0.337193	0.779973	-0.693134
Ca	0.434731	-0.485723	1.898902

4

O	-0.073419	0.025567	0.163405
H	-0.435624	0.856718	0.521314
H	-0.275803	-0.657177	0.828019
Ca	0.931181	-0.243167	-1.761825

4

O	-0.108652	-0.152171	-0.045185
H	-0.434551	-0.344805	-0.943052
H	-0.794471	-0.486916	0.560661
Ca	1.557935	1.163626	0.494167

4

O	0.016466	0.023262	-0.183608
H	-0.600212	0.424475	-0.821901
H	0.609808	-0.542653	-0.711125
Ca	-0.045468	0.134402	2.001154

4

O	-0.140354	-0.072447	-0.078503
H	-1.005161	-0.289979	0.332852
H	-0.201452	-0.393941	-1.004245
Ca	1.568539	0.881034	0.873265

4

O	-0.039720	0.046140	-0.163582
H	-0.669966	-0.407386	-0.764936
H	0.339177	0.784626	-0.688354
Ca	0.433689	-0.481333	1.893629

4

O -0.078251 0.025019 0.154140
H -0.434431 0.862508 0.522954
H -0.271279 -0.661705 0.829156
Ca 0.930295 -0.243881 -1.755337
4

O -0.138119 -0.097187 -0.042057
H -0.416205 -0.361686 -0.945875
H -0.788711 -0.511904 0.565211
Ca 1.563296 1.150511 0.489312
4

O 0.002434 -0.004825 -0.174940
H -0.597318 0.437725 -0.814366
H 0.621549 -0.536368 -0.721284
Ca -0.046072 0.142953 1.995109

Ca – 2 water molecules

7

O -0.030902 0.030598 -2.228029
H 0.546632 -0.467567 -2.832009
H -0.597911 0.576534 -2.800221
O 0.014950 -0.032018 2.228197
H -0.477072 -0.633049 2.814077
H 0.551705 0.525713 2.817885
Ca -0.007366 -0.000187 0.000101
7

O -0.808223 -0.260463 -2.069532
H -0.357866 0.012357 -2.888012
H -1.746786 -0.349644 -2.311500
O 0.822568 0.190486 2.060487
H 0.495018 -0.256706 2.860192
H 1.594855 0.708166 2.346342
Ca 0.000434 -0.044198 0.002023
7

O -0.977402 -0.808062 1.033664
H -0.949147 -1.718785 1.375999
H -1.189297 -0.246166 1.798546
O 0.956121 0.894452 -1.048051
H 1.595497 0.835391 -0.316365
H 1.454882 1.267703 -1.795442
Ca -0.966921 -0.205758 -1.099778
7

O 1.308589 1.111944 -0.102357
H 2.178254 1.414549 0.213660
H 0.685716 1.821907 0.129531
O -1.290029 -1.085923 0.005585
H -1.547826 -1.022876 0.942472
H -2.096832 -1.344268 -0.472102
Ca 0.776662 -0.932305 -0.780743
7

O -0.051149 -1.302348 -1.325188
H -0.494690 -1.717778 -2.085712
H 0.868178 -1.156413 -1.610982
O -0.027750 1.254824 1.464413
H -0.118119 2.181936 1.181538
H 0.832910 1.207813 1.918300
Ca -1.027894 -0.490464 0.497024
7

O -0.025805 0.038555 -2.226700
H 0.556412 -0.459580 -2.838460
H -0.617760 0.562380 -2.806811
O 0.025321 -0.040577 2.226679
H -0.499477 -0.619881 2.818552
H 0.561138 0.519926 2.826738
Ca 0.000207 -0.000798 0.000001
7

O -0.824112 -0.177342 -2.062628
H -0.414240 0.134938 -2.896698
H -1.683956 -0.565282 -2.329621
O 0.826651 0.172364 2.062001
H 0.403772 -0.113705 2.898985
H 1.690601 0.551566 2.328267
Ca 0.001284 -0.002540 -0.000305
7

O -1.096811 -0.839302 1.063238
H -0.820705 -1.713392 1.411209
H -1.398702 -0.330855 1.845538
O 1.032548 0.851486 -1.099953

H 1.713617 0.851450 -0.394879
H 1.442619 1.317945 -1.858477
Ca -0.948833 -0.118559 -1.018104
7

O 1.252413 1.200160 -0.098370
H 1.004903 1.566709 0.776374
H 2.159021 1.530889 -0.271771
O -1.252895 -1.192594 0.056153
H -0.987147 -1.596520 0.909080
H -2.200342 -1.420300 -0.054870
Ca 0.038583 -0.125316 -1.380550
7

O -0.078676 -1.165139 -1.281203
H -0.551654 -1.508048 -2.068642
H 0.850874 -1.045158 -1.568692
O 0.056560 1.140044 1.308096
H 0.143553 1.947581 0.758897
H 0.470012 1.365587 2.168063
Ca -0.909182 -0.757295 0.722875

Ca – 4 water molecules

13

O -0.491662 2.276270 0.636079
H -0.805088 2.632175 1.488907
H -0.453955 3.054749 0.049778
O 2.266020 -0.416433 -0.147889
H 3.024783 0.196620 -0.160354
H 2.667113 -1.299633 -0.248164
O -0.698019 -1.628464 1.464078
H -0.312907 -1.970025 2.292227
H -1.472438 -2.198898 1.300929
O -1.072953 -0.212954 -1.903299
H -1.959357 0.104132 -2.158682
H -0.718618 -0.622749 -2.714816
Ca 0.027082 0.085211 0.101207
13

O 1.165940 1.473485 1.698712
H 0.827057 1.723976 2.578654
H 2.048676 1.887539 1.656370
O 0.104184 0.256977 -2.224534
H 0.835370 0.311747 -2.867237
H -0.703000 0.342315 -2.764919
O -2.195855 0.192608 0.162567
H -2.781724 -0.582651 0.249563
H -2.796079 0.957502 0.244272
O 0.993405 -1.917259 0.357364
H 1.021099 -2.625207 -0.312741
H 1.442082 -2.297636 1.135272
Ca 0.113668 0.183873 0.077494
13

O 2.102167 0.520821 0.456467
H 2.575236 1.270344 0.048385
H 2.744953 0.142414 1.085305
O -0.843838 0.039581 2.248724
H -0.492268 0.651383 2.921431
H -1.563046 -0.436673 2.704737
O 0.119854 -1.822880 -1.540906
H -0.587925 -2.286001 -2.026234
H 0.944155 -2.214946 -1.885480
O -1.397433 1.211239 -1.148010
H -2.060950 1.844763 -0.816884
H -1.409498 1.326884 -2.116373
Ca -0.059894 -0.184574 0.079987
13

O 0.846674 -1.539131 0.948798
H 1.074768 -2.353143 0.462434
H 1.088635 -1.728438 1.874306
O 1.838900 1.682299 0.455147
H 1.926384 2.654041 0.449113
H 2.713443 1.359853 0.738987
O -2.231287 0.080091 0.757645
H -2.987370 0.696544 0.762222
H -2.579993 -0.731756 1.171005
O -0.453998 -0.105918 -2.146642
H -1.290226 -0.449602 -2.512128
H 0.113366 0.041856 -2.926004
Ca -0.044232 0.378314 0.058260
13

O -1.144898 -1.045513 -1.553697
H -0.849742 -0.984796 -2.481063
H -1.912433 -1.646978 -1.579643
O -1.230220 1.962148 0.548695

H -1.176531 2.590036 1.293430
H -1.851069 2.379834 -0.077021
O 1.802116 0.618566 -0.809406
H 2.529305 0.050096 -1.125004
H 2.092267 1.524837 -1.023149
O 0.512701 -1.543989 1.905183
H 1.389735 -1.600179 2.329333
H -0.026054 -2.201760 2.383449
Ca -0.126535 -0.048614 0.251466
13

O -0.435864 1.929514 0.857404
H 0.177346 2.590838 1.238187
H -1.326385 2.326338 0.947687
O 2.331264 -0.268085 -0.208590
H 2.890555 0.037649 -0.951868
H 2.960066 -0.604661 0.462212
O -0.889506 -1.583683 1.374627
H -1.244998 -1.403757 2.268981
H -1.121017 -2.517638 1.193521
O -0.969970 -0.129996 -2.028114
H -1.000525 0.588101 -2.692954
H -1.452771 -0.876199 -2.438728
Ca 0.081804 -0.088419 -0.022363
13

O 1.086230 1.532444 1.353103
H 1.418169 1.340266 2.253814
H 1.415592 2.431311 1.147827
O 0.270471 0.439542 -2.242442
H 0.582761 -0.212723 -2.902339
H 0.022984 1.230775 -2.763411
O -2.220767 -0.041897 0.434142
H -2.932028 -0.312992 -0.181675
H -2.681970 0.228633 1.254273
O 0.884900 -1.916673 0.485196
H 1.830181 -2.170242 0.460393
H 0.406543 -2.739916 0.712402
Ca -0.008246 0.098738 -0.020446
13

O 2.055750 0.688535 0.295433
H 2.480171 1.510409 -0.024997
H 2.746703 0.233528 0.819110
O -0.917332 -0.318299 2.091079
H -0.753026 0.214680 2.895692
H -1.383103 -1.119307 2.407152
O -0.025708 -1.897879 -1.129020
H -0.781264 -2.455152 -1.407082
H 0.771459 -2.393435 -1.407479
O -1.127484 1.595224 -1.293945
H -1.462418 2.476459 -1.029844
H -1.436128 1.472725 -2.215045
Ca -0.096108 0.054869 0.010095
13

O 0.985683 -1.833497 0.805183
H 1.905038 -1.931769 1.126896
H 0.551846 -2.686689 1.011320
O 1.406976 1.819019 0.328813
H 2.063272 2.111962 -0.336293
H 1.588463 2.363617 1.122056
O -2.107552 0.194953 0.991346
H -2.372791 0.529867 1.871995
H -2.928455 -0.165376 0.598374
O -0.322940 -0.137658 -2.117988
H -0.709076 0.522182 -2.729557
H -0.024173 -0.872663 -2.691618
Ca -0.021225 0.071060 0.112617
13

O -1.211652 -1.049962 -1.462819
H -0.872753 -1.321266 -2.340493
H -2.109590 -1.435993 -1.407843
O -1.168794 1.946498 0.535587
H -0.928893 2.669168 1.151338
H -2.040155 2.204840 0.171633
O 1.911487 0.677387 -0.768184
H 2.721165 0.139328 -0.882723
H 2.118436 1.539654 -1.182496
O 0.506218 -1.526019 1.725901
H 0.963270 -1.364750 2.576689
H 0.164086 -2.440836 1.792615
Ca -0.044183 0.015639 0.153369

Ca – 8 water molecules

25

O 0.370550 -2.288007 0.506655

H	-0.487423	-2.772864	0.568411
H	1.021938	-2.832396	0.973331
O	-0.204749	2.297359	0.063158
H	-0.138956	2.665882	-0.851672
H	-0.834519	2.857672	0.539732
O	2.674424	0.068674	0.408622
H	3.340907	-0.274269	-0.205492
H	3.093949	0.044157	1.283644
O	0.835379	0.586232	2.615564
H	0.925365	1.513763	2.887452
H	0.442161	0.145497	3.385698
O	0.510968	0.124262	-1.984588
H	0.433523	1.027347	-2.377882
H	1.236385	-0.305309	-2.463030
O	0.180205	2.777571	-2.563130
H	0.954482	3.290805	-2.846713
H	-0.545161	3.083242	-3.131400
O	-1.954525	-0.448882	0.489928
H	-2.238590	-1.395772	0.498057
H	-2.663344	0.041236	0.048127
O	-2.202408	-3.115074	0.563173
H	-2.580480	-3.539605	1.350617
H	-2.565103	-3.608566	-0.190103
Ca	0.328514	0.043085	0.361160
25			
O	-2.885515	0.944002	-2.132461
H	-3.214538	0.601178	-2.980295
H	-3.546942	1.599128	-1.857782
O	2.228226	0.731091	0.789544
H	2.576150	1.422785	1.371425
H	2.916764	0.022917	0.740950
O	-0.245690	1.291342	-1.795759
H	-1.190281	1.318169	-2.086133
H	0.152273	2.126001	-2.084154
O	-1.952634	-0.939681	-0.435908
H	-2.503463	-0.364366	-1.019170
H	-2.574111	-1.442639	0.110718
O	1.163991	-1.750885	-0.678374
H	0.748197	-2.626019	-0.647458
H	2.080721	-1.878532	-0.335118
O	3.649571	-1.516932	0.401021
H	3.953199	-1.983502	1.196986
H	4.435917	-1.449312	-0.164461
O	-0.358419	-0.934619	2.263636
H	0.031535	-0.619562	3.094822

H	-1.222199	-1.294549	2.520038
O	-1.077335	2.003834	1.087696
H	-1.494389	2.630002	0.474715
H	-1.679004	1.969088	1.848121
Ca	0.051374	0.116979	0.203246
25			
O	1.443504	-1.715447	0.508733
H	1.515398	-2.587326	0.094689
H	1.615431	-1.843561	1.473268
O	-1.830639	1.407692	-0.420748
H	-2.021484	1.514219	-1.384027
H	-2.686560	1.324061	0.024299
O	1.807636	1.800712	0.022912
H	2.420574	2.014108	-0.697694
H	2.190827	2.205239	0.816724
O	1.594999	-1.507643	3.193266
H	2.457604	-1.327365	3.602946
H	1.184053	-2.177460	3.763535
O	0.479083	0.174127	-2.310366
H	-0.270578	0.587292	-2.805903
H	0.807406	-0.545431	-2.869697
O	-1.759285	1.430609	-3.120608
H	-1.636588	2.280489	-3.575052
H	-2.403410	0.948813	-3.664552
O	0.164360	0.596336	2.314175
H	0.642068	-0.096795	2.833516
H	-0.562313	0.898708	2.878913
O	-1.543420	-1.544352	-0.053104
H	-2.374430	-1.467730	-0.546123
H	-1.315773	-2.486512	-0.087592
Ca	0.114871	0.152276	0.008290
25			
O	1.932651	-0.536943	-1.371367
H	2.506388	-0.671428	-0.576161
H	2.231265	-1.184945	-2.027243
O	0.486159	2.207530	-0.491423
H	0.870319	2.532280	0.338416
H	1.059854	2.582383	-1.179286
O	-2.302208	0.417087	0.439019
H	-2.833172	1.206493	0.253720
H	-2.214555	0.379982	1.422177
O	-1.616836	0.127407	3.052130
H	-1.472784	0.889367	3.636480
H	-2.020061	-0.549591	3.619248

O	-1.215340	0.981781	-2.656647
H	-1.254894	1.929882	-2.857373
H	-1.607256	0.541678	-3.426591
O	3.057182	-0.778191	1.065192
H	3.469773	-1.643730	1.224086
H	3.743601	-0.137155	1.310288
O	0.346554	-0.676937	1.377857
H	-0.164753	-0.419568	2.177083
H	1.306422	-0.682288	1.582157
O	-1.176197	-1.959369	-1.714293
H	-2.092109	-2.002841	-2.032973
H	-0.693398	-2.591673	-2.269682
Ca	-0.295328	-0.006979	-0.750702
25			
O	-0.099008	-2.734918	1.629892
H	0.653528	-3.195370	2.035812
H	-0.880577	-3.215616	1.948246
O	-0.193914	-0.019699	1.552719
H	-1.117161	0.289644	1.696542
H	-0.188448	-0.977838	1.783560
O	2.660251	-0.462533	-0.226193
H	3.100881	-1.303178	-0.422506
H	3.361739	0.132756	0.080558
O	1.478920	2.215456	0.307588
H	1.433957	3.126993	-0.021117
H	1.391574	2.292440	1.270908
O	1.050475	0.836903	-2.889191
H	1.948512	0.829319	-3.257330
H	0.521410	1.333774	-3.532567
O	-1.534976	1.432239	-1.022758
H	-2.105592	1.363305	-1.803330
H	-2.136761	1.344905	-0.241720
O	-0.024565	-1.940791	-0.969663
H	-0.083770	-2.433577	-0.116209
H	-0.568746	-2.428011	-1.605520
O	-2.740389	0.986970	1.358703
H	-3.500556	0.382701	1.359343
H	-3.044282	1.765037	1.854280
Ca	0.507120	0.312737	-0.676964
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O	0.521909	-2.260011	0.384082
H	-0.387378	-2.669804	0.486029
H	1.113706	-2.805534	0.936997
O	0.235766	2.391218	0.030634
H	0.062516	2.649534	-0.922090
H	-0.326423	2.980629	0.569092
O	2.831723	0.113597	0.712282
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H	3.297085	0.793468	1.239506
O	0.389508	0.359858	2.703451
H	1.030415	-0.015641	3.339286
H	-0.469942	0.297681	3.166364
O	0.685704	0.069121	-1.971509
H	0.425822	0.936061	-2.402689
H	0.311070	-0.626649	-2.545194
O	-0.038134	2.555520	-2.615517
H	0.583313	3.117726	-3.122441
H	-0.908370	2.705676	-3.038458
O	-1.821479	-0.202062	0.458117
H	-2.117305	-1.159409	0.485773
H	-2.469126	0.250087	-0.115743
O	-2.071549	-2.854098	0.568798
H	-2.419381	-3.272958	1.382667
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Ca	0.504197	0.085784	0.365256
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O	-2.534269	0.752175	-2.608197
H	-2.595151	0.318786	-3.484143
H	-3.202551	1.467277	-2.637541
O	1.972404	0.812561	0.977541
H	2.282189	1.728010	0.838093
H	2.715601	0.227233	0.644543
O	-0.115544	1.184026	-1.574257
H	-0.973225	1.170873	-2.092875
H	0.247124	2.083107	-1.690167
O	-2.200361	-0.761050	-0.436429
H	-2.516107	-0.269645	-1.250352
H	-3.003976	-0.942560	0.087525
O	1.028516	-1.860062	-0.327831
H	0.834559	-2.787914	-0.091967
H	2.023090	-1.765808	-0.235589
O	3.558419	-1.100996	0.019056
H	4.143640	-1.564799	0.652667
H	4.118665	-0.943563	-0.768656
O	-0.531288	-1.169293	2.453287
H	-0.339174	-2.120027	2.575831
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O	-1.149397	1.788756	1.633792
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Ca -0.164760 0.003493 0.449244
25

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H 1.551387 -2.541114 0.117693
H 1.777478 -1.698529 1.429713
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H -1.858296 1.668345 -1.489039
H -2.649402 1.442676 -0.146248
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H 2.587733 -1.109980 3.495755
H 1.434693 -2.130896 3.653869
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H -3.458369 0.512531 1.590367
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Ca 0.564343 0.412640 -0.529627

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O -2.202257 1.910818 0.065854
H -2.958428 1.964473 -0.537742

H	-1.607767	2.671065	-0.183668
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H	-1.525009	-2.029758	-1.557179
H	-2.335233	-2.519106	-0.307135
O	-1.406095	-0.379161	2.431878
H	-1.760516	0.331766	2.986791
H	-0.619035	-0.732254	2.917585
O	-0.271106	3.619800	-0.610006
H	-0.356583	4.576499	-0.479391
H	-0.137346	3.491316	-1.582288
O	1.008052	-1.289911	3.220929
H	1.623301	-0.518602	3.296834
H	1.303856	-1.947437	3.868600
O	-0.228386	-2.320539	-2.674114
H	-0.549876	-2.784343	-3.463047
H	0.145708	-3.023778	-2.091971
O	0.766700	1.606308	0.908000
H	1.434476	1.575221	1.627147
H	0.697995	2.509912	0.537321
O	0.514822	-3.969747	-0.643312
H	-0.234420	-4.502877	-0.331071
H	1.246689	-4.602448	-0.728597
O	2.452551	0.952171	2.983437
H	2.496141	1.551290	3.746581
H	3.379246	0.812239	2.727281
O	0.865251	-1.558687	0.563209
H	1.058384	-1.638857	1.527987
H	0.806529	-2.475227	0.210213
O	-0.285624	0.390017	-2.080962
H	-0.155548	1.181873	-2.647276
H	-0.120167	-0.418454	-2.604783
O	-0.014284	2.902616	-3.192952
H	0.836126	3.103853	-3.618544
H	-0.680953	3.236084	-3.815243
Ca	-0.781048	0.042827	0.179264

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O	-1.642206	2.127317	0.039213
H	-2.055720	1.728841	0.840698
H	-2.320540	2.123868	-0.672372
O	-1.206277	-1.009091	-0.816220
H	-1.735234	-1.289535	-0.033680
H	-0.720785	-1.827300	-1.073887
O	-2.493238	-1.826044	1.430786
H	-2.042045	-2.472611	1.997680
H	-3.379527	-2.199178	1.290531
O	2.224463	2.114188	-0.452528
H	2.978900	1.522227	-0.199348
H	2.254245	2.849841	0.178091
O	-2.233774	0.706914	2.265457
H	-2.481336	-0.232492	2.089381
H	-2.637821	0.943623	3.114014
O	1.830036	-0.739063	-1.341959
H	2.708663	-0.641773	-0.907037
H	1.573577	-1.686117	-1.308560
O	3.872754	0.127847	0.170298
H	3.560267	-0.277313	1.016701
H	4.829377	-0.019795	0.123653
O	0.454749	-3.111545	-1.292493
H	0.485804	-3.799143	-0.608158
H	0.377139	-3.604426	-2.125813
O	2.541918	-0.866821	2.306299
H	2.953442	-0.668367	3.164081
H	2.442033	-1.833027	2.312457
O	0.382425	0.693564	1.696036
H	-0.485250	0.622826	2.156515
H	1.030007	0.078982	2.103649
O	-0.329908	1.489215	-2.843343
H	-1.294053	1.707793	-2.863166
H	0.109215	2.198018	-3.336913
O	-2.954015	1.967867	-2.343609
H	-3.381246	2.763149	-2.701949
H	-3.580727	1.250057	-2.529314
Ca	0.232844	0.849558	-0.639881

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O	-1.368192	1.437139	-3.016992
H	-1.536108	1.670803	-3.942650
H	-1.833399	2.122240	-2.476257
O	1.632076	0.773290	1.749362
H	2.405107	0.277822	2.096036
H	1.568659	1.657968	2.168666
O	-2.443764	3.182022	-1.229148
H	-2.259861	4.119476	-1.405730
H	-3.406025	3.143276	-1.099042
O	1.713962	-1.749400	0.157703
H	1.244947	-2.584456	0.396785
H	2.415901	-1.641433	0.840331
O	1.008684	1.099378	-1.793350
H	0.251116	1.321398	-2.393754
H	1.563272	1.893312	-1.768237
O	-1.015210	1.984857	0.762482

H	-1.546235	2.518525	0.127020
H	-0.478725	2.610722	1.300885
O	-0.977090	-3.489218	-1.792178
H	-0.323677	-3.744189	-2.464151
H	-1.780279	-3.973875	-2.045844
O	-1.187807	-1.358284	1.556355
H	-0.926428	-2.300905	1.397398
H	-2.149617	-1.334455	1.438008
O	-0.085683	-3.668749	0.758557
H	-0.446307	-3.814916	-0.150869
H	-0.037546	-4.537485	1.185417
O	0.791396	3.246572	2.394618
H	1.237884	4.051020	2.085054
H	0.443802	3.480855	3.270566
O	3.489374	-1.113671	2.178893
H	4.427751	-0.982866	1.968274
H	3.485244	-1.652974	2.986097
O	-1.381394	-0.754304	-1.446623
H	-1.310732	-1.688601	-1.744276
H	-1.488197	-0.180016	-2.236605
Ca	0.136137	0.042003	0.152637

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O	-2.054364	0.019077	-1.245586
H	-2.497886	-0.811060	-0.934331
H	-2.018755	-0.057440	-2.211299
O	-1.074352	1.041557	1.874948
H	-1.964850	0.651852	2.029362
H	-1.147117	2.017078	1.989222
O	-3.407049	-0.409407	2.041935
H	-4.223796	0.102517	1.921426
H	-3.500871	-0.803812	2.925166
O	2.409613	-2.476021	-1.943680
H	3.294318	-2.570242	-2.334666
H	1.850133	-3.059737	-2.482223
O	2.167430	-2.813770	0.735005
H	2.725632	-3.476455	1.168327
H	2.374410	-2.859530	-0.230336
O	2.320343	2.595509	-2.150700
H	3.210451	2.845430	-1.853603
H	2.193188	3.098466	-2.971363
O	-2.944252	-2.201954	0.041050
H	-3.700058	-2.741015	-0.235910
H	-3.254819	-1.663452	0.809290
O	1.241815	0.026996	-2.067990
H	1.797176	-0.785235	-2.100769
H	1.826386	0.799354	-2.230053
O	-0.324373	-1.921976	0.462329
H	0.403035	-2.547094	0.667891
H	-1.170925	-2.395617	0.326866
O	0.240673	2.605438	-0.431499
H	0.034941	3.246825	0.281165
H	1.022323	2.901314	-0.948015
O	-0.879593	3.762042	1.815420
H	-0.394894	4.159442	2.556963
H	-1.686457	4.295087	1.734645
O	2.022653	-0.132914	1.081843
H	2.851159	0.348918	0.944094
H	2.258439	-1.094518	1.036348
Ca	0.001979	0.312594	-0.072363

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O	-0.822907	1.392155	-0.268154
H	-0.847191	2.163543	-0.879613
H	-1.768029	1.186777	-0.088549
O	-1.627973	-1.568187	-0.183049
H	-1.567225	-2.264966	0.512649
H	-2.389567	-0.984607	0.037713
O	-3.375335	0.419560	0.204605
H	-3.806186	0.590976	1.058031
H	-4.075572	0.546283	-0.455424
O	-0.810390	3.447489	-2.087027
H	-1.642213	3.550960	-2.577345
H	-0.628019	4.323533	-1.709105
O	-0.237179	-1.797869	3.733020
H	0.326649	-2.146794	4.442854
H	-0.978924	-1.373011	4.194380
O	-0.795015	-3.375924	1.613167
H	-1.227475	-4.219915	1.813158
H	-0.633041	-2.931509	2.481447
O	2.860454	1.492157	1.597015
H	2.637337	2.360992	1.969178
H	3.751002	1.305471	1.936966
O	1.111152	-2.888485	-0.262547
H	0.516237	-3.242645	0.445654
H	0.991798	-3.499310	-1.006261
O	1.113633	-0.537494	1.721189
H	0.663589	-0.847746	2.537652
H	1.711845	0.208256	1.950393
O	2.393994	0.740762	-0.980508
H	2.653797	1.230242	-0.167778
H	2.147632	1.399853	-1.669828

O	0.352026	-0.520359	-2.870807
H	0.602343	0.398805	-3.152407
H	-0.462438	-0.731115	-3.351714
O	1.189249	1.996055	-3.087041
H	0.471498	2.629315	-2.835842
H	1.636137	2.389356	-3.851987
Ca	0.471171	-0.583869	-0.508700

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O	-2.005196	1.876258	0.050312
H	-2.807058	1.925209	-0.503928
H	-1.443604	2.675966	-0.206291
O	-2.258245	-1.435922	-0.668637
H	-1.890523	-1.883016	-1.496074
H	-2.664519	-2.151647	-0.143006
O	-1.247002	-0.436168	2.418721
H	-1.623239	0.255367	2.996512
H	-0.443574	-0.796163	2.914473
O	-0.146252	3.615116	-0.602361
H	-0.255995	4.585538	-0.565621
H	-0.022454	3.381725	-1.572272
O	1.093542	-1.288174	3.270731
H	1.548814	-0.398269	3.375607
H	1.226827	-1.762617	4.114565
O	-0.858547	-2.330051	-2.708157
H	-1.205493	-2.805050	-3.488198
H	-0.268723	-2.982536	-2.222075
O	1.047473	1.593565	0.713363
H	1.414199	1.648267	1.637483
H	0.792419	2.508836	0.420381
O	0.692199	-3.777720	-1.077122
H	0.282920	-4.602623	-0.742803
H	1.545620	-4.074693	-1.455665
O	2.056949	1.207716	3.200966
H	1.778404	1.786895	3.940456
H	3.034643	1.274004	3.204915
O	1.000281	-1.676845	0.604090
H	1.157198	-1.838505	1.571277
H	0.952155	-2.554606	0.135606
O	0.157256	0.063107	-2.026452
H	0.097884	0.895522	-2.570014
H	-0.185112	-0.695921	-2.570017
O	0.098569	2.572939	-3.052798
H	0.917616	2.815409	-3.532383
H	-0.619778	2.811724	-3.674590
Ca	-0.583802	-0.003543	0.191290

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O	-1.459017	1.909754	0.142407
H	-1.834157	1.529487	0.990449
H	-2.213933	2.082755	-0.479830
O	-1.291836	-1.296220	-1.073951
H	-1.944355	-1.442132	-0.331971
H	-0.743874	-2.130356	-1.097035
O	-2.993869	-1.575221	1.041387
H	-2.891124	-2.444562	1.481089
H	-3.940874	-1.550577	0.790624
O	2.071146	1.963345	-0.609658
H	2.846021	1.390879	-0.308849
H	2.065684	2.728876	-0.003331
O	-1.987046	0.521253	2.342474
H	-2.491285	-0.281347	2.013912
H	-2.393282	0.774086	3.194033
O	1.904542	-0.955965	-1.500571
H	2.718460	-0.796776	-0.944339
H	1.622292	-1.899988	-1.346956
O	3.781738	0.081973	0.111470
H	3.607926	-0.093175	1.086157
H	4.752069	0.139029	0.008734
O	0.569338	-3.272687	-1.135653
H	0.732642	-3.824007	-0.343488
H	0.572071	-3.911261	-1.878013
O	2.893647	-0.294487	2.590460
H	3.140265	0.384707	3.251726
H	3.112291	-1.144758	3.024536
O	0.449237	-0.112907	1.434037
H	-0.323736	0.101599	2.025222
H	1.265582	-0.184090	1.997489
O	-0.528549	1.471952	-2.833448
H	-1.461419	1.821635	-2.709653
H	-0.030588	2.226364	-3.204385
O	-2.965080	2.310860	-2.071729
H	-3.201223	3.231699	-2.305640
H	-3.739998	1.785096	-2.356537
Ca	0.198446	0.517224	-0.785862

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O	-1.248957	1.319853	-3.091487
H	-1.358758	1.517353	-4.042138
H	-1.674802	2.083361	-2.594828
O	1.852679	1.158103	1.471239
H	2.451439	0.517872	1.942934

H	1.467496	1.788360	2.138330
O	-2.153640	3.170048	-1.393976
H	-1.824445	4.079017	-1.552947
H	-3.127123	3.275183	-1.352329
O	1.847604	-1.645775	-0.028736
H	1.356789	-2.494755	0.171919
H	2.490329	-1.537759	0.728172
O	1.062905	1.265028	-1.813399
H	0.286080	1.336868	-2.454716
H	1.776216	0.848110	-2.335378
O	-1.155699	1.859778	0.769858
H	-1.530734	2.463367	0.070130
H	-0.738342	2.438830	1.466139
O	-1.384530	-3.381301	-1.666863
H	-0.963854	-3.724260	-2.482357
H	-2.269477	-3.801559	-1.659388
O	-0.669596	-1.313980	1.761559
H	-0.510741	-2.259096	1.451939
H	-1.629128	-1.265308	1.938284
O	0.058871	-3.555240	0.563227
H	-0.496537	-3.667840	-0.267463
H	0.165171	-4.446304	0.950061
O	0.323057	2.973750	2.748836
H	0.631736	3.901765	2.709716
H	-0.025409	2.873749	3.657975
O	3.354635	-0.969187	2.135809
H	4.326621	-0.884273	2.052794
H	3.228352	-1.468393	2.968305
O	-1.406429	-0.697718	-1.335396
H	-1.461964	-1.658398	-1.596923
H	-1.472275	-0.154280	-2.166745
Ca	0.255499	0.117909	0.103280
37			
O	-1.506840	0.411819	-0.982316
H	-2.071932	-0.400454	-0.807759
H	-0.866846	0.120830	-1.676969
O	-1.155887	1.131953	2.195896
H	-2.031938	0.650884	2.229925
H	-1.373095	2.067819	1.919723
O	-3.447695	-0.337239	2.106733
H	-4.269543	0.187019	2.008608
H	-3.597224	-0.853766	2.925796
O	2.432287	-2.300994	-2.257756
H	3.359676	-2.203557	-2.557928
H	2.009699	-2.850044	-2.950354
O	2.055506	-2.936824	0.296935
H	2.518956	-3.739459	0.606684
H	2.264264	-2.855409	-0.682745
O	1.895749	2.434088	-2.278354
H	2.848717	2.621404	-2.401284
H	1.459222	2.891241	-3.025703
O	-2.746326	-1.755365	-0.049798
H	-3.441121	-2.318216	-0.443864
H	-3.160630	-1.326149	0.757918
O	1.070871	-0.050045	-1.664916
H	1.605744	-0.828597	-1.990390
H	1.483825	0.773662	-2.051388
O	-0.305589	-1.920143	0.996293
H	0.412618	-2.537421	0.680814
H	-1.162305	-2.156444	0.543895
O	0.971939	2.541920	0.260344
H	0.187450	3.132821	0.433372
H	1.270842	2.709766	-0.676179
O	-1.328892	3.625257	1.152693
H	-1.284561	4.395370	1.755440
H	-2.059928	3.841679	0.538726
O	2.447407	-0.493876	1.283086
H	2.717962	-0.506186	2.221932
H	2.464929	-1.461567	0.998682
Ca	0.334375	0.302474	0.583116
37			
O	-1.032891	1.556183	-0.430417
H	-1.052919	2.174248	-1.211355
H	-1.978261	1.411790	-0.149102
O	-1.884380	-1.481479	-0.068735
H	-1.779818	-2.221857	0.590614
H	-2.578062	-0.854013	0.272697
O	-3.420829	0.665832	0.491652
H	-3.678232	0.948536	1.392518
H	-4.228019	0.805016	-0.044093
O	-0.700656	3.194979	-2.572160
H	-1.367348	3.188913	-3.289994
H	-0.627250	4.139086	-2.320739
O	0.369823	-2.301711	3.517079
H	1.190354	-2.742111	3.820502
H	-0.132811	-2.135718	4.341424
O	-0.893503	-3.441594	1.472500
H	-1.170572	-4.369340	1.603866
H	-0.488090	-3.144876	2.342838
O	2.559947	1.691738	1.816711

H	2.367803	2.614556	2.080089
H	3.438453	1.507868	2.207311
O	0.996607	-2.668919	-0.216378
H	0.344333	-3.140937	0.393133
H	0.990007	-3.194424	-1.040358
O	0.552877	-0.128061	1.910891
H	0.609832	-0.866904	2.577172
H	1.306958	0.496438	2.096047
O	2.236843	0.730779	-0.684039
H	2.458646	1.283842	0.114219
H	2.173973	1.335015	-1.474088
O	0.374465	-0.514941	-2.740824
H	0.796912	0.353321	-3.033998
H	-0.404886	-0.629495	-3.318000
O	1.541433	1.844952	-3.025098
H	0.762195	2.477079	-2.970720
H	2.049448	2.101937	-3.819486
Ca	0.204481	-0.426997	-0.376294

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O	0.455751	-2.260530	0.465298
H	-0.443265	-2.526226	0.145909
H	1.078581	-2.433124	-0.283382
O	0.537495	-1.109249	-3.236671
H	-0.391967	-1.457925	-3.279474
H	0.735368	-0.745731	-4.113414
O	1.447711	-0.168027	3.302259
H	0.739326	-0.183536	3.964100
H	1.991445	0.630961	3.524550
O	-1.996176	-2.793745	-0.474485
H	-2.651934	-2.152000	-0.084907
H	-2.356897	-3.675957	-0.289298
O	1.236416	2.329584	1.263619
H	1.763024	2.492962	2.079186
H	0.363770	2.764926	1.392188
O	2.289829	-2.208829	-1.529332
H	1.730065	-1.871281	-2.272384
H	2.683627	-3.032916	-1.853845
O	2.984348	-0.563366	0.507180
H	3.104898	-1.064129	-0.326100
H	3.791597	-0.057747	0.741874
O	-1.428869	0.245112	1.740026
H	-2.219175	-0.151966	1.301832
H	-1.595011	1.220544	1.727127
O	-3.464788	0.213419	-2.127790
H	-2.977076	-0.514664	-2.598614
H	-4.276987	0.367152	-2.635595
O	-3.521269	-0.800618	0.344281
H	-3.661060	-0.377921	-0.544582
H	-4.403681	-0.967369	0.710731
O	2.904322	2.078158	3.356611
H	3.725599	1.794050	2.884650
H	3.189158	2.581852	4.134062
O	-2.020268	-1.871763	-2.997850
H	-2.025281	-2.359824	-2.129125
H	-2.418228	-2.480255	-3.640982
O	4.823290	1.022790	1.755407
H	5.477622	0.495902	2.243317
H	5.357127	1.659802	1.252895
O	0.203068	0.575012	-1.157442
H	0.322580	0.058322	-1.989481
H	-0.526996	1.223179	-1.304491
O	-1.928646	2.253751	-1.288567
H	-2.575069	1.588434	-1.641795
H	-1.863504	2.939707	-1.971173
O	-1.443631	2.879913	1.330848
H	-1.748049	2.811617	0.392195
H	-2.034816	3.515958	1.761300
Ca	0.788516	-0.011040	1.013457

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O	0.547814	-2.180285	0.083182
H	-0.328549	-2.578927	-0.136048
H	1.187775	-2.419455	-0.626772
O	0.684564	-0.738323	-3.094771
H	-0.226191	-1.136743	-3.098109
H	0.829292	-0.409725	-3.995972
O	1.385163	-0.985306	2.991036
H	0.865078	-0.661314	3.742030
H	2.288782	-0.602295	3.115131
O	-1.961839	-2.915779	-0.476224
H	-2.625176	-2.351310	0.004543
H	-2.299424	-3.824440	-0.430317
O	1.044442	2.057807	1.982386
H	1.888704	2.560335	2.011448
H	0.301346	2.675668	1.825413
O	2.528283	-2.163431	-1.756174

H	1.945091	-1.691210	-2.403018
H	2.938151	-2.891098	-2.247532
O	3.001915	-0.162907	0.074443
H	3.133316	-0.928259	-0.526845
H	3.556268	-0.281254	0.876536
O	-1.417636	0.186379	1.656140
H	-2.242056	-0.272135	1.364759
H	-1.629280	1.152833	1.682813
O	-3.499459	0.154988	-1.793095
H	-2.943296	-0.481106	-2.317920
H	-4.315491	0.275786	-2.304615
O	-3.534540	-1.058091	0.584246
H	-3.707289	-0.577693	-0.267939
H	-4.397918	-1.246205	0.983502
O	3.631552	2.833151	2.193147
H	4.071104	3.178806	1.399030
H	3.858608	3.466334	2.893258
O	-1.833782	-1.692477	-2.845269
H	-1.884260	-2.281123	-2.042666
H	-2.177259	-2.230398	-3.577262
O	3.794180	0.132024	2.639228
H	4.629637	-0.167207	3.029163
H	3.865312	1.115395	2.577559
O	0.365926	1.112590	-1.144076
H	0.471022	0.534623	-1.939072
H	-0.483181	1.607202	-1.257510
O	-2.036112	2.320655	-1.186119
H	-2.652341	1.584678	-1.445955
H	-2.170718	3.016598	-1.848128
O	-1.536330	2.854593	1.432398
H	-1.825333	2.817665	0.486817
H	-2.223978	3.354160	1.898012
Ca	0.771545	-0.002969	0.884652

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O	0.660977	-2.300684	1.104462
H	1.469378	-2.722391	0.727844
H	-0.077080	-2.766417	0.642001
O	0.818659	-2.606029	-2.252056
H	0.055279	-2.996497	-1.750673
H	0.807582	-3.035813	-3.121401
O	1.284566	0.156786	2.871668
H	1.790172	-0.567640	3.269181
H	1.795594	0.985352	3.056079
O	-3.763577	0.655626	-1.943069
H	-4.525279	0.864227	-2.507006
H	-3.955762	1.065978	-1.060250
O	0.834196	2.345692	0.723485
H	1.364370	2.690029	1.473666
H	0.010843	2.882574	0.634660
O	2.803615	-3.018073	-0.444197
H	3.310593	-3.842115	-0.494517
H	2.198808	-3.011100	-1.228585
O	2.942615	-0.361883	0.024107
H	3.641842	0.008456	0.608624
H	3.164484	-1.306201	-0.137916
O	-1.650298	-0.195940	0.713380
H	-2.328998	0.510191	0.839676
H	-2.157525	-0.871019	0.205608
O	-1.425435	1.950000	-2.222391
H	-1.351012	2.469637	-3.038253
H	-2.313104	1.509013	-2.271431
O	-3.225800	-1.745125	-0.930224
H	-3.482338	-0.944399	-1.459489
H	-4.020716	-1.994895	-0.433476
O	2.619570	2.482786	2.788922
H	3.458614	2.074125	2.463715
H	2.858019	2.992027	3.578254
O	-1.143707	-3.329602	-0.603693
H	-1.955551	-2.807509	-0.826916
H	-1.423196	-4.257881	-0.571172
O	4.626635	1.007987	1.681551
H	5.156717	0.483550	2.304226
H	5.284711	1.497028	1.160302
O	0.488857	0.054780	-1.763050
H	-0.248755	0.603050	-2.114807
H	0.489155	-0.835366	-2.182606
O	-3.635534	1.641116	0.554236
H	-3.022503	2.418648	0.515108
H	-4.259510	1.812563	1.276022
O	-1.586672	3.314181	0.100986
H	-1.503522	2.941744	-0.818632
H	-1.751168	4.263075	-0.016891
Ca	0.680837	0.014711	0.573970

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O	-2.824853	-3.022407	0.637737
H	-2.950266	-2.969531	-0.343757
H	-3.205222	-3.869474	0.915274
O	1.823593	-0.366613	-0.694674
H	1.822894	-0.578687	-1.658604
H	2.440869	0.390948	-0.559329

O	2.524083	1.991711	2.492221
H	1.662494	2.368557	2.805088
H	3.168450	2.187334	3.190148
O	-2.685588	-2.597238	-2.011580
H	-3.269736	-2.895094	-2.725005
H	-1.775432	-2.916532	-2.242968
O	-0.406046	2.006988	0.477157
H	0.085456	2.508639	-0.216367
H	-0.273876	2.449336	1.348429
O	-0.059722	-3.057671	-2.219415
H	0.453711	-2.343379	-2.681178
H	0.317559	-3.892845	-2.538257
O	1.327363	-0.392882	2.309029
H	1.946863	-1.136610	2.256375
H	1.897317	0.406591	2.445281
O	-0.042423	2.629224	3.065302
H	-0.343097	3.493319	3.388795
H	-0.668755	1.970469	3.459270
O	-0.138783	1.203201	-3.328502
H	-0.488303	1.670935	-4.102166
H	0.342380	1.877928	-2.782161
O	-1.812206	0.736562	3.923171
H	-2.599769	1.162050	4.301929
H	-1.449968	0.214175	4.658012
O	1.072596	2.870929	-1.584391
H	1.148229	3.812258	-1.805542
H	1.927630	2.624435	-1.144427
O	1.330797	-0.999553	-3.238978
H	2.015816	-1.098956	-3.917584
H	0.814323	-0.182639	-3.469383
O	3.126015	1.927962	-0.139977
H	4.065706	2.095434	-0.308654
H	2.989665	2.064698	0.832286
O	-0.154915	-2.676270	0.456769
H	0.005832	-2.935235	-0.484137
H	-1.082882	-2.974517	0.625101
O	-1.518048	-0.185086	-1.463945
H	-1.163657	0.301000	-2.245073
H	-2.036488	-0.948912	-1.804454
O	-2.246466	-0.561085	1.583910
H	-2.260904	-0.276669	2.523869
H	-2.637596	-1.457660	1.499173
Ca	-0.198755	-0.311908	0.477353
49			
O	0.374787	-2.420608	0.706210
H	-0.532270	-2.613729	0.357133
H	1.000493	-2.615328	-0.034726
O	0.491381	-1.385743	-3.044972
H	-0.453509	-1.687085	-3.109800
H	0.720359	-1.008271	-3.908113
O	1.452534	-0.177980	3.540190
H	0.826721	0.188757	4.183440
H	2.261767	0.387140	3.625100
O	-2.109469	-2.755272	-0.290364
H	-2.705023	-2.029238	0.044832
H	-2.555363	-3.585600	-0.057576
O	1.252451	2.128272	1.423845
H	2.094599	2.391967	0.998281
H	0.515430	2.706506	1.132851
O	2.220598	-2.434569	-1.288430
H	1.669014	-2.140962	-2.055704
H	2.665199	-3.246991	-1.574611
O	2.980832	-0.684079	0.642013
H	2.951327	-1.212313	-0.187466
H	3.470653	0.152100	0.469365
O	-1.480043	0.385733	1.864086
H	-2.246167	0.012506	1.363324
H	-1.522455	1.356981	1.671583
O	-3.327283	0.347427	-2.158536
H	-2.912990	-0.461454	-2.563495
H	-4.156388	0.490510	-2.641913
O	-3.479526	-0.601693	0.343655
H	-3.551576	-0.180488	-0.554844
H	-4.383269	-0.670774	0.689034
O	3.671834	1.419348	3.526877
H	4.440358	1.047445	3.990290
H	3.487325	2.249436	3.996848
O	-2.107432	-1.947888	-2.855859
H	-2.136128	-2.390790	-1.963469
H	-2.556480	-2.556610	-3.463868
O	3.844917	1.900865	0.806569
H	4.622776	2.366914	0.464978
H	3.987356	1.809768	1.777752
O	0.125240	0.299894	-0.960126
H	0.289550	-0.237927	-1.771139
H	-0.422018	1.068078	-1.244118
O	-1.614128	2.334645	-1.586434
H	-2.315242	1.704025	-1.893721
H	-1.384119	2.882338	-2.352515
O	-1.268285	2.927611	1.002507
H	-1.510604	2.857871	0.044998

H	-1.760524	3.686023	1.351351
Ca	0.736625	-0.165823	1.259188
49			
O	0.363230	-2.348419	0.485651
H	-0.514217	-2.644532	0.102317
H	1.034584	-2.499126	-0.247161
O	0.611922	-1.113791	-3.117277
H	-0.358485	-1.396334	-3.176203
H	0.840348	-0.741146	-3.991677
O	1.345658	-0.226819	3.391746
H	0.605544	-0.048552	4.005065
H	1.971072	0.553625	3.526713
O	-2.017483	-2.900810	-0.632453
H	-2.648351	-2.267739	-0.148727
H	-2.410993	-3.792058	-0.541964
O	1.101445	2.246850	1.343833
H	1.632617	2.415501	2.168251
H	0.218682	2.700221	1.444418
O	2.258313	-2.297021	-1.417445
H	1.718626	-1.930070	-2.183239
H	2.644959	-3.132755	-1.743738
O	2.926831	-0.729054	0.665300
H	2.981670	-1.202665	-0.207020
H	3.667057	-0.068094	0.735434
O	-1.487968	0.285560	1.830825
H	-2.259569	-0.165340	1.376297
H	-1.652563	1.268126	1.706176
O	-3.322017	0.324481	-1.896393
H	-2.842039	-0.399283	-2.425492
H	-4.163667	0.484069	-2.369469
O	-3.404966	-0.939285	0.412928
H	-3.527764	-0.407157	-0.441366
H	-4.301998	-1.072012	0.780058
O	2.885525	1.929526	3.309300
H	3.665311	1.728373	2.707896
H	3.248614	2.406897	4.080442
O	-1.953988	-1.677552	-2.939772
H	-2.004163	-2.288220	-2.124641
H	-2.390822	-2.169906	-3.664232
O	4.659693	1.194955	1.434209
H	5.519465	0.848618	1.751327
H	4.908652	1.919531	0.823872
O	0.378460	0.616008	-1.097234
H	0.466607	0.049130	-1.918956
H	-0.333797	1.293610	-1.289584
O	-1.681986	2.306731	-1.349302
H	-2.390679	1.636514	-1.621738
H	-1.665103	2.981879	-2.056506
O	-1.500399	2.886203	1.219880
H	-1.671336	2.807157	0.228020
H	-2.111641	3.572409	1.551179
Ca	0.713000	-0.094873	1.084577
49			
O	0.419224	-2.346799	0.397077
H	-0.448210	-2.647440	-0.004851
H	1.100590	-2.473696	-0.331155
O	0.642770	-0.806681	-3.013321
H	-0.308069	-1.134972	-3.128843
H	0.890409	-0.396774	-3.865680
O	1.865070	-0.864720	3.088116
H	1.544084	-0.526334	3.946697
H	2.797713	-0.489000	3.002372
O	-1.939739	-2.906272	-0.761562
H	-2.596949	-2.324439	-0.247635
H	-2.308188	-3.812328	-0.735892
O	0.848551	1.996481	2.125081
H	1.716387	2.480561	2.068326
H	0.115840	2.590496	1.811713
O	2.283184	-2.220738	-1.506390
H	1.731572	-1.771896	-2.221384
H	2.706420	-2.992014	-1.930463
O	2.848274	-0.184977	0.153578
H	2.926586	-0.974157	-0.449165
H	3.570321	-0.238774	0.834888
O	-1.536446	0.163453	1.872982
H	-2.284429	-0.296881	1.389787
H	-1.705340	1.145816	1.743235
O	-3.440774	0.294866	-1.858767
H	-2.894135	-0.355196	-2.418432
H	-4.290627	0.403446	-2.331686
O	-3.405858	-1.070684	0.391047
H	-3.575861	-0.507818	-0.435345
H	-4.286960	-1.275577	0.763423
O	3.437857	2.779927	2.191489
H	3.819606	3.231719	1.410806
H	3.644061	3.382036	2.936275
O	-1.894570	-1.527129	-2.980190
H	-1.928491	-2.192918	-2.208410
H	-2.269041	-2.000102	-3.750943
O	4.187093	0.213328	2.428170

H	5.055486	0.045900	2.843095
H	4.069525	1.210837	2.412017
O	0.195600	0.815900	-0.923657
H	0.379340	0.305939	-1.765621
H	-0.566949	1.432344	-1.126623
O	-1.957190	2.370889	-1.244485
H	-2.616803	1.661994	-1.540964
H	-1.932377	3.038135	-1.958529
O	-1.587061	2.802296	1.332981
H	-1.819368	2.782268	0.353293
H	-2.252704	3.380535	1.753833
Ca	0.684011	-0.130046	1.139177

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O	0.537945	-2.576256	0.811173
H	1.401115	-2.799353	0.348576
H	-0.145067	-2.983369	0.199519
O	0.864717	-2.461690	-2.559966
H	0.054799	-2.922192	-2.166255
H	0.856199	-2.661035	-3.516637
O	0.938601	0.277171	3.207978
H	1.414706	-0.393051	3.735932
H	1.536090	1.090860	3.225364
O	-3.615617	0.570806	-1.589047
H	-4.471489	0.745273	-2.030251
H	-3.628748	1.119156	-0.731365
O	0.797695	2.113368	0.711460
H	1.290062	2.537825	1.463293
H	0.104439	2.749332	0.377832
O	2.747223	-2.838884	-0.726489
H	3.170366	-3.718716	-0.762735
H	2.173429	-2.778526	-1.552038
O	2.806332	-0.569203	0.707920
H	3.581095	-0.014324	0.990952
H	3.118953	-1.339055	0.167797
O	-1.788299	-0.317122	1.356049
H	-2.316341	0.529458	1.270878
H	-2.284591	-0.945044	0.750433
O	-1.385860	1.704215	-2.438694
H	-1.378328	2.000808	-3.370401
H	-2.289702	1.276270	-2.290201
O	-3.072715	-1.773244	-0.520787
H	-3.358044	-0.955276	-1.046839
H	-3.904105	-2.197408	-0.228081
O	2.412676	2.438032	2.822375
H	3.299772	2.111236	2.482380
H	2.613291	3.107373	3.505505
O	-1.120626	-3.411876	-1.135234
H	-1.937551	-2.824316	-1.020053
H	-1.450688	-4.330207	-1.190789
O	4.536130	1.252197	1.704438
H	5.228841	0.928700	2.316783
H	5.030056	1.778869	1.042465
O	0.310053	-0.104906	-1.414594
H	-0.280589	0.520827	-1.922699
H	0.477190	-0.900811	-1.995421
O	-3.176124	1.874085	0.643954
H	-2.520412	2.583522	0.330021
H	-3.876994	2.343525	1.138441
O	-1.287507	3.360852	-0.400057
H	-1.294536	2.872220	-1.290043
H	-1.425567	4.305757	-0.611563
Ca	0.517371	-0.197520	0.897754

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O	-2.885936	-2.943959	0.602695
H	-2.977384	-2.864054	-0.396494
H	-3.273254	-3.810119	0.836047
O	1.815074	-0.367483	-0.566943
H	1.856149	-0.654219	-1.526605
H	2.377759	0.456205	-0.483456
O	2.272550	1.923478	2.449634
H	1.457886	2.450768	2.748258
H	2.952127	2.071165	3.138085
O	-2.602428	-2.497783	-2.017882
H	-3.191193	-2.708067	-2.769168
H	-1.698389	-2.881972	-2.255186
O	-0.540536	2.035774	0.504438
H	-0.060006	2.531983	-0.221588
H	-0.416064	2.541496	1.356373
O	-0.071572	-3.177732	-2.268736
H	0.509249	-2.467646	-2.695216
H	0.247273	-4.034767	-2.613518
O	0.887307	-0.295428	2.501075
H	1.369972	-1.107907	2.751768
H	1.565939	0.461701	2.547132
O	-0.098530	2.881256	3.008835
H	-0.344310	3.723256	3.439674
H	-0.601454	2.149807	3.489146
O	0.090935	1.064788	-3.317915
H	-0.190355	1.470580	-4.161409
H	0.452872	1.819055	-2.745511

O	-1.227451	0.604734	3.838172
H	-1.352535	0.385724	4.783114
H	-0.383621	0.134191	3.563669
O	0.910974	2.882437	-1.571020
H	0.963834	3.822942	-1.833090
H	1.781738	2.677949	-1.096092
O	1.443658	-1.162003	-3.082841
H	2.176208	-1.271318	-3.721018
H	0.969371	-0.304490	-3.340538
O	2.924059	2.028045	-0.128028
H	3.862961	2.260145	-0.268829
H	2.757509	2.106428	0.864843
O	-0.240883	-2.643452	0.364342
H	-0.060441	-2.961085	-0.569737
H	-1.188364	-2.931530	0.535337
O	-1.571053	-0.081630	-1.558719
H	-1.093629	0.326683	-2.337908
H	-2.029281	-0.911311	-1.883982
O	-2.339491	-0.477186	1.597170
H	-2.187777	-0.256162	2.554052
H	-2.689181	-1.403972	1.526497
Ca	-0.314397	-0.278082	0.392243

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O	0.264730	-2.324314	0.768458
H	-0.616426	-2.594123	0.372145
H	0.943129	-2.550570	0.062520
O	0.608240	-1.291928	-2.892664
H	-0.362923	-1.565215	-2.986022
H	0.884883	-0.953589	-3.767058
O	1.515617	-0.306400	3.501277
H	0.988923	0.046526	4.245051
H	2.367651	0.222994	3.530901
O	-2.100297	-2.832628	-0.396569
H	-2.710390	-2.129886	0.011477
H	-2.540923	-3.692121	-0.240160
O	1.073727	2.257925	1.630135
H	1.924409	2.448920	1.151002
H	0.339369	2.781349	1.205969
O	2.156014	-2.462435	-1.128554
H	1.640956	-2.126737	-1.926694
H	2.595782	-3.286500	-1.414310
O	2.872664	-0.626291	0.681693
H	2.824875	-1.210397	-0.125765
H	3.305425	0.234911	0.428062
O	-1.552365	0.609323	1.810426
H	-2.309378	0.125966	1.362903
H	-1.623151	1.558874	1.490391
O	-3.307569	0.280677	-1.993778
H	-2.839647	-0.502203	-2.444151
H	-4.140327	0.413870	-2.490089
O	-3.423712	-0.728297	0.437005
H	-3.531188	-0.285892	-0.469024
H	-4.327214	-0.815520	0.802449
O	3.798572	1.149651	3.343833
H	4.579889	0.594000	3.545464
H	3.844792	1.866712	4.009885
O	-1.962580	-1.831403	-2.807260
H	-2.042259	-2.360596	-1.939329
H	-2.374381	-2.390030	-3.497284
O	3.592078	1.950878	0.771234
H	4.326627	2.475751	0.397116
H	3.853137	1.769539	1.720653
O	0.369552	0.536306	-0.943169
H	0.488829	-0.096760	-1.711096
H	-0.310762	1.196679	-1.266534
O	-1.582644	2.227451	-1.679323
H	-2.322436	1.564827	-1.880293
H	-1.448218	2.749648	-2.494457
O	-1.326823	3.083345	0.781614
H	-1.518292	2.916695	-0.194018
H	-1.868955	3.853133	1.041741
Ca	0.646823	-0.061170	1.298699

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O	-2.471413	-2.144197	2.346087
H	-2.387963	-1.441894	3.038038
H	-3.385168	-2.464360	2.378942
O	0.408492	3.087298	3.273361
H	-0.565525	2.925675	3.374701
H	0.514481	4.051300	3.298012
O	2.507793	1.366672	3.479960
H	1.827533	2.072875	3.575300
H	2.965108	1.321167	4.333125
O	-2.214570	2.463422	3.159992
H	-2.421312	2.505136	2.195633
H	-2.889487	3.003160	3.601014

O	3.843975	0.199453	-1.446696
H	4.738934	-0.038538	-1.733060
H	3.368903	0.465835	-2.269439
O	0.672767	-0.573153	2.931697
H	1.321328	0.080655	3.283268
H	-0.182693	-0.391818	3.389198
O	0.446547	0.553356	-1.527672
H	-0.373357	1.043517	-1.756066
H	1.087328	0.726267	-2.251648
O	-1.999665	-0.864388	-3.143186
H	-2.678745	-1.135150	-3.782038
H	-1.153519	-0.848113	-3.666547
O	-1.299038	-2.982323	-1.585737
H	-1.655518	-2.163882	-2.022557
H	-1.953422	-3.674929	-1.768113
O	0.544332	1.965614	0.865443
H	1.043311	2.447824	0.189412
H	0.633521	2.484345	1.706742
O	2.183751	-1.903557	-0.788341
H	2.870109	-1.281055	-1.121632
H	1.846891	-2.384824	-1.581095
O	-1.648863	-0.363591	0.489648
H	-2.017679	0.541195	0.588407
H	-2.146285	-0.955461	1.096631
O	-2.108903	2.320829	0.465708
H	-2.296379	2.211285	-0.495133
H	-1.121808	2.296251	0.513378
O	-2.021043	1.651696	-2.151941
H	-2.026533	2.250098	-2.914797
H	-2.197262	0.748345	-2.522015
O	1.002331	-3.097157	-2.882593
H	0.119906	-3.229042	-2.440219
H	1.274865	-3.962912	-3.223999
O	-0.208842	-2.793941	0.915874
H	-0.640892	-2.954129	0.043277
H	-0.972248	-2.714091	1.528766
O	2.247272	0.745329	-3.565696
H	1.645414	0.098868	-4.021421
H	2.180428	1.573740	-4.065105
O	0.400648	-0.990917	-4.385769
H	0.349958	-1.205845	-5.331202
H	0.694511	-1.834923	-3.942360
O	-1.806662	-0.090561	3.929403
H	-2.080570	0.829383	3.677706
H	-1.957114	-0.154628	4.885480
O	2.974093	0.050983	1.124534
H	3.436791	0.388584	0.330295
H	3.013090	0.725507	1.832915
Ca	0.718068	-0.556284	0.544132
61			
O	-3.135657	-0.359565	1.546013
H	-2.905173	-0.351575	2.513045
H	-4.096185	-0.477875	1.500014
O	1.427359	2.198159	3.975729
H	1.645925	2.883985	3.291527
H	2.156607	2.186053	4.613885
O	0.894468	0.254012	2.156592
H	1.180423	0.916679	2.825483
H	0.643461	-0.540861	2.696175
O	-1.215446	2.255102	4.155234
H	-1.540408	2.722338	4.941884
H	-0.226108	2.230210	4.259961
O	3.080982	1.238523	-2.322333
H	4.015742	1.272176	-2.576291
H	2.606303	0.848553	-3.099160
O	0.155228	-1.699828	3.851837
H	0.678934	-1.527616	4.649746
H	-0.715971	-1.272978	4.037190
O	-0.417497	0.466841	-2.329033
H	-1.246563	-0.031641	-2.562001
H	0.224369	0.311268	-3.061053
O	-1.323808	-3.113604	-3.843613
H	-1.708397	-3.856907	-4.333915
H	-0.416959	-2.970034	-4.221874
O	-0.597721	-3.553427	-1.328077
H	-0.974403	-3.493024	-2.247876
H	-0.850863	-4.429323	-0.995794
O	1.548541	3.776632	1.834798
H	1.947482	4.659081	1.893074
H	0.567209	3.930812	1.830824
O	2.231625	-0.670619	-0.617377
H	2.710241	-0.066598	-1.234668
H	2.207657	-1.550346	-1.067111
O	-1.799960	1.625599	0.347823
H	-1.702920	2.435123	0.903252
H	-2.421205	1.018839	0.821537
O	-1.165710	3.739682	1.918392
H	-1.301869	3.292245	2.795047
H	-1.706466	4.544304	1.942726
O	-2.638936	-0.927707	-2.880582
H	-3.085172	-0.478030	-3.614673

H	-2.253901	-1.733199	-3.298419
O	1.961003	-3.032124	-1.908344
H	1.069525	-3.348542	-1.595499
H	2.584281	-3.737158	-1.670965
O	-0.961104	-1.508748	0.371585
H	-0.993809	-2.273304	-0.250777
H	-1.865910	-1.338695	0.715448
O	1.517497	0.068567	-4.176066
H	1.493018	-0.902082	-4.388808
H	1.350296	0.526294	-5.014491
O	1.250595	-2.590760	-4.444357
H	1.731082	-3.097496	-5.117957
H	1.648292	-2.855533	-3.570344
O	-2.186865	-0.249745	4.048330
H	-1.855454	0.684901	4.126705
H	-2.777739	-0.380357	4.806521
O	1.373996	2.482834	-0.571544
H	2.143668	2.282025	-1.146706
H	1.686336	2.990972	0.211235
Ca	0.215014	0.458611	-0.074461
61			
O	-3.567857	-0.558070	1.283590
H	-3.356568	-0.588467	2.252232
H	-4.510583	-0.344334	1.219085
O	1.544670	1.446688	4.113500
H	0.605393	1.449805	4.436541
H	2.105775	1.344189	4.897295
O	0.992523	-0.462890	2.219220
H	1.296369	0.191686	2.887288
H	0.477753	-1.143956	2.732726
O	-1.111647	1.517180	4.495260
H	-1.275890	2.241979	3.829201
H	-1.396810	1.893024	5.344254
O	3.464963	1.125494	-1.408885
H	4.420636	1.244826	-1.513687
H	3.072058	1.168120	-2.317109
O	-0.499759	-2.256598	3.499820
H	-0.160352	-2.382063	4.399420
H	-1.331111	-1.735580	3.627486
O	-0.300950	0.547237	-2.146111
H	-1.104006	0.565978	-2.723950
H	0.461614	0.758903	-2.733404
O	-0.902845	-1.853606	-4.467431
H	-1.177261	-2.406873	-5.215754
H	0.069911	-1.693992	-4.604775

O	-0.877558	-3.151827	-2.137597
H	-1.001865	-2.694287	-3.014304
H	-1.306348	-4.016760	-2.234557
O	1.405084	3.452514	2.399488
H	1.912291	4.254486	2.599205
H	1.615190	2.800221	3.119635
O	2.067650	-1.056590	-0.718031
H	2.752476	-0.406268	-1.002454
H	2.106723	-1.825313	-1.332278
O	-1.698313	1.309171	0.748141
H	-1.662191	2.066684	1.376338
H	-2.494898	0.770313	0.968850
O	-1.268189	3.297388	2.539909
H	-1.763239	4.126180	2.629412
H	-0.307315	3.543351	2.470327
O	-2.327243	0.399749	-3.906919
H	-2.113862	1.058970	-4.585613
H	-1.894140	-0.426169	-4.232777
O	1.805900	-3.133592	-2.413722
H	0.840523	-3.311608	-2.257502
H	2.266160	-3.983673	-2.339656
O	-1.438366	-1.719288	0.068270
H	-1.437940	-2.254028	-0.760863
H	-2.357972	-1.489903	0.318832
O	1.957114	0.942481	-3.622164
H	2.008270	0.043563	-4.041353
H	1.964610	1.576964	-4.355296
O	1.764206	-1.567589	-4.531289
H	1.921361	-2.223792	-3.798282
H	2.244795	-1.908875	-5.302082
O	-2.628510	-0.594372	3.791618
H	-2.112499	0.201265	4.094618
H	-3.229760	-0.812638	4.520725
O	1.388718	2.020230	0.126291
H	2.264001	1.902971	-0.304436
H	1.521589	2.604428	0.910408
Ca	0.142843	0.029451	0.083767
61			
O	-2.988365	-1.074564	1.995023
H	-2.550910	-0.817473	2.847340
H	-3.938745	-1.121337	2.177616
O	1.448704	2.640750	4.307524
H	1.474896	3.012489	3.383560
H	1.842324	3.326049	4.870412
O	0.727032	-0.728044	2.471738

H	1.513847	-0.375238	2.964350
H	-0.024989	-0.630518	3.105950
O	-1.215700	2.365039	4.323400
H	-1.678014	2.837177	5.033632
H	-0.243918	2.522757	4.473864
O	3.477176	0.049753	-1.585860
H	4.424235	-0.045399	-1.767563
H	3.040942	0.168893	-2.466151
O	2.715375	0.228938	4.023097
H	2.332926	1.120567	4.212788
H	2.573762	-0.267129	4.844199
O	-0.237362	0.017625	-2.038206
H	-1.013435	0.458799	-2.464880
H	0.512856	0.198402	-2.650942
O	-1.904098	-1.571859	-4.368828
H	-2.421589	-2.000712	-5.068051
H	-0.952996	-1.662721	-4.646169
O	-1.797187	-2.991135	-2.107427
H	-1.945303	-2.407935	-2.901105
H	-2.344777	-3.776653	-2.263455
O	1.225753	3.394420	1.734308
H	1.540745	4.279366	1.490107
H	0.236784	3.433310	1.642132
O	1.888701	-1.925076	-0.610521
H	2.587691	-1.344433	-1.001078
H	1.576469	-2.509867	-1.343437
O	-1.767506	0.808013	0.518399
H	-1.769517	1.703919	0.931855
H	-2.396932	0.255609	1.039774
O	-1.467117	3.195503	1.786580
H	-1.516436	2.979440	2.754956
H	-2.022755	3.979706	1.655979
O	-2.213186	0.995830	-3.595440
H	-1.741091	1.548681	-4.236991
H	-2.214067	0.097541	-4.006348
O	0.799655	-3.393710	-2.612040
H	-0.173467	-3.377606	-2.397348
H	1.045231	-4.329798	-2.681189
O	-1.160637	-2.366753	0.454732
H	-1.520689	-2.596712	-0.434879
H	-1.938572	-2.099583	0.996025
O	1.878318	0.290310	-3.727931
H	1.585182	-0.500044	-4.255011
H	1.894175	1.038383	-4.344693
O	0.737458	-1.868554	-4.760573
H	1.054638	-2.317547	-5.560584
H	0.864323	-2.523723	-4.018155
O	-1.430484	-0.294509	4.035360
H	-1.427644	0.679496	4.237955
H	-1.476840	-0.749141	4.890531
O	1.843734	1.233185	0.215526
H	2.616599	1.157322	-0.380417
H	1.814595	2.104815	0.670022
Ca	0.223824	-0.442709	0.201877
61			
O	-3.622047	-0.508224	1.777474
H	-3.322583	-0.576026	2.717263
H	-4.471246	-0.044092	1.835295
O	1.192288	1.730486	3.953015
H	1.337193	2.467307	3.299844
H	1.902349	1.798135	4.610036
O	0.887600	-0.270474	2.189508
H	1.088031	0.403911	2.880138
H	0.376883	-0.982659	2.645404
O	-1.407594	1.865589	4.403937
H	-1.610066	2.333919	5.229917
H	-0.412656	1.799340	4.380942
O	2.805616	1.504038	-2.269194
H	3.679827	1.838226	-2.519925
H	2.363283	1.225069	-3.116356
O	-0.718519	-2.222531	3.128864
H	-0.300806	-2.841840	3.746149
H	-1.387247	-1.713002	3.654509
O	-0.913757	1.796966	-3.856016
H	-1.562533	1.550091	-4.533488
H	-0.053319	1.474419	-4.220232
O	-0.949342	-2.582579	-3.492179
H	-1.698055	-2.760330	-4.081901
H	-0.149516	-2.471367	-4.069161
O	-0.029705	-3.856774	-1.346202
H	-0.178348	-4.810241	-1.248468
H	-0.506986	-3.579832	-2.171271
O	1.151252	3.522120	1.973747
H	1.552343	4.397716	2.090478
H	0.169987	3.664855	2.042486
O	2.385807	-0.574180	-0.619025
H	2.439206	-1.412512	-1.137639
H	2.701431	0.124651	-1.242639
O	-1.809076	1.141474	0.717208
H	-1.806041	1.996625	1.205521
H	-2.504823	0.564206	1.133291

O	-1.513992	3.386204	2.205741
H	-1.610738	2.930280	3.083182
H	-2.143022	4.124128	2.210063
O	-0.590994	-0.237013	-2.159275
H	-0.810494	0.511237	-2.772375
H	-0.820178	-1.064100	-2.643023
O	2.309675	-2.839803	-2.125152
H	1.526659	-3.345280	-1.775628
H	3.061121	-3.451170	-2.064180
O	-0.869135	-1.966608	0.393584
H	-0.597728	-2.750565	-0.140431
H	-0.863604	-2.252962	1.333059
O	1.487940	0.672676	-4.453447
H	1.460983	-0.321486	-4.494173
H	1.916895	0.946346	-5.279596
O	1.433188	-2.014508	-4.496043
H	1.892134	-2.362325	-3.681930
H	1.854561	-2.459823	-5.248195
O	-2.530283	-0.571390	4.235914
H	-2.132218	0.329446	4.376650
H	-3.014199	-0.785651	5.048180
O	0.923918	2.309778	-0.468184
H	1.695041	2.261413	-1.078066
H	1.189696	2.838798	0.318864
Ca	0.154008	0.111180	-0.004505
61			
O	-3.244482	-0.810015	1.661933
H	-2.826325	-0.692304	2.572952
H	-4.205137	-0.897058	1.815794
O	1.300218	2.542396	4.398200
H	0.312984	2.399008	4.580298
H	1.632426	3.093583	5.134619
O	2.546200	0.304414	3.654510
H	2.155352	1.149827	4.028360
H	2.582126	-0.291421	4.429177
O	-1.309402	2.135593	4.469030
H	-1.497948	2.637516	3.601000
H	-1.848073	2.580599	5.154294
O	3.257608	0.794270	-1.656198
H	4.219689	0.868029	-1.808390
H	2.839523	0.685440	-2.568017
O	0.392845	-0.368532	2.273768
H	1.226086	-0.141606	2.799426
H	-0.352194	-0.432125	2.934827
O	-0.367900	0.319340	-2.247966
H	-1.212685	0.134375	-2.771190
H	0.370884	0.402594	-2.913080
O	-1.321894	-2.506147	-4.400219
H	-1.664990	-3.052788	-5.135018
H	-0.335409	-2.369634	-4.590620
O	-1.146009	-3.550149	-1.987210
H	-1.338258	-3.226080	-2.928525
H	-1.473052	-4.471280	-1.957834
O	1.137231	3.562202	1.973590
H	1.465585	4.482329	1.931294
H	1.324655	3.251404	2.920024
O	2.002749	-1.230275	-0.434838
H	2.617759	-0.594930	-0.906892
H	1.881799	-2.006332	-1.054509
O	-1.974109	1.198557	0.433804
H	-1.866861	1.987117	1.040130
H	-2.600752	0.572724	0.902169
O	-1.464827	3.245819	2.112128
H	-1.960941	4.081071	1.997900
H	-0.483493	3.488063	1.982672
O	-2.546618	-0.265431	-3.628171
H	-2.576522	0.344204	-4.392303
H	-2.164950	-1.107998	-4.017320
O	1.457679	-3.248698	-2.140520
H	0.474838	-3.483954	-2.008198
H	1.945976	-4.090548	-2.041272
O	-1.307435	-1.968834	0.178543
H	-1.471829	-2.548574	-0.615266
H	-2.176969	-1.761229	0.615365
O	1.814529	0.371358	-3.831145
H	1.722026	-0.574318	-4.181291
H	1.841651	0.945396	-4.621942
O	1.291431	-2.124524	-4.489688
H	1.819689	-2.570723	-5.182131
H	1.481076	-2.632739	-3.625262
O	-1.803022	-0.373414	3.834899
H	-1.720645	0.577040	4.174389
H	-1.852543	-0.936643	4.632380
O	1.321202	1.929427	-0.151123
H	2.191625	1.733170	-0.590008
H	1.474959	2.533790	0.626257
Ca	0.012875	-0.022352	0.012416
61			
O	-2.942053	-0.646814	1.748395
H	-2.755816	-0.432425	2.717965

H	-3.902678	-0.814628	1.689724
O	1.390909	2.350558	3.750984
H	1.517609	3.037302	3.013117
H	2.120493	2.483874	4.387910
O	1.045668	0.173550	2.203828
H	1.264733	0.942147	2.801163
H	0.685953	-0.534545	2.832426
O	-1.166327	2.430612	4.248539
H	-1.393152	2.961978	5.038643
H	-0.147515	2.410088	4.221042
O	3.191231	1.090459	-2.155516
H	4.125699	1.189925	-2.422177
H	2.693403	0.826591	-2.991005
O	0.031596	-1.567161	3.925291
H	0.556207	-1.441687	4.740992
H	-0.807613	-1.043236	4.105079
O	-0.373162	0.230851	-2.221456
H	-1.255502	-0.079205	-2.602594
H	0.271704	0.267733	-2.982468
O	-1.335162	-2.909872	-3.863641
H	-1.717483	-3.576258	-4.469394
H	-0.402726	-2.720005	-4.214698
O	-0.711328	-3.630814	-1.407281
H	-1.068606	-3.443223	-2.337905
H	-0.944047	-4.562749	-1.222694
O	1.324698	3.881422	1.628729
H	1.632213	4.809601	1.659314
H	0.312058	3.931163	1.662724
O	2.303835	-0.902208	-0.605442
H	2.787103	-0.261621	-1.207159
H	2.195621	-1.745254	-1.134278
O	-1.728515	1.347638	0.450159
H	-1.672317	2.186928	0.991535
H	-2.321895	0.715744	0.953258
O	-1.290665	3.586779	1.875177
H	-1.367284	3.261233	2.830318
H	-1.914546	4.336680	1.800671
O	-2.644635	-0.667582	-3.248754
H	-2.774218	-0.164893	-4.077759
H	-2.244534	-1.532806	-3.563621
O	1.800346	-3.148098	-2.006221
H	0.878691	-3.449993	-1.697888
H	2.393611	-3.913035	-1.866202
O	-0.818214	-1.790367	0.546516
H	-0.957781	-2.488191	-0.153335
H	-1.701920	-1.584915	0.960091
O	1.576849	0.241718	-4.078236
H	1.525612	-0.740425	-4.319719
H	1.424153	0.729508	-4.911505
O	1.187094	-2.341249	-4.409342
H	1.635396	-2.831982	-5.127468
H	1.553392	-2.728987	-3.540495
O	-2.131906	-0.024852	4.184161
H	-1.809524	0.933821	4.264888
H	-2.703822	-0.181851	4.961778
O	1.375428	2.238634	-0.506024
H	2.199411	2.070430	-1.036166
H	1.573970	2.907844	0.205827
Ca	0.289245	0.207238	-0.002356
61			
O	-3.181024	-0.665011	1.297870
H	-3.082178	-0.654298	2.304362
H	-4.140193	-0.712851	1.118317
O	1.203028	1.444019	4.225689
H	0.238600	1.524847	4.524053
H	1.734637	1.324421	5.037298
O	0.858904	-0.422570	2.324007
H	1.070089	0.224992	3.054497
H	0.346609	-1.165372	2.785580
O	-1.405580	1.669255	4.523731
H	-1.467794	2.359165	3.775030
H	-1.757344	2.115369	5.320515
O	3.527312	1.077644	-1.524104
H	4.490248	1.145087	-1.674412
H	3.106356	1.062846	-2.439728
O	-0.541893	-2.281874	3.587322
H	-0.133235	-2.358685	4.472454
H	-1.358648	-1.719987	3.755710
O	-0.056535	0.508250	-2.127043
H	-0.925224	0.520227	-2.642114
H	0.666545	0.699773	-2.787247
O	-1.125037	-1.830707	-4.535737
H	-1.494561	-2.323118	-5.295662
H	-0.139692	-1.706394	-4.741502
O	-0.908459	-3.109249	-2.239010
H	-1.113974	-2.674816	-3.132695
H	-1.271085	-4.015358	-2.299951
O	1.391273	3.350564	2.437365
H	1.845319	4.166482	2.727584
H	1.479542	2.696412	3.205362
O	2.301321	-1.093238	-0.536481

H	2.902565	-0.395114	-0.932678
H	2.156836	-1.769385	-1.260830
O	-1.602316	1.351367	0.557361
H	-1.569009	2.076035	1.243983
H	-2.328508	0.722010	0.842277
O	-1.238851	3.240550	2.450636
H	-1.695178	4.104451	2.406131
H	-0.243506	3.446111	2.414631
O	-2.276196	0.374667	-3.559229
H	-2.229583	1.073371	-4.241792
H	-1.931233	-0.438848	-4.034122
O	1.694236	-2.879892	-2.462807
H	0.708447	-3.095444	-2.317931
H	2.159869	-3.740172	-2.447782
O	-1.051916	-1.835068	0.131989
H	-1.182556	-2.282775	-0.750453
H	-1.952011	-1.581554	0.480461
O	2.078554	0.861318	-3.729605
H	1.982462	-0.028531	-4.202827
H	2.039638	1.542132	-4.430088
O	1.497264	-1.522945	-4.683451
H	1.696462	-2.122266	-3.881974
H	1.997846	-1.905743	-5.432095
O	-2.589759	-0.594407	3.868447
H	-2.199913	0.297233	4.157285
H	-3.285404	-0.803936	4.523287
O	1.600040	2.063512	0.094313
H	2.471413	1.918185	-0.361714
H	1.747484	2.586530	0.930343
Ca	0.330817	0.075273	0.107648
61			
O	-3.316456	-0.388388	1.637012
H	-2.870952	-0.379123	2.542223
H	-4.275481	-0.320592	1.810551
O	1.629454	2.055018	4.506114
H	1.747274	2.588077	3.645394
H	2.131674	2.545376	5.187941
O	0.362181	-0.380044	2.180492
H	1.226314	-0.375389	2.702704
H	-0.376708	-0.421153	2.849760
O	-0.991053	2.086587	4.579594
H	-1.353674	2.505758	5.385501
H	0.020472	2.068838	4.703029
O	3.252478	0.601456	-1.767893
H	4.213155	0.556267	-1.940082
H	2.807339	0.525950	-2.670371
O	2.606230	-0.264724	3.585016
H	2.337806	0.592943	4.031657
H	2.526645	-0.926910	4.300296
O	-0.404302	0.545326	-2.295663
H	-1.268614	0.361873	-2.788694
H	0.328353	0.524009	-2.973367
O	-1.657370	-2.337872	-4.395102
H	-2.055878	-2.845794	-5.129538
H	-0.667801	-2.264720	-4.607867
O	-1.506377	-3.389160	-1.988926
H	-1.693683	-3.056599	-2.928806
H	-1.921382	-4.273215	-1.937559
O	1.647753	3.252516	2.169428
H	2.062827	4.138649	2.140697
H	0.646429	3.433950	2.151753
O	1.824589	-1.298879	-0.537932
H	2.494057	-0.724228	-1.013379
H	1.635292	-2.064125	-1.153792
O	-1.834757	1.535986	0.505483
H	-1.615551	2.251358	1.170444
H	-2.520243	0.950148	0.943772
O	-0.978527	3.374447	2.281443
H	-1.100282	2.985326	3.208842
H	-1.417048	4.248472	2.306130
O	-2.655848	-0.003472	-3.564369
H	-2.706466	0.592917	-4.337744
H	-2.362470	-0.875866	-3.963831
O	1.105768	-3.292272	-2.208665
H	0.113311	-3.457429	-2.047122
H	1.540520	-4.162651	-2.107103
O	-1.539970	-1.666255	0.060094
H	-1.742869	-2.289017	-0.691602
H	-2.384229	-1.414269	0.519641
O	1.734665	0.301774	-3.911956
H	1.537793	-0.632236	-4.250275
H	1.821923	0.861872	-4.708389
O	0.967951	-2.139042	-4.545254
H	1.436583	-2.619563	-5.257447
H	1.138630	-2.673465	-3.692914
O	-1.792532	-0.289083	3.793636
H	-1.579472	0.611518	4.203616
H	-1.886715	-0.909220	4.543468
O	1.503097	1.919874	-0.183145
H	2.326283	1.627973	-0.660507
H	1.771284	2.386435	0.656511

Ca -0.017801 0.115666 -0.047607
61

O -3.832267 -0.347059 2.011137
H -3.353868 -0.444825 2.889587
H -4.597556 0.221147 2.228244
O 1.245228 1.830891 3.784542
H 1.287523 2.579234 3.100005
H 2.036472 1.924121 4.351140
O 0.826632 -0.177777 2.051501
H 1.062858 0.510584 2.734559
H 0.389871 -0.929533 2.551615
O -1.251572 1.825996 4.539459
H -1.398133 2.260917 5.403693
H -0.241324 1.816840 4.409642
O 2.807896 1.513910 -2.092017
H 3.756053 1.747687 -2.103913
H 2.566989 1.257222 -3.038780
O -0.614177 -2.173777 3.058648
H -0.215810 -2.820290 3.673023
H -1.287817 -1.647732 3.599359
O -0.530840 1.698166 -3.978105
H -1.072863 1.511202 -4.770017
H 0.380904 1.357919 -4.231306
O -0.880634 -2.486093 -3.408044
H -1.537256 -2.832997 -4.044263
H -0.040667 -2.305705 -3.945033
O 0.068939 -3.857136 -1.379347
H -0.154841 -4.809467 -1.379660
H -0.407135 -3.467086 -2.186859
O 0.926351 3.541875 1.824407
H 1.258527 4.460553 1.878506
H -0.070566 3.604388 2.006647
O 1.937674 -0.673863 -0.846000
H 2.201318 -1.514337 -1.314773
H 2.409817 0.070478 -1.322465
O -2.066539 1.150445 0.735840
H -1.979193 1.973013 1.295964
H -2.771239 0.593567 1.205953
O -1.632522 3.258290 2.356324
H -1.610142 2.808148 3.263317
H -2.242715 4.017205 2.446824
O -1.198909 -0.110614 -2.169316
H -0.971041 0.588042 -2.868117
H -1.166748 -0.979579 -2.662254
O 2.390241 -2.949824 -2.201699
H 1.596134 -3.469594 -1.845293
H 3.177280 -3.516831 -2.080191
O -0.988182 -2.109869 0.387123
H -0.595221 -2.863889 -0.139182
H -0.877473 -2.341293 1.350695
O 1.900428 0.681148 -4.426755
H 1.793288 -0.327366 -4.486498
H 2.356620 0.950942 -5.248456
O 1.492412 -1.921030 -4.420800
H 1.981025 -2.369575 -3.648007
H 1.758779 -2.418429 -5.220639
O -2.338825 -0.559295 4.221717
H -1.930909 0.348020 4.418022
H -2.774235 -0.840252 5.050951
O 0.724254 2.199043 -0.514596
H 1.561365 2.138885 -1.053062
H 0.934608 2.761168 0.285210
Ca -0.170199 0.055352 -0.075843

Zn – 1 water molecule

4

Zn 0.736787 -1.462450 -0.307579
O -0.060650 0.222980 -0.104873
H -1.041186 0.314608 -0.030818
H 0.365049 0.924862 0.443269
4

Zn -0.059345 1.418493 0.867276
O -0.098599 -0.113662 -0.216684
H -0.534921 -0.940586 0.101637
H 0.692864 -0.364244 -0.752229
4

Zn -0.949895 0.242307 1.343046
O 0.242136 0.060715 -0.096511
H 0.649709 -0.817901 -0.292180
H 0.058050 0.514879 -0.954355
4

Zn 1.014430 -0.872456 1.014949
O -0.115293 0.097266 -0.107112
H -0.244130 1.073679 -0.077410
H -0.655008 -0.298489 -0.830428

4

Zn -0.626152 -1.012089 -1.160450
O -0.042972 0.074536 0.257078
H 0.819281 -0.117750 0.700035
H -0.150157 1.055303 0.203337
4

Zn 0.749738 -1.463215 -0.344978
O -0.080403 0.160302 0.033684
H -1.049909 0.341217 -0.085575
H 0.380573 0.961696 0.396869
4

Zn -0.118673 1.443758 0.800440
O 0.145478 -0.256241 0.038517
H -0.633103 -0.879276 0.005735
H 0.606297 -0.308241 -0.844693
4

Zn -0.880134 0.289209 1.373887
O -0.037780 -0.140545 -0.251270
H 0.754314 -0.746259 -0.231682
H 0.163601 0.597595 -0.890935
4

Zn 1.038568 -0.849119 0.968967
O -0.287240 0.079916 0.009446
H -0.171291 1.063599 -0.110836
H -0.580038 -0.294396 -0.867577
4

Zn -0.686545 -1.034642 -1.097558
O 0.221753 0.187034 0.006287
H 0.722574 -0.164010 0.794096
H -0.257782 1.011618 0.297175

Zn – 2 water molecules

7

Zn 0.039040 0.025798 -0.006530
O 1.008143 -1.566241 -0.029321
H 1.899217 -1.644927 -0.440982
H 0.585218 -2.454574 -0.004887
O -0.884393 1.644543 0.099054
H -1.107560 2.066463 0.960231
H -1.539664 1.928939 -0.577566
7

Zn 0.009030 -0.000088 -0.005976
O -0.926787 1.092477 1.171563
H -1.866767 1.367144 1.084225
H -0.569430 1.403967 2.034079
O 1.059559 -1.054922 -1.130694
H 1.027100 -2.038453 -1.102911
H 1.267297 -0.770124 -2.050287
7

Zn -0.005024 0.042668 -0.000290
O 1.280222 0.541095 1.259322
H 2.210770 0.732803 0.999818
H 1.273644 0.188666 2.178795
O -1.278887 -0.393715 -1.287034
H -1.469807 -1.312088 -1.583830
H -2.010918 0.200573 -1.566780
7

Zn -0.027537 0.074210 0.025732
O 1.617100 0.646296 0.702992
H 2.259316 -0.010975 1.059766
H 2.128343 1.357467 0.250891
O -1.653950 -0.515901 -0.666640
H -2.512407 -0.112677 -0.401630
H -1.810864 -1.438420 -0.971112
7

Zn -0.002533 0.038475 -0.061876
O 1.199494 1.218775 0.736683
H 0.919765 2.054325 1.176032
H 2.061917 0.930925 1.114145
O -1.178776 -1.094879 -0.971934
H -0.883105 -1.970660 -1.312290
H -2.116761 -1.176963 -0.680760
7

Zn -0.035325 -0.024898 0.039038
O 1.031377 -1.559940 0.040376
H 1.881507 -1.568332 -0.474726
H 0.608096 -2.453984 -0.059577

O -1.133501 1.480506 0.184421
H -0.958866 2.144288 0.904074
H -1.393287 1.982361 -0.633606
7

Zn 0.087060 0.064956 0.008372
O -0.892750 1.222396 1.099974
H -1.884367 1.156401 1.124673
H -0.577996 1.420549 2.021773
O 1.084510 -1.062313 -1.099109
H 0.862672 -2.030930 -1.135916
H 1.320872 -0.771058 -2.019767
7

Zn 0.026865 -0.001804 -0.029176
O 1.367731 0.227017 1.253769
H 2.220316 0.670744 0.999100
H 1.125906 0.539885 2.165931
O -1.238620 -0.313707 -1.368591
H -1.368556 -1.237123 -1.713555
H -2.133642 0.114987 -1.307478
7

Zn 0.040437 -0.016401 -0.101391
O 1.765207 0.461068 0.438118
H 2.098020 0.168330 1.327891
H 2.090287 1.387601 0.282950
O -1.671209 -0.461513 -0.705998
H -2.468883 -0.162222 -0.194090
H -1.853859 -1.376862 -1.047480
7

Zn 0.003430 0.018879 -0.030337
O 1.306599 1.128304 0.720310
H 1.219504 2.114880 0.631822
H 1.648134 0.935529 1.633746
O -1.282331 -1.037843 -0.883474
H -1.048028 -1.507019 -1.728130
H -1.847308 -1.652729 -0.343936

Zn – 4 water molecules

13

Zn -0.042040 0.025970 -0.036434
O 0.428455 0.522503 -1.880734
H 1.043766 -0.024796 -2.411830
H -0.210759 0.916197 -2.508538
O -1.164910 1.208519 1.065603
H -2.105155 1.392048 0.866110
H -0.795481 2.022939 1.463781
O 1.708199 0.086981 0.855668
H 2.555855 0.248694 0.395959
H 1.918602 -0.320758 1.719071
O -1.055791 -1.657235 0.048816
H -1.459858 -1.964122 0.886046
H -0.820882 -2.456939 -0.463518
13

Zn 0.034851 -0.033019 0.031680
O -0.188775 1.811155 0.675614
H -0.246939 2.072184 1.615937
H -0.494029 2.568783 0.139510
O 1.906601 -0.373113 -0.460411
H 2.546128 0.354027 -0.601207
H 2.203807 -1.127903 -1.007285
O -0.430927 -1.254412 1.499910
H 0.192547 -1.903468 1.881632
H -1.335269 -1.583178 1.675350
O -1.150708 -0.137296 -1.524309
H -0.957008 -0.560309 -2.383530
H -2.080278 0.166549 -1.542888
13

Zn 0.002220 0.042167 0.087380
O 1.381678 1.329617 0.633772
H 1.770907 1.983067 0.018736
H 1.452401 1.705123 1.534977
O -1.663568 -0.129464 1.106765
H -1.727043 -0.283678 2.070590
H -2.519920 0.237977 0.809478
O -0.501573 0.376602 -1.783892
H -0.779456 1.222019 -2.187234
H -0.252915 -0.230037 -2.508990
O 0.816730 -1.751625 -0.084890
H 0.293858 -2.562134 0.080982
H 1.726681 -1.939634 0.222324
13

Zn -0.053283 -0.005912 0.012817

O 0.117621 -0.863120 1.777545
H -0.331993 -1.702111 2.004639
H 0.962728 -0.851058 2.271070
O -1.210903 -1.067970 -1.164254
H -2.174259 -1.180568 -1.036534
H -1.030368 -1.182403 -2.119151
O -0.663246 1.827121 0.351480
H -0.729863 2.243072 1.233642
H -1.055959 2.440694 -0.299471
O 1.697700 0.089789 -0.874598
H 2.294683 -0.660816 -1.063714
H 2.177143 0.913283 -1.093471
13

Zn 0.006441 0.008578 0.035575
O -0.960515 -0.515229 1.665227
H -1.411457 -1.378667 1.758753
H -1.428331 0.116581 2.247782
O -0.885964 0.798242 -1.533515
H -0.935762 1.761112 -1.697699
H -1.648173 0.388223 -1.988618
O 1.254838 1.440238 0.554289
H 1.586629 1.562026 1.466765
H 1.930524 1.813104 -0.046836
O 0.577073 -1.734037 -0.689207
H 0.882324 -1.840864 -1.612685
H 1.032372 -2.419306 -0.159831
13

Zn 0.001888 -0.016957 0.018272
O 0.165985 0.340139 -1.907734
H 0.870972 -0.076637 -2.459044
H 0.013325 1.240308 -2.282522
O -1.190909 1.252651 0.933079
H -2.112457 1.429098 0.628900
H -0.852341 2.097940 1.312528
O 1.715671 0.117868 0.979142
H 2.537345 0.425577 0.527997
H 1.997087 -0.570326 1.628040
O -0.745599 -1.829706 0.193515
H -1.239072 -2.115814 0.998396
H -1.161897 -2.294140 -0.570569
13

Zn -0.003201 0.002462 -0.001046
O -0.038363 1.843208 0.694439
H -0.269326 2.033313 1.634583
H -0.388687 2.597868 0.164417
O 1.820423 -0.227267 -0.708768
H 2.597205 0.216484 -0.294005
H 2.145219 -1.086758 -1.067053
O -0.397742 -1.154099 1.541183
H 0.016654 -2.045334 1.632963
H -1.310231 -1.234230 1.909178
O -1.113040 -0.407125 -1.571651
H -0.981093 0.064442 -2.428502
H -2.077819 -0.602964 -1.505738
13

Zn 0.005386 0.007278 -0.020361
O 1.146066 1.490045 0.585225
H 1.972597 1.730418 0.102772
H 1.318674 1.666914 1.540328
O -1.651609 -0.185299 1.021409
H -1.649763 -0.442910 1.973780
H -2.431087 0.405189 0.889919
O -0.338543 0.467873 -1.903629
H -0.788073 1.306567 -2.163420
H -0.611822 -0.212694 -2.563318
O 0.868671 -1.762054 -0.009857
H 0.369734 -2.579087 0.228639
H 1.789770 -1.892241 0.318513
13

Zn 0.007413 0.013792 -0.009716
O -0.005993 -0.865888 1.754029
H -0.156898 -1.837056 1.840392
H 0.625318 -0.617107 2.470454
O -1.161003 -1.154624 -1.079235
H -2.113738 -1.282623 -0.855926
H -1.100534 -1.182921 -2.063920
O -0.468153 1.877702 0.408537
H -1.023457 2.096563 1.194195
H -0.711964 2.526392 -0.294124
O 1.642914 0.160972 -1.093697
H 2.182520 -0.632209 -1.326177
H 2.283574 0.897008 -0.944812
13

Zn -0.012563 -0.002323 -0.006222
O -1.066719 -0.497712 1.583832
H -2.011028 -0.775388 1.519070

H -0.978365 -0.005311 2.433942
O -1.216675 0.687375 -1.398093
H -1.595484 1.597918 -1.371721
H -1.087689 0.463345 -2.350398
O 1.328607 1.299302 0.601564
H 2.219014 1.014021 0.918026
H 1.459417 2.162822 0.141895
O 0.722570 -1.689425 -0.707581
H 1.590051 -1.729347 -1.176095
H 0.648864 -2.525275 -0.188219

Zn – 8 water molecules

25

Zn -0.002562 -0.307600 0.063409
O 2.055455 -0.270421 0.415867
H 2.529849 -1.117889 0.456976
H 2.363620 0.273735 1.178963
O 0.323209 -2.089600 -1.075561
H -0.443804 -2.654135 -1.280615
H 0.740514 -1.898062 -1.934904
O -2.045158 -0.189674 -0.326490
H -2.630364 -0.899967 -0.015904
H -2.338034 0.075456 -1.229158
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Zn – 12 water molecules

37

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37

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Zn – 16 water molecules

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SO_4 – 1 water molecule

8

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H	-0.450796	1.399868	-0.029625
S	0.445870	-1.038001	-0.597790
O	0.500337	-0.862632	0.934933
O	0.392547	0.355135	-1.258885
O	1.701673	-1.760549	-1.059837
O	-0.798011	-1.828145	-0.974421
8			

O	-0.498091	1.657795	0.885087
H	-0.185264	1.454847	-0.039137
H	-0.325271	0.735004	1.219929
S	0.247491	-1.104867	-0.602409
O	1.356973	-2.054143	-1.027125
O	0.272652	-0.953947	0.933127
O	0.493565	0.277055	-1.244657
O	-1.109969	-1.633241	-1.039290
8			

O	-0.110284	-1.878423	0.479895
H	-0.522912	-1.059443	0.869197
H	0.246145	-1.401592	-0.319874
S	0.142507	1.246004	-0.281863
O	0.459472	0.114570	-1.282962
O	1.420447	1.676083	0.422165
O	-0.476622	2.414552	-1.032713
O	-0.869535	0.722832	0.759472
8			

O	-0.557849	1.895836	-0.163190
H	-0.508172	1.141991	-0.812843
H	-0.194715	1.352684	0.589469
S	0.364427	-1.254278	0.108205
O	1.776661	-1.771886	-0.123960
O	-0.151248	-0.585275	-1.182844

O	-0.566878	-2.396150	0.487776
O	0.386001	-0.215389	1.249158

SO_4 – 2 water molecules

11

O	0.000190	-0.000333	3.310179
H	-0.443042	-0.579182	2.654000
H	0.443169	0.578709	2.653986
O	0.000051	-0.000428	-3.310166
H	-0.578815	0.443128	-2.654222
H	0.578811	-0.443436	-2.653739
S	-0.000090	0.000313	-0.000048
O	0.761583	0.980938	0.869783
O	-0.761916	-0.980441	0.869501
O	-0.980552	0.762119	-0.869720
O	0.980609	-0.761386	-0.869556

11

O	1.644863	1.801027	-0.709557
H	0.749375	1.742114	-1.103654
H	1.637921	0.911381	-0.296507
O	-0.897988	-0.476473	2.250022
H	-0.078226	-0.418310	1.715575
H	-1.472958	-0.820245	1.533986
S	-0.455209	-0.735212	-0.963300
O	-1.650595	-1.352846	-0.259764
O	-0.802128	0.674840	-1.397003
O	0.726580	-0.685335	0.010818
O	-0.074405	-1.569825	-2.150778

11

O	1.700620	0.088600	0.576248
H	1.212846	-0.762308	0.471210
H	1.401615	0.486952	-0.273605
O	-0.677889	1.114996	1.653953
H	0.232974	0.833661	1.425767
H	-1.183718	0.728039	0.900766
S	-0.740113	-0.710610	-1.350168
O	0.267613	0.350127	-1.769390
O	-1.850411	-0.052630	-0.545750
O	-1.325700	-1.378601	-2.561566
O	-0.039462	-1.738778	-0.475089

11

O	-0.696273	0.465243	-2.814091
H	-1.437686	0.312916	-2.190641
H	0.015960	0.433319	-2.141129
O	1.911663	-0.516297	2.060848
H	1.839366	-0.092388	1.183848
H	1.010307	-0.905178	2.090021
S	-0.780063	0.131625	0.516835
O	-0.680524	-1.145582	1.335584
O	0.501857	0.277059	-0.308730
O	-1.975781	0.029602	-0.409335
O	-0.929208	1.320951	1.419510

11

O	3.077988	-0.601643	0.737844
H	2.295567	-0.294405	1.243591
H	2.583034	-0.944820	-0.034953
O	-2.884061	1.321347	-0.584517
H	-2.737640	0.405543	-0.268667
H	-1.939429	1.527413	-0.754394
S	-0.090737	-0.305549	-0.018148
O	-0.193167	0.998595	-0.789652
O	-1.457763	-0.948349	0.105754
O	0.838591	-1.245209	-0.758955
O	0.446425	-0.029008	1.374086

11

O	-0.000469	0.000097	3.302291
H	-0.444750	-0.577460	2.626635
H	0.444293	0.577468	2.626781
O	-0.000388	-0.000151	-3.302289
H	-0.577538	0.444644	-2.626621
H	0.577143	-0.444703	-2.626774
S	0.000337	0.000020	-0.000065
O	0.771068	0.994120	0.876156
O	-0.770317	-0.994391	0.875868
O	-0.993837	0.770866	-0.875822
O	0.994458	-0.770509	-0.876161

11

O	1.786183	1.814006	-1.082105
H	0.909949	1.659842	-1.526580
H	1.658475	1.103963	-0.401160
O	-0.964067	-1.056732	2.385700
H	-0.181108	-0.726636	1.870905

H -1.555451 -1.130055 1.590704
S -0.466726 -0.529458 -0.853388
O -1.800031 -0.933328 -0.215218
O -0.674692 0.763893 -1.651664
O 0.572581 -0.261059 0.268293
O 0.042115 -1.633319 -1.755648
11

O 1.710040 0.084406 0.559279
H 1.184602 -0.763872 0.452640
H 1.380110 0.477964 -0.301524
O -0.654665 1.088176 1.626791
H 0.254995 0.787560 1.356810
H -1.188530 0.710389 0.871777
S -0.740970 -0.690706 -1.313058
O 0.271589 0.401319 -1.701244
O -1.906312 -0.043023 -0.548230
O -1.264467 -1.378120 -2.554973
O -0.048017 -1.714643 -0.395893
11

O -0.669872 0.686436 -2.684637
H -1.387552 0.320309 -2.103534
H 0.044726 0.610278 -1.999864
O 1.997688 -0.628959 1.929033
H 1.801965 -0.260629 1.028267
H 1.054587 -0.871526 2.129511
S -0.822788 0.104469 0.498005
O -0.716335 -0.909335 1.643096
O 0.527545 0.129246 -0.268506
O -1.922872 -0.354797 -0.465273
O -1.127474 1.485776 1.036620
11

O 2.746708 -1.453213 0.643858
H 2.242310 -0.846160 1.247020
H 2.251526 -1.186608 -0.175534
O -2.926284 0.647280 -1.037239
H -2.479249 -0.084652 -0.533928
H -2.201540 1.307895 -0.884125
S 0.060183 0.298266 0.197051
O -0.530367 1.671528 -0.137153
O -1.065059 -0.714574 0.438984
O 0.930833 -0.174244 -0.973264
O 0.909746 0.418398 1.466320

SO_4 – 4 water molecules

17

O -2.289346 0.337559 0.120280
H -1.480101 0.758217 0.512415
H -1.921365 -0.119135 -0.668243
O -1.427376 -2.137170 1.061007
H -0.533612 -1.776530 1.289957
H -1.934823 -1.305928 0.923102
O -0.848922 -1.379226 -1.564382
H -0.065097 -0.819155 -1.331052
H -0.998519 -1.884463 -0.734812
O 2.395000 2.794950 -0.949085
H 2.641974 2.449421 -0.067057
H 1.928919 2.004284 -1.280314
S 1.169148 0.402154 0.796194
O 1.216912 0.167175 -0.713202
O 0.974724 -0.922978 1.501302
O 2.463367 1.033560 1.238265
O 0.017938 1.331091 1.115303
17

O -3.167014 -0.607872 1.581871
H -2.878087 0.204889 1.128923
H -2.284914 -1.016440 1.710581
O -0.636771 2.339315 -2.039099
H -0.887941 1.938789 -1.179044
H 0.217704 1.890897 -2.212097
O 2.196250 -2.090958 1.647345
H 2.218918 -1.199835 1.240388
H 1.235148 -2.134658 1.811608
O 1.656530 0.714977 -2.197540
H 0.974612 0.013347 -2.097125
H 1.858832 0.827631 -1.243618
S -0.103927 -0.180451 0.361824
O -0.244684 -0.880035 -0.966517
O -1.030418 1.018889 0.420267
O -0.455272 -1.139784 1.486800
O 1.331033 0.301302 0.545435
17

O -2.184359 -0.221731 -1.362437
H -1.315752 -0.468332 -1.750659

H	-1.996515	-0.275792	-0.391302
O	-0.722412	2.149965	-1.442319
H	-0.368273	2.019178	-0.524836
H	-1.447254	1.486129	-1.467267
O	0.523755	-0.267465	-2.064766
H	0.279748	0.684181	-2.032290
H	0.717500	-0.461225	-1.111708
O	2.460253	-1.925285	2.484242
H	2.114950	-1.717692	1.592408
H	1.853617	-1.343549	2.983519
S	-0.006995	0.150720	1.448370
O	0.141610	1.606113	1.051461
O	0.888993	-0.708928	0.555704
O	0.403612	-0.029079	2.884843
O	-1.446864	-0.280608	1.261242

17

O	-1.476467	-1.808044	-1.693091
H	-1.811628	-0.901524	-1.851740
H	-0.658758	-1.624568	-1.181999
O	-0.514005	-0.079840	3.312693
H	0.348638	0.266830	3.018533
H	-0.988467	-0.001266	2.458621
O	3.514053	-0.155000	-0.134778
H	3.073629	0.458010	0.484280
H	2.730032	-0.671067	-0.407261
O	-2.176175	0.933217	-1.825348
H	-2.166900	0.782641	-0.854683
H	-1.235412	1.201457	-1.916265
S	0.355235	0.476805	0.143057
O	0.791729	-0.919084	-0.280491
O	-1.082123	0.409740	0.642293
O	1.253485	0.965548	1.258448
O	0.430715	1.408618	-1.039597

17

O	-2.419742	2.340934	-0.639548
H	-1.521132	2.453402	-0.265826
H	-2.462836	1.367904	-0.762176
O	1.303515	-2.144480	1.536408
H	0.795201	-2.535589	0.793672
H	0.751478	-1.337281	1.649365
O	0.227619	2.224534	0.341112
H	-0.083771	1.458531	0.877236
H	0.416178	1.726651	-0.482365
O	2.675376	-0.813241	-0.541766
H	1.829026	-0.495816	-0.925649
H	2.356337	-1.288055	0.254275
S	-0.827893	-0.750835	-0.428755
O	-2.247587	-0.451274	-0.840885
O	-0.605217	-0.273632	1.008967
O	-0.553266	-2.231502	-0.504246
O	0.130151	-0.001103	-1.346133

17

O	-2.552787	-0.008548	0.321450
H	-1.808618	0.535901	0.726935
H	-2.123331	-0.289040	-0.538696
O	-1.082103	-2.249846	0.879826
H	-0.256224	-1.732556	1.131214
H	-1.764624	-1.516772	0.879841
O	-0.943925	-1.117412	-1.601293
H	-0.231861	-0.458307	-1.336431
H	-0.907900	-1.748517	-0.823504
O	3.137362	2.202184	-1.131374
H	2.997271	2.178859	-0.150197
H	2.367474	1.621409	-1.351004
S	0.896805	0.704705	0.855999
O	0.917749	0.605339	-0.686895
O	1.045249	-0.697619	1.448397
O	2.047760	1.579569	1.326983
O	-0.429474	1.324480	1.298430

17

O	-2.687542	-0.338132	1.962118
H	-2.250458	0.453177	1.558245
H	-2.053935	-0.999089	1.585687
O	-1.700149	2.078449	-1.989509
H	-1.612965	2.026308	-1.004750
H	-1.115729	1.301775	-2.177939
O	1.717047	-2.071076	1.984396
H	1.939728	-1.195251	1.579351
H	0.806207	-2.124142	1.600014
O	2.676606	0.339836	-1.967367
H	1.719667	0.173688	-2.160140
H	2.571267	0.369983	-0.983578
S	-0.002164	-0.003442	0.003007
O	-0.018504	-0.064993	-1.530455
O	-0.890716	1.150276	0.487128
O	-0.528450	-1.334338	0.554774
O	1.430090	0.236972	0.499017

17

O	-2.024233	-0.430854	-1.248303
H	-1.122962	-0.553717	-1.665543
H	-1.776004	-0.415173	-0.271959
O	-0.962672	2.079962	-1.462122
H	-0.523761	2.039894	-0.558107
H	-1.572346	1.287005	-1.406378
O	0.560399	-0.114274	-2.112075
H	0.171814	0.804295	-2.032166
H	0.860848	-0.272746	-1.165263
O	1.910428	-2.245860	2.490972
H	1.815651	-1.879227	1.576805
H	1.507550	-1.468999	2.954795
S	0.203732	0.316094	1.408546
O	0.162498	1.781219	0.972442
O	1.180578	-0.453882	0.488603
O	0.693765	0.228376	2.844538
O	-1.189672	-0.305511	1.299422

17

O	-0.655213	-1.500286	-2.351858
H	-1.463303	-1.004738	-2.051053
H	0.052797	-0.982976	-1.883332
O	0.933009	0.227496	2.830069
H	1.228560	1.006561	2.284790
H	0.135865	0.012557	2.271419
O	2.290497	-1.424434	1.043132
H	1.878996	-0.909316	1.787495
H	1.918118	-0.931327	0.264210
O	-2.654791	0.103520	-1.266346
H	-2.197058	-0.079611	-0.400564
H	-2.084147	0.881650	-1.515147
S	0.200649	1.081699	-0.175392
O	1.118240	0.113711	-0.950474
O	-0.768455	0.256883	0.700775
O	1.052747	1.976297	0.713102
O	-0.598927	1.914787	-1.168157

17

O	-2.386962	2.321573	-0.572635
H	-1.436312	2.412003	-0.295220
H	-2.448734	1.338168	-0.694512
O	1.293794	-2.118688	1.549729
H	0.793335	-2.533836	0.798072
H	0.701139	-1.318289	1.632077
O	0.304485	2.174246	0.167575
H	-0.002723	1.443284	0.774272
H	0.408546	1.589995	-0.632159
O	2.642151	-0.655705	-0.394707
H	1.789519	-0.389100	-0.828872
H	2.290655	-1.191483	0.366441
S	-0.845593	-0.776026	-0.434399
O	-2.278515	-0.468680	-0.837910
O	-0.594142	-0.248814	1.000692
O	-0.586776	-2.273430	-0.473607
O	0.119572	-0.056072	-1.401148

SO_4 – 8 water molecules

29

O	0.286551	2.792653	0.527147
H	0.503266	1.834114	0.484579
H	-0.696797	2.789744	0.543020
O	0.670561	-3.168209	1.950729
H	1.153383	-2.358305	2.231573
H	0.311601	-2.891463	1.077293
O	-2.378540	2.442421	-0.114092
H	-1.917024	2.511057	-0.979310
H	-2.285059	1.494786	0.125809
O	2.309135	0.526514	-2.215099
H	1.819831	0.509070	-1.369134
H	1.920038	-0.250965	-2.666948
O	1.362610	-0.583529	2.662236
H	1.231054	-0.279326	1.735844
H	0.437771	-0.655591	2.991608
O	-1.251681	-1.350886	3.067533
H	-1.510067	-0.929603	2.214651
H	-0.804042	-2.174337	2.776584
O	-0.447504	2.561834	-2.135166
H	0.046438	2.771635	-1.311983
H	-0.472849	1.579890	-2.130764
O	0.832141	-1.684874	-3.121129
H	0.874937	-2.226934	-2.314541
H	0.085329	-1.089379	-2.887922
S	-0.579308	-0.587837	-0.369990
O	-0.356094	-2.074607	-0.375944
O	0.712703	0.112408	0.060718
O	-0.950692	-0.118217	-1.761415
O	-1.679452	-0.204347	0.596327

29

O	-0.993432	2.298368	1.108808
H	-0.224910	2.365265	0.504743
H	-1.175092	1.332556	1.146690
O	0.918543	-2.672154	2.538872
H	1.390971	-1.810347	2.561142
H	0.511777	-2.674928	1.643076
O	-2.011257	1.978015	-1.516425
H	-1.878161	1.004637	-1.549462
H	-1.941225	2.183231	-0.560073
O	2.266794	-0.593923	-2.445837
H	1.831859	-0.561832	-1.572204
H	1.529915	-0.392602	-3.061787
O	1.554736	0.032947	2.614368
H	1.336201	0.067700	1.656180
H	0.668237	-0.025876	3.039332
O	-0.930552	-0.805727	3.491267
H	-1.285013	-0.654765	2.584649
H	-0.430068	-1.642176	3.359593
O	0.721876	2.305004	-1.191629
H	0.870965	1.370531	-0.932474
H	-0.196795	2.279606	-1.541691
O	-0.037060	-0.159934	-3.962279
H	-0.130187	-0.982545	-4.466418
H	-0.466348	-0.369657	-3.099128
S	-0.566349	-0.932552	-0.175392
O	-0.341825	-2.395074	0.037729
O	0.764097	-0.184671	-0.054874
O	-1.155169	-0.666037	-1.545699
O	-1.520805	-0.386068	0.870205

29

O	-3.280522	-0.550068	-0.714646
H	-2.768733	0.045599	-1.318623
H	-2.676397	-0.612469	0.056762
O	-1.643937	-0.723499	3.742261
H	-1.739855	-1.039877	2.823073
H	-0.744914	-0.354709	3.677691
O	-1.715163	-2.738319	-1.253456
H	-2.450352	-2.078397	-1.222166
H	-1.261006	-2.509055	-0.418210
O	-1.517710	0.987163	-2.137072
H	-0.966104	0.226421	-2.451150
H	-1.102025	1.181446	-1.265082
O	0.058298	-1.180009	-2.610700
H	0.541356	-1.021860	-1.768294
H	-0.614467	-1.835392	-2.300446
O	2.921998	0.867694	-1.045412
H	2.489460	1.711819	-0.785526
H	2.245921	0.200641	-0.786268
O	1.704003	2.935393	0.398748
H	0.889526	2.381124	0.431867
H	2.288266	2.493283	1.053387
O	3.283352	1.054973	1.742289
H	2.453038	0.593148	1.995808
H	3.385868	0.830910	0.791789
S	0.059641	-0.205424	0.889137
O	0.722364	-0.014104	2.230257
O	-1.156608	-1.107527	1.021845
O	-0.375631	1.142705	0.347037
O	1.042446	-0.849715	-0.073248

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O	1.724041	-0.704614	2.210978
H	1.401689	-1.627847	2.100542
H	1.020639	-0.190012	1.752313
O	-2.642622	-0.210560	2.240865
H	-3.089101	-0.645979	1.485875
H	-1.783834	0.046385	1.851513
O	-0.070337	3.093139	0.095685
H	-0.410967	3.056449	-0.823132
H	-0.233347	2.181045	0.430371
O	-0.379683	2.474180	-2.666953
H	-0.830421	1.663113	-2.342683
H	0.562695	2.323685	-2.446570
O	2.133009	2.121350	-1.294609
H	1.536765	2.563845	-0.649356
H	1.815011	1.193034	-1.266445
O	1.014124	-3.170695	1.142674
H	0.254244	-2.752333	0.676177
H	1.768897	-2.865305	0.592133
O	-3.594539	-1.388445	-0.167515
H	-2.714252	-1.822840	-0.163371
H	-3.358886	-0.569709	-0.643142
O	2.880882	-1.557818	-0.171643
H	2.702779	-1.109857	0.686405
H	2.172969	-1.173317	-0.736649
S	-0.490824	-0.327235	-0.564807
O	0.792630	-0.308873	-1.367146
O	-0.877286	-1.749673	-0.236240
O	-0.278191	0.439486	0.742651

O	-1.587387	0.345167	-1.345250

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O	0.487867	-1.070954	-3.660300
H	-0.241462	-0.955584	-3.008702
H	1.281695	-1.116929	-3.085072
O	0.999109	1.616759	-2.924815
H	0.513963	1.606862	-2.069256
H	0.674741	0.810560	-3.378666
O	-0.947834	1.958344	2.703241
H	-1.273684	1.790369	1.801221
H	-0.999080	1.048781	3.094717
O	-1.046087	-0.682689	3.252192
H	-0.096244	-0.878253	3.045591
H	-1.434032	-0.662369	2.348574
O	-3.468559	-1.922859	-0.915363
H	-2.833000	-1.466642	-1.501377
H	-3.232705	-1.491230	-0.075566
O	1.625620	1.603744	1.823673
H	1.264393	1.497451	0.914675
H	0.793066	1.853590	2.294791
O	1.463365	-1.066956	2.261488
H	1.064591	-1.248597	1.378690
H	1.650070	-0.096383	2.191417
O	2.493617	-0.492899	-1.758944
H	2.174017	0.378927	-2.078398
H	1.807676	-0.748735	-1.101052
S	-0.720116	-0.107236	-0.419801
O	-0.018170	1.238883	-0.386404
O	0.312740	-1.201673	-0.204177
O	-1.776206	-0.159355	0.659564
O	-1.368601	-0.295073	-1.776152

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O	0.328351	2.901906	0.389421
H	0.563839	1.939067	0.270460
H	-0.634707	2.828519	0.652060
O	0.696541	-2.956349	1.814456
H	1.155855	-2.119154	2.113765
H	0.384627	-2.698187	0.903323
O	-2.368006	2.416066	0.420434
H	-2.134174	2.601521	-0.535783
H	-2.207852	1.432743	0.468144
O	2.813800	-0.367361	-1.805566
H	2.171537	-0.095320	-1.105107
H	2.229079	-0.925305	-2.384673
O	1.288786	-0.396805	2.619055
H	1.172627	-0.110741	1.670772
H	0.337392	-0.557267	2.888641
O	-1.261921	-1.350598	2.869149
H	-1.508853	-0.935162	1.996526
H	-0.717348	-2.132151	2.562890
O	-1.069647	2.755064	-1.967926
H	-0.388800	2.943496	-1.258645
H	-0.992791	1.764594	-2.058513
O	0.882698	-1.856716	-3.157070
H	0.634235	-2.229802	-2.271483
H	0.302174	-1.055879	-3.124315
S	-0.499906	-0.503606	-0.540008
O	-0.199632	-1.997440	-0.604254
O	0.742033	0.234018	0.016522
O	-0.804046	0.019218	-1.937187
O	-1.687651	-0.250654	0.387127

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O	-1.766578	2.579513	1.087558
H	-0.834618	2.794749	0.789666
H	-1.762035	1.583124	1.052009
O	0.935927	-2.934692	1.788919
H	1.529991	-2.136242	1.899458
H	0.439424	-2.691339	0.958479
O	-1.850028	2.647765	-1.654230
H	-1.684239	1.670998	-1.764936
H	-2.072219	2.693755	-0.679365
O	2.314352	-0.532990	-2.354897
H	1.846145	-0.216818	-1.542865
H	1.600578	-1.087611	-2.768095
O	1.912340	-0.413418	2.207593
H	1.562951	-0.140309	1.313520
H	1.059180	-0.468693	2.729569
O	-0.548885	-1.109661	3.179886
H	-0.998080	-0.734715	2.372722
H	-0.155243	-1.951216	2.804393
O	0.539394	2.914559	-0.354792
H	0.703269	1.932779	-0.278695
H	-0.205680	2.934768	-1.024644
O	0.079522	-1.986767	-3.177810
H	0.041378	-2.354960	-2.258817
H	-0.465770	-1.175687	-3.015042
S	-0.638454	-0.507512	-0.366911
O	-0.410371	-2.013202	-0.417746
O	0.723404	0.202983	-0.168902

O	-1.257841	-0.039795	-1.677221
O	-1.556095	-0.152374	0.802475

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O	-3.272725	-0.484636	-0.683886
H	-2.736197	0.103264	-1.310596
H	-2.628291	-0.579333	0.064844
O	-1.451045	-0.769964	3.673324
H	-1.646563	-1.099850	2.765030
H	-0.544959	-0.427561	3.490550
O	-1.911362	-2.739584	-1.250895
H	-2.599149	-2.005535	-1.202424
H	-1.403393	-2.493878	-0.435568
O	-1.543291	0.960843	-2.127453
H	-1.015023	0.149314	-2.425743
H	-1.104501	1.159022	-1.254132
O	-0.149010	-1.261069	-2.644969
H	0.424014	-1.103023	-1.842800
H	-0.824703	-1.901292	-2.254129
O	3.155006	0.882544	-0.778114
H	2.628459	1.721976	-0.631179
H	2.454230	0.186110	-0.640802
O	1.689220	2.932116	0.281374
H	0.877463	2.351231	0.283172
H	2.205825	2.543218	1.046240
O	3.144572	1.304800	1.928408
H	2.326784	0.759089	2.099050
H	3.374471	1.025451	0.995200
S	0.127734	-0.272597	0.782639
O	0.830462	-0.164063	2.130518
O	-1.082943	-1.207455	0.907931
O	-0.353583	1.113997	0.338550
O	1.100612	-0.851240	-0.252491

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O	1.520246	-0.873943	2.400368
H	1.298923	-1.817541	2.144917
H	0.870019	-0.368282	1.836435
O	-2.681867	0.194318	2.009041
H	-3.117132	-0.344527	1.296031
H	-1.776496	0.302429	1.625735
O	0.290875	2.956026	0.257208
H	-0.270363	3.050274	-0.566585
H	0.109079	2.005196	0.500419
O	-0.780034	2.720007	-2.246398
H	-1.131222	1.815044	-2.019412
H	0.196213	2.529521	-2.354484
O	1.853638	2.066013	-1.812248
H	1.516840	2.445242	-0.948961
H	1.570935	1.113373	-1.729729
O	1.170606	-3.233195	1.079591
H	0.396190	-2.852319	0.581436
H	1.937126	-2.782302	0.620455
O	-3.534326	-1.285763	-0.195222
H	-2.718099	-1.837590	-0.089261
H	-3.138651	-0.578518	-0.764951
O	2.980211	-1.396351	0.142970
H	2.632572	-1.034798	1.009580
H	2.289630	-1.070495	-0.496964
S	-0.411156	-0.485395	-0.641693
O	0.904044	-0.484758	-1.421300
O	-0.813806	-1.914290	-0.301591
O	-0.217662	0.311316	0.672402
O	-1.507635	0.177067	-1.465117

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O	0.499626	-1.060642	-3.734615
H	-0.217298	-1.087845	-3.041026
H	1.308264	-1.273890	-3.184561
O	1.377319	1.334472	-2.770377
H	0.778855	1.331294	-1.971612
H	0.962946	0.604649	-3.319248
O	-1.518950	1.255625	2.873957
H	-1.767791	0.863992	1.996592
H	-1.095032	0.431967	3.269677
O	-0.357194	-1.144917	3.247779
H	0.553292	-0.823933	2.941489
H	-0.820671	-1.228931	2.375698
O	-3.874132	-0.143765	-0.838179
H	-3.181605	-0.429473	-1.477543
H	-3.342930	-0.251824	-0.014290
O	0.737801	2.142732	1.706481
H	0.447913	1.832014	0.803403
H	-0.090821	1.926950	2.240174
O	1.902916	-0.225589	2.141875
H	1.566825	-0.640145	1.299778
H	1.557779	0.720984	2.039141
O	2.574558	-0.977093	-1.941839
H	2.360327	-0.023881	-2.164241
H	1.924018	-1.148114	-1.204442
S	-0.624603	-0.446587	-0.376633
O	-0.253656	1.026580	-0.583898

O	0.628031	-1.268165	-0.047149
O	-1.608361	-0.559545	0.797495
O	-1.276676	-0.997067	-1.638095

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O	2.691471	-2.293514	0.032989
H	3.006742	-1.467763	0.458441
H	1.715407	-2.222051	0.068165
O	-3.047440	-0.378652	-2.268086
H	-2.686891	-0.102399	-1.400984
H	-2.580252	-1.231353	-2.421477
O	3.342145	0.431615	0.508301
H	3.334493	0.308644	-0.466265
H	2.398711	0.522962	0.748875
O	-1.407479	-2.595596	2.349025
H	-1.909929	-1.769055	2.524899
H	-1.012102	-2.442805	1.468020
O	2.957596	-0.551886	-2.083125
H	2.945528	-1.363417	-1.526689
H	2.047438	-0.212517	-1.962058
O	0.979084	3.136902	-0.634002
H	0.965767	3.104684	0.347982
H	0.961652	2.195675	-0.902816
O	-0.712820	0.298714	-3.702398
H	-0.213183	0.478303	-2.878597
H	-1.638782	0.294569	-3.370788
O	0.383280	-0.893095	3.688713
H	0.687311	-0.526562	2.832665
H	-0.085452	-1.705312	3.394976
O	-1.710930	3.020639	0.003819
H	-0.855099	3.181902	-0.453042
H	-1.799966	2.045587	-0.023948
O	0.174235	2.815976	2.023619
H	-0.656208	2.963988	1.517055
H	0.344311	1.861417	1.888028
O	-2.134262	0.015779	2.912982
H	-1.235302	-0.064256	3.303120
H	-1.977933	0.248682	1.976860
O	-1.114277	-2.296202	-2.768432
H	-0.707247	-2.236778	-1.880205
H	-0.780089	-1.496874	-3.234051
S	-0.140239	-0.221668	-0.019547
O	0.497778	0.420613	-1.236379
O	-0.088492	-1.727566	-0.130664
O	0.638923	0.219473	1.204719
O	-1.577504	0.233199	0.110307

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O	3.036314	-1.716247	-0.107492
H	3.206779	-0.802402	0.232386
H	2.094391	-1.850437	0.127143
O	-2.225534	-0.909586	-2.451334
H	-2.217623	-0.696531	-1.496875
H	-1.438092	-1.503413	-2.546467
O	3.164885	0.809007	0.949322
H	2.971319	1.537399	0.312797
H	2.282636	0.673636	1.353679
O	-0.960487	-2.983357	2.381243
H	-1.815210	-2.496088	2.374699
H	-0.495917	-2.612744	1.600564
O	2.185662	-0.973333	-2.592104
H	1.572502	-0.332253	-2.176957
H	2.638510	-1.327457	-1.784870
O	2.046308	2.731977	-0.767051
H	1.419041	3.115528	-0.102436
H	1.547104	1.932017	-1.028938
O	-1.387282	1.678087	-2.741933
H	-0.584595	1.438981	-2.235482
H	-1.808020	0.783570	-2.800933
O	-0.496414	-0.610878	3.810360
H	-0.124675	-0.117920	3.046934
H	-0.453184	-1.540413	3.493924
O	-2.150109	2.685472	-0.327051
H	-1.956752	2.471063	-1.273922
H	-2.161061	1.784848	0.056195
O	0.141312	3.301008	1.066233
H	-0.685913	3.217323	0.527164
H	0.252796	2.386246	1.398664
O	-2.930198	-1.025618	2.522149
H	-2.229272	-0.698243	3.130627
H	-2.632216	-0.663432	1.660831
O	-0.061663	-2.563940	-2.351094
H	-0.033152	-2.440137	-1.379352
H	0.759654	-2.086125	-2.622088
S	-0.133524	-0.157359	0.222929
O	0.449815	0.498209	-1.010951
O	0.254188	-1.624667	0.248802

O	0.416502	0.525506	1.461194
O	-1.643390	-0.042883	0.200711

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O	1.616796	-2.850042	1.023853
H	2.304865	-2.160456	1.196691
H	1.177437	-2.498405	0.222303
O	-3.212805	-2.044709	-1.135950
H	-2.631945	-1.593338	-0.486149
H	-2.561439	-2.352078	-1.807812
O	3.221218	-0.634971	1.295243
H	3.425930	-0.554111	0.329633
H	2.353127	-0.186645	1.311601
O	-0.477137	-2.030969	2.608592
H	-0.969051	-1.622647	1.866740
H	0.319997	-2.394662	2.146995
O	3.211156	-0.414431	-1.416048
H	2.930318	0.520899	-1.573847
H	2.350471	-0.878911	-1.406942
O	2.041868	2.083370	-1.914529
H	1.926497	2.597177	-1.077993
H	1.153908	1.686000	-2.007835
O	-2.838198	0.166501	-2.810764
H	-2.092331	0.567912	-2.317173
H	-3.197164	-0.492176	-2.174934
O	0.237116	0.517872	3.336672
H	0.531334	0.667296	2.415836
H	-0.010891	-0.439887	3.277177
O	-1.383728	3.129631	0.238837
H	-1.224044	2.429723	-0.427090
H	-1.645392	2.615543	1.042545
O	1.357861	3.129582	0.521574
H	0.395325	3.333288	0.422562
H	1.311245	2.168663	0.703939
O	-2.119103	1.420363	2.296601
H	-1.320070	1.202022	2.836920
H	-2.107223	0.694657	1.639683
O	-1.268323	-2.152485	-3.086138
H	-0.549057	-1.911182	-2.463868
H	-1.707882	-1.291991	-3.263791
S	-0.171796	-0.122661	-0.337968
O	-0.553459	0.935459	-1.351927
O	0.486708	-1.289477	-1.046198
O	0.800984	0.458228	0.666484
O	-1.415696	-0.589953	0.390242

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O	2.590004	-2.466858	-0.716128
H	2.956828	-2.038969	0.090754
H	1.633392	-2.267734	-0.641643
O	-3.083938	-0.361363	-2.037939
H	-2.681883	-0.154403	-1.168719
H	-2.534995	0.194144	-2.637181
O	3.439334	-0.622126	1.174399
H	3.598875	-0.171123	0.313377
H	2.509732	-0.366815	1.348221
O	-1.729198	-2.769595	1.550949
H	-2.226211	-1.985646	1.870614
H	-1.224590	-2.436492	0.780487
O	3.306983	0.127441	-1.485908
H	3.135189	-0.841033	-1.497538
H	2.394864	0.484697	-1.455162
O	0.751233	3.447905	-0.645842
H	1.053166	3.353300	0.285788
H	0.741899	2.519090	-0.957592
O	-0.958536	0.656771	-3.532447
H	-0.408134	0.866696	-2.749810
H	-0.837330	-0.318080	-3.584597
O	0.038913	-1.455162	3.295124
H	0.399198	-0.847059	2.615128
H	-0.417367	-2.135555	2.752011
O	-1.593845	3.159764	0.789886
H	-0.929058	3.441138	0.120377
H	-1.696783	2.207639	0.583498
O	0.844441	2.816871	2.065938
H	-0.104631	2.989536	1.869737
H	0.927873	1.863652	1.854084
O	-2.459394	-0.322569	2.716533
H	-1.607766	-0.561441	3.145601
H	-2.175441	0.063871	1.862378
O	-1.029819	-2.051699	-2.946959
H	-1.905518	-1.707279	-2.659524
H	-0.523991	-1.973303	-2.111712
S	-0.041400	-0.065990	-0.058189
O	0.572689	0.708988	-1.204299
O	-0.046335	-1.544604	-0.386943
O	0.777771	0.167334	1.197203
O	-1.464578	0.393601	0.182566

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O	2.384346	-2.153631	1.773414
H	2.449293	-1.311643	2.276790

H	1.534908	-2.073929	1.293894
O	-1.854481	-0.486005	-3.239065
H	-1.772957	-0.118394	-2.335544
H	-0.919191	-0.539125	-3.542754
O	2.720547	0.502648	2.512095
H	3.208887	0.421489	1.661428
H	1.814085	0.680693	2.186969
O	-1.223320	-2.172995	2.757091
H	-1.170007	-1.271880	3.148665
H	-0.738812	-2.080571	1.912048
O	3.561827	-0.332870	-0.007685
H	3.311483	-1.162265	0.457143
H	2.737431	-0.102868	-0.485456
O	0.981246	2.834286	-1.933465
H	0.924658	3.196291	-1.019924
H	1.079719	1.874104	-1.762015
O	0.804417	-1.151647	-3.524799
H	1.016407	-0.673548	-2.693530
H	0.405829	-1.979390	-3.182113
O	-1.453286	0.542766	3.302456
H	-0.786243	0.718080	2.606227
H	-2.255021	0.364246	2.758098
O	-1.728909	2.858045	-1.438539
H	-0.841083	2.885927	-1.864140
H	-1.770810	1.936166	-1.112243
O	0.104639	3.434288	0.623649
H	-0.714793	3.389094	0.082936
H	0.208079	2.510057	0.934194
O	-3.201551	-0.558836	1.500642
H	-2.693845	-0.308445	0.700087
H	-2.722334	-1.342430	1.844284
O	-1.034187	-2.908215	-2.149971
H	-1.539074	-2.143959	-2.507932
H	-0.721968	-2.595337	-1.278622
S	-0.022099	-0.138702	-0.051884
O	1.015545	0.165070	-1.115408
O	0.023149	-1.610176	0.300790
O	0.285041	0.698787	1.172283
O	-1.407570	0.204826	-0.560095

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O	2.667075	-2.463672	-0.272328
H	3.036654	-1.787903	0.369493
H	1.698383	-2.256007	-0.239606
O	-3.077322	-0.399361	-1.942777
H	-2.615868	-0.028742	-1.147829
H	-2.634572	-1.294227	-2.027853
O	3.500125	-0.175629	0.960796
H	3.547223	0.027736	-0.018769
H	2.566992	0.087981	1.167500
O	-1.087393	-2.822620	2.054576
H	-1.830586	-2.160712	2.169511
H	-0.650272	-2.480095	1.233780
O	3.166632	-0.214796	-1.754804
H	3.016658	-1.155902	-1.445813
H	2.253565	0.164977	-1.678405
O	0.645881	3.414249	-1.112085
H	0.917274	3.439034	-0.148271
H	0.652129	2.439022	-1.291761
O	-0.906235	0.000547	-3.553324
H	-0.294576	0.288971	-2.828630
H	-1.795943	0.068031	-3.097339
O	-0.022394	-0.795997	3.551975
H	0.351617	-0.284944	2.788495
H	-0.224046	-1.678528	3.121692
O	-1.684438	3.231478	0.304904
H	-0.987278	3.399925	-0.395612
H	-1.744513	2.241963	0.290453
O	0.718447	3.203237	1.617649
H	-0.249948	3.283670	1.372762
H	0.844810	2.221006	1.575971
O	-2.558030	-0.572172	2.538768
H	-1.715594	-0.470972	3.070806
H	-2.295232	-0.162310	1.675828
O	-1.304981	-2.432438	-2.379237
H	-0.811043	-2.227779	-1.544478
H	-1.010434	-1.679689	-2.971436
S	-0.018047	0.006794	-0.003138
O	0.558416	0.641873	-1.268721
O	0.042476	-1.516016	-0.125594
O	0.804262	0.451937	1.207223
O	-1.469879	0.448082	0.175632

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O	3.011953	-1.553659	-0.245531
H	3.163784	-0.658278	0.197954
H	2.085687	-1.754045	0.041551
O	-2.295735	-0.826741	-2.369263
H	-2.267723	-0.609829	-1.403175
H	-1.505961	-1.451639	-2.453418
O	3.129119	0.818705	1.062522
H	2.921378	1.553692	0.403919

H	2.226020	0.671841	1.443276
O	-0.959271	-2.999755	2.399078
H	-1.812615	-2.474380	2.381882
H	-0.477292	-2.617265	1.620035
O	2.035726	-0.914382	-2.656354
H	1.448659	-0.251820	-2.215746
H	2.545309	-1.219075	-1.836703
O	2.155629	2.649403	-0.673924
H	1.449272	3.046082	-0.066451
H	1.639530	1.868598	-0.994130
O	-1.200199	1.580123	-2.851166
H	-0.440567	1.325278	-2.271420
H	-1.705145	0.703876	-2.812082
O	-0.489124	-0.743993	3.863910
H	-0.112162	-0.203534	3.121714
H	-0.466387	-1.664806	3.468450
O	-2.092252	2.632611	-0.516821
H	-1.807015	2.375799	-1.449391
H	-2.135761	1.735957	-0.097998
O	0.105013	3.281221	0.937157
H	-0.710484	3.150060	0.356034
H	0.193753	2.382556	1.343580
O	-2.863191	-1.052587	2.556739
H	-2.132218	-0.765525	3.179351
H	-2.556436	-0.656932	1.700478
O	-0.140695	-2.475840	-2.325479
H	-0.082838	-2.398784	-1.340153
H	0.680436	-1.951959	-2.589283
S	-0.144000	-0.146586	0.292039
O	0.451959	0.522981	-0.943201
O	0.248030	-1.626192	0.311892
O	0.391352	0.538943	1.552223
O	-1.670099	-0.025707	0.259123

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O	1.626975	-2.759727	1.133824
H	2.343422	-2.053803	1.192871
H	1.159974	-2.460940	0.312709
O	-3.283639	-1.850651	-1.252627
H	-2.732865	-1.435040	-0.539684
H	-2.575849	-2.284417	-1.814114
O	3.260283	-0.596109	1.040026
H	3.344218	-0.516305	0.035470
H	2.384873	-0.143843	1.139320
O	-0.483223	-2.065292	2.684379
H	-0.995673	-1.671057	1.934104
H	0.354314	-2.365863	2.205229
O	3.003462	-0.322614	-1.621724
H	2.690653	0.631383	-1.731431
H	2.137811	-0.796848	-1.548414
O	1.864837	2.121448	-1.899041
H	1.838325	2.578071	-1.000085
H	0.959105	1.721437	-1.911608
O	-2.511771	0.041384	-3.068843
H	-1.827473	0.465765	-2.487600
H	-3.020252	-0.508102	-2.402959
O	0.117066	0.439919	3.444823
H	0.496199	0.598694	2.544947
H	-0.114633	-0.538535	3.330694
O	-1.194405	3.178525	0.310617
H	-1.098878	2.469234	-0.374309
H	-1.523308	2.641591	1.100746
O	1.471831	3.083260	0.600295
H	0.481983	3.281830	0.518235
H	1.405455	2.119342	0.811196
O	-2.069207	1.485477	2.234714
H	-1.300059	1.190015	2.816007
H	-2.096237	0.734981	1.589275
O	-1.204805	-2.352326	-2.945230
H	-0.531342	-2.077034	-2.269363
H	-1.573720	-1.465343	-3.231080
S	-0.220891	-0.140532	-0.238998
O	-0.593611	0.931680	-1.266796
O	0.443382	-1.320699	-0.953171
O	0.750183	0.449492	0.782011
O	-1.485083	-0.620448	0.479352

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O	2.619211	-2.477317	-0.545342
H	2.996137	-1.898626	0.180497
H	1.656785	-2.242518	-0.507637
O	-2.968634	0.232425	-2.101977
H	-2.526224	0.341918	-1.221679
H	-2.236259	0.507173	-2.726047
O	3.500071	-0.382948	0.973533
H	3.564066	-0.066405	0.025864
H	2.567303	-0.138964	1.203222
O	-1.226693	-3.063825	1.580117
H	-1.956291	-2.402207	1.762300
H	-0.744648	-2.620057	0.836788
O	3.208159	-0.084296	-1.733893
H	3.020600	-1.050197	-1.546568

H	2.311292	0.318780	-1.607460
O	0.799636	3.524635	-0.562430
H	1.014974	3.394659	0.406797
H	0.785916	2.588788	-0.889057
O	-0.654206	0.332717	-3.574612
H	-0.129966	0.593089	-2.775043
H	-0.825672	-0.637396	-3.393135
O	-0.171277	-1.310103	3.396256
H	0.249366	-0.705859	2.732482
H	-0.380716	-2.113798	2.835466
O	-1.618870	3.214144	0.677939
H	-0.877093	3.453939	0.048170
H	-1.690170	2.235876	0.536318
O	0.703275	2.901918	2.102988
H	-0.247265	3.053632	1.826991
H	0.816552	1.936817	1.904250
O	-2.658184	-0.861749	2.343605
H	-1.835490	-0.864552	2.915128
H	-2.350118	-0.336364	1.561888
O	-1.540500	-2.053462	-2.574242
H	-2.261497	-1.394283	-2.355133
H	-0.946368	-1.966516	-1.785408
S	0.004123	0.007959	0.006792
O	0.636668	0.800241	-1.138169
O	0.019551	-1.482239	-0.336445
O	0.802863	0.242156	1.291007
O	-1.438766	0.470355	0.212399

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O	2.512457	-2.170206	1.496024
H	2.630914	-1.300581	1.978312
H	1.617050	-2.055688	1.088223
O	-1.956989	-0.953038	-2.930782
H	-1.880945	-0.453541	-2.077781
H	-1.017875	-0.909043	-3.276139
O	2.904237	0.459183	2.151614
H	3.304363	0.344145	1.240379
H	1.958193	0.659867	1.934931
O	-1.628138	-2.168478	2.442624
H	-1.514516	-1.302783	2.933670
H	-1.001914	-2.050088	1.683274
O	3.601997	-0.447365	-0.331334
H	3.310184	-1.258349	0.178763
H	2.741144	-0.121528	-0.697925
O	1.151034	3.064616	-1.609704
H	0.953104	3.353028	-0.670987
H	1.192001	2.078793	-1.516486
O	0.733677	-1.277661	-3.331363
H	0.928652	-0.644282	-2.593769
H	0.436519	-2.091349	-2.828647
O	-1.657250	0.459533	3.212459
H	-0.901576	0.660262	2.603837
H	-2.417386	0.359298	2.567770
O	-1.577888	2.989348	-1.367193
H	-0.638665	3.038815	-1.709741
H	-1.640730	2.040556	-1.087939
O	-0.023814	3.555472	0.812845
H	-0.779196	3.458822	0.162313
H	0.128879	2.614663	1.083436
O	-3.391445	-0.417809	1.284076
H	-2.777584	-0.096642	0.575192
H	-2.913768	-1.233601	1.613157
O	-0.652815	-3.095139	-1.825147
H	-1.339825	-2.462249	-2.185798
H	-0.369654	-2.631888	-0.996219
S	-0.004701	0.000964	-0.001394
O	1.032564	0.324465	-1.076224
O	0.063605	-1.487064	0.341802
O	0.287638	0.827234	1.250725
O	-1.401540	0.339311	-0.520854

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O	-0.479760	-0.590418	3.171529
H	-0.937565	-0.357625	2.335623
H	0.159718	-1.293104	2.861839
O	-3.252876	-2.255430	1.016812
H	-2.667724	-1.472146	0.918385
H	-2.705372	-2.986747	0.640451
O	-3.368102	-1.950357	-1.789046
H	-3.642673	-1.889890	-0.852088
H	-2.709825	-1.235352	-1.895316
O	2.926782	2.022884	-2.723861
H	2.312945	2.597334	-2.212775
H	3.237667	1.364706	-2.062487
O	1.074297	0.269788	-3.680125
H	0.285937	0.326640	-3.106120
H	1.702030	0.967683	-3.361392

O	2.088012	-1.882169	-2.454279
H	1.372258	-2.015980	-1.800504
H	1.726691	-1.154653	-3.027162
O	1.273698	-2.250362	2.022906
H	2.112419	-1.719812	1.975219
H	0.905753	-2.178962	1.117998
O	3.231594	-0.061420	-0.881775
H	3.018902	-0.833455	-1.476160
H	2.325844	0.222822	-0.627540
O	3.412925	-0.616859	1.834107
H	2.881041	0.156228	2.124724
H	3.512544	-0.476125	0.864347
O	0.186307	3.607520	1.528285
H	0.684165	2.869081	1.945529
H	0.539748	3.642551	0.611865
O	1.409535	1.255892	2.304392
H	0.787980	0.713955	2.847141
H	1.145152	1.013214	1.386767
O	-1.682702	2.775489	-1.863020
H	-1.971261	2.785475	-0.912179
H	-1.587736	1.818203	-2.037044
O	-2.207187	2.572500	0.792728
H	-1.358268	2.956918	1.134430
H	-2.063302	1.605421	0.819323
O	-3.039363	-1.771361	3.773382
H	-2.133684	-1.406876	3.733650
H	-3.198215	-2.065121	2.853812
O	-1.728298	-3.846719	-0.649872
H	-2.306383	-3.348852	-1.272961
H	-0.963199	-3.240294	-0.573506
O	0.890963	3.176488	-1.173727
H	0.853344	2.258904	-0.821460
H	-0.016331	3.230428	-1.578354
S	-0.486042	-0.326933	-0.488438
O	0.650073	0.656205	-0.240703
O	0.076083	-1.727624	-0.457466
O	-1.509962	-0.160844	0.618600
O	-1.117154	-0.041879	-1.825720

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O	-0.786870	-0.667755	2.735100
H	-1.199646	-0.313620	1.913319
H	-0.177604	-1.357815	2.364529
O	-3.707722	-1.791484	0.295459
H	-3.118138	-1.017473	0.188537
H	-3.152042	-2.537846	-0.050035
O	-1.933322	-3.663470	-0.473810
H	-1.642347	-3.942079	0.432558
H	-1.298293	-2.965939	-0.733114
O	2.948134	2.218953	-2.577994
H	2.344112	2.760203	-2.019990
H	3.170273	1.437392	-2.026634
O	1.041733	0.833050	-3.921274
H	0.257745	0.877376	-3.336826
H	1.727282	1.397443	-3.479759
O	1.753549	-1.610021	-3.053888
H	1.011844	-1.751471	-2.432103
H	1.505093	-0.753522	-3.493826
O	0.859074	-2.406396	1.405392
H	1.741358	-1.950079	1.507394
H	0.559565	-2.152744	0.505184
O	3.059701	-0.228338	-1.160996
H	2.785939	-0.862077	-1.877883
H	2.180432	0.109251	-0.872918
O	3.072861	-0.918366	1.543613
H	2.608228	-0.121649	1.882802
H	3.228707	-0.725899	0.590832
O	0.314592	3.698028	1.661515
H	0.719169	2.876362	2.017411
H	0.665459	3.749913	0.742987
O	1.251689	1.118732	2.222584
H	0.560796	0.591450	2.686488
H	1.006605	0.982871	1.276837
O	-1.588558	3.366915	-1.821094
H	-1.890587	3.286637	-0.878168
H	-1.558469	2.430180	-2.101681
O	-2.124672	2.865034	0.794912
H	-1.263805	3.161965	1.188459
H	-2.033779	1.895553	0.700177
O	-3.025397	-2.311996	2.872668
H	-2.326015	-1.643324	3.034725
H	-3.365791	-2.082585	1.968873
O	-1.191269	-4.151998	2.117576
H	-0.372525	-3.619366	2.051049
H	-1.878548	-3.523851	2.462136
O	0.963911	3.337941	-1.012718
H	0.837269	2.389626	-0.776367
H	0.086774	3.539483	-1.440309
S	-0.614321	-0.016432	-0.820671
O	0.646106	0.731711	-0.373696
O	-0.237707	-1.473311	-0.993629
O	-1.663857	0.119552	0.267797

O	-1.116024	0.576934	-2.097869
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O	-1.090779	0.243434	3.263124
H	-1.436770	0.224166	2.351049
H	-0.898348	-0.720719	3.442090
O	-2.788679	-2.531876	1.683069
H	-2.493467	-1.654889	1.368613
H	-2.668854	-3.072903	0.865277
O	-3.642292	-1.128010	-1.632446
H	-3.659622	-0.750218	-0.737415
H	-2.821039	-0.738175	-1.997638
O	2.935883	1.732396	-2.723091
H	2.274241	2.337951	-2.317323
H	3.218104	1.167965	-1.967355
O	1.290120	-0.195894	-3.654211
H	0.444875	-0.062916	-3.182249
H	1.865591	0.562415	-3.370215
O	2.188563	-2.128560	-1.988081
H	1.382726	-2.188928	-1.436247
H	1.904009	-1.503504	-2.706249
O	1.349353	-2.515813	1.737205
H	1.989370	-1.770347	1.881493
H	0.838556	-2.261838	0.941989
O	3.171874	-0.065943	-0.630643
H	3.017604	-0.923545	-1.117475
H	2.241694	0.189555	-0.439590
O	3.099443	-0.480058	2.089551
H	2.502886	0.266416	2.322353
H	3.328373	-0.311971	1.147041
O	0.068368	3.707384	1.225349
H	0.504123	3.003791	1.760669
H	0.476975	3.622361	0.335523
O	1.092466	1.442847	2.347775
H	0.347821	1.027880	2.867996
H	0.897083	1.108479	1.443293
O	-1.716607	2.732770	-2.119728
H	-2.031925	2.793113	-1.179801
H	-1.596096	1.767889	-2.231243
O	-2.301044	2.623977	0.525762
H	-1.451007	3.019563	0.856707
H	-2.172109	1.657463	0.594163
O	-0.691156	-2.380407	3.481604
H	0.092598	-2.468644	2.875467
H	-1.460021	-2.595063	2.902378
O	-2.417844	-3.485406	-0.865524

H	-2.968100	-2.747185	-1.219914
H	-1.524645	-3.086276	-0.861428
O	0.856318	2.966594	-1.354511
H	0.773222	2.088538	-0.919792
H	-0.038052	3.050458	-1.783401
S	-0.603071	-0.371091	-0.520771
O	0.562077	0.535099	-0.149493
O	-0.151046	-1.812004	-0.478944
O	-1.719360	-0.154186	0.479863
O	-1.067885	-0.023185	-1.914954
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O	-0.028543	-0.982058	3.168611
H	-0.389327	-0.612804	2.332749
H	0.659718	-1.620165	2.833570
O	-3.596618	-0.245222	0.816224
H	-2.619735	-0.118251	0.805285
H	-3.714499	-0.723921	-0.045409
O	-3.223063	-1.640077	-1.479172
H	-2.776399	-2.372015	-0.980134
H	-2.467185	-1.084817	-1.753860
O	2.496802	2.050688	-2.857679
H	1.886244	2.591004	-2.321957
H	3.038245	1.556086	-2.204095
O	1.078742	-0.086670	-3.767316
H	0.307710	-0.098095	-3.164637
H	1.566144	0.733620	-3.499965
O	2.567758	-1.807626	-2.322594
H	1.899088	-1.977758	-1.630714
H	2.058322	-1.242190	-2.962508
O	1.821696	-2.461539	1.915815
H	2.624610	-1.879751	1.868750
H	1.378476	-2.304145	1.057003
O	3.665409	0.251328	-0.980506
H	3.464706	-0.557980	-1.523389
H	2.765774	0.439076	-0.630347
O	3.873344	-0.688140	1.767016
H	3.279703	0.003490	2.148441
H	3.979871	-0.405636	0.833512
O	-0.770136	2.680220	1.544725
H	-0.348008	3.049891	0.738018
H	-0.755554	1.716375	1.380633
O	1.905132	1.039440	2.574744
H	1.257356	0.416969	2.972356
H	1.578372	1.154858	1.663134
O	-2.246852	2.419313	-1.696406

H	-2.722533	2.496100	-0.829264
H	-1.924104	1.496985	-1.723385
O	-3.407256	2.566166	0.760113
H	-2.521984	2.681685	1.178682
H	-3.617295	1.613296	0.870542
O	-2.546996	-2.312332	2.445760
H	-1.765435	-1.895858	2.861571
H	-3.037721	-1.570478	2.028942
O	-1.787301	-3.407655	0.054420
H	-0.945373	-2.944091	-0.127295
H	-2.045362	-3.077015	0.951799
O	0.324402	3.163632	-1.023203
H	0.651256	2.261190	-0.813089
H	-0.589910	3.003960	-1.372467
S	-0.059888	-0.288906	-0.413146
O	1.102674	0.674004	-0.308030
O	0.439386	-1.711070	-0.387204
O	-0.950406	-0.029666	0.790875
O	-0.842191	-0.036733	-1.678283

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O	-0.767746	-0.984831	3.050551
H	-1.076825	-0.710505	2.159168
H	0.086974	-1.458394	2.844299
O	-3.942920	-1.200449	0.653031
H	-3.121055	-0.678512	0.576771
H	-3.654464	-1.898398	1.293361
O	-3.045668	-2.139394	-1.755457
H	-3.510994	-1.789254	-0.955459
H	-2.376835	-1.460783	-1.964486
O	2.761587	2.032457	-2.737916
H	2.077278	2.586528	-2.298528
H	3.193556	1.565454	-1.989024
O	1.452160	-0.163441	-3.674666
H	0.615260	-0.165401	-3.168128
H	1.897239	0.679504	-3.398257
O	2.742418	-1.790288	-1.929119
H	1.971240	-1.965684	-1.353672
H	2.333519	-1.267728	-2.668818
O	1.503445	-2.098067	2.191354
H	2.196090	-1.387054	2.228678
H	1.206246	-2.079431	1.259054
O	3.410277	0.401121	-0.547913
H	3.378190	-0.464937	-1.039350
H	2.449459	0.549450	-0.396042
O	3.225938	-0.021844	2.207502
H	2.512696	0.609805	2.439192
H	3.431667	0.165036	1.263542
O	-0.229917	3.674741	1.412306
H	0.175157	2.953837	1.941536
H	0.222460	3.639592	0.541780
O	0.763681	1.331742	2.548708
H	0.180062	0.665906	2.976441
H	0.733989	1.080361	1.597656
O	-1.800880	2.513308	-2.087958
H	-2.144644	2.535509	-1.157252
H	-1.535781	1.578364	-2.196515
O	-2.455050	2.391373	0.568074
H	-1.697160	2.916157	0.936741
H	-2.146656	1.467294	0.648303
O	-2.656416	-2.992386	2.296741
H	-2.022961	-2.377653	2.721328
H	-2.194776	-3.287403	1.468158
O	-1.541771	-3.666819	-0.079870
H	-2.134662	-3.235897	-0.744731
H	-0.741982	-3.105950	-0.140911
O	0.694133	3.165277	-1.225220
H	0.738564	2.267926	-0.822959
H	-0.191769	3.119341	-1.672681
S	-0.251510	-0.358785	-0.477096
O	0.767466	0.719123	-0.119158
O	0.410858	-1.707523	-0.327167
O	-1.398524	-0.231718	0.500939
O	-0.750592	-0.159756	-1.881984

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O	-0.401448	-0.570998	3.171029
H	-0.905187	-0.349183	2.344192
H	0.266143	-1.264723	2.817070
O	-3.346361	-2.127152	0.916165
H	-2.729245	-1.349084	0.881754
H	-2.811225	-2.836057	0.438325
O	-3.427423	-1.654574	-1.906211
H	-3.705136	-1.625829	-0.955856
H	-2.688684	-0.996712	-1.947729
O	2.684097	1.842446	-2.789883
H	2.078629	2.452613	-2.280955
H	3.075562	1.268262	-2.073203
O	1.044156	-0.077943	-3.676548
H	0.237195	0.001862	-3.111037
H	1.629502	0.696317	-3.382849
O	2.211112	-1.979921	-2.200473

H	1.466775	-2.103167	-1.560155
H	1.796500	-1.325708	-2.857351
O	1.331457	-2.211545	2.060408
H	2.146479	-1.610343	1.990906
H	0.940535	-2.174807	1.151425
O	3.245614	0.002787	-0.795602
H	3.032708	-0.838465	-1.331989
H	2.318234	0.265302	-0.546734
O	3.351737	-0.473064	1.911847
H	2.777960	0.294765	2.186463
H	3.472261	-0.326452	0.929287
O	0.208287	3.717799	1.453513
H	0.661210	2.962540	1.922282
H	0.563592	3.656317	0.522184
O	1.319075	1.359104	2.376829
H	0.698897	0.761366	2.899173
H	1.084870	1.090314	1.446199
O	-1.682532	2.778361	-1.842073
H	-1.953139	2.790005	-0.862812
H	-1.572290	1.809231	-2.001599
O	-2.151204	2.636138	0.776898
H	-1.283260	3.045468	1.100551
H	-1.991545	1.661745	0.838295
O	-2.512534	-2.422007	3.618749
H	-1.767211	-1.771976	3.591607
H	-2.864118	-2.384819	2.693249
O	-1.927654	-3.648562	-0.810018
H	-2.453309	-3.064300	-1.431379
H	-1.106827	-3.106600	-0.690951
O	0.853219	3.121784	-1.172279
H	0.825335	2.205093	-0.783706
H	-0.088914	3.150723	-1.559352
S	-0.468475	-0.323567	-0.426425
O	0.704411	0.636658	-0.160783
O	0.056845	-1.754280	-0.383532
O	-1.509192	-0.108216	0.675124
O	-1.084062	-0.017982	-1.783275

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O	-0.410207	-0.823890	3.090588
H	-0.836500	-0.553947	2.232231
H	0.365721	-1.398172	2.758886
O	-3.964667	-1.095388	0.863673
H	-3.149088	-0.539444	0.823541
H	-3.845197	-1.594488	-0.006289
O	-3.197512	-2.332844	-1.393075
H	-2.609990	-2.947650	-0.839127
H	-2.567370	-1.648465	-1.714254
O	2.583018	1.980183	-2.853328
H	1.952541	2.552449	-2.331249
H	3.022152	1.426664	-2.148096
O	1.048375	-0.045382	-3.707556
H	0.237770	-0.018336	-3.142038
H	1.579417	0.767502	-3.418340
O	2.350957	-1.869950	-2.245897
H	1.624516	-2.042739	-1.596973
H	1.887656	-1.242720	-2.895654
O	1.576628	-2.191781	1.992567
H	2.328459	-1.513282	1.942494
H	1.176164	-2.147593	1.089040
O	3.297246	0.177988	-0.863139
H	3.126767	-0.676657	-1.391919
H	2.354840	0.389309	-0.617577
O	3.420585	-0.257223	1.858116
H	2.757289	0.436772	2.126540
H	3.529663	-0.108121	0.874871
O	0.078125	3.721953	1.427618
H	0.531111	2.960010	1.882330
H	0.415808	3.670766	0.488527
O	1.186558	1.330737	2.331032
H	0.612165	0.687946	2.840504
H	0.990339	1.074139	1.387215
O	-1.819472	2.637092	-1.857085
H	-2.066766	2.651696	-0.872567
H	-1.665224	1.672423	-2.009313
O	-2.226035	2.524036	0.776325
H	-1.394246	3.009219	1.090025
H	-1.961082	1.572877	0.838468
O	-2.536985	-2.708499	2.507960
H	-1.840932	-2.097803	2.862362
H	-3.147047	-2.100600	1.982203
O	-1.600837	-3.747333	0.214638
H	-0.856357	-3.127664	0.011884
H	-1.924318	-3.412745	1.112867
O	0.694907	3.161004	-1.212517
H	0.729880	2.239799	-0.832425
H	-0.248942	3.124942	-1.593565
S	-0.402846	-0.358542	-0.467238
O	0.733576	0.662819	-0.255211
O	0.202614	-1.756300	-0.396438
O	-1.406519	-0.145949	0.666442
O	-1.076019	-0.137167	-1.808414

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O	-1.079505	0.291937	3.228872
H	-1.416175	0.275585	2.301577
H	-0.925171	-0.709491	3.396856
O	-2.787080	-2.432893	1.626274
H	-2.515340	-1.548125	1.279935
H	-2.608169	-3.010768	0.820285
O	-3.509969	-1.435584	-1.819494
H	-3.786361	-1.002420	-0.986032
H	-2.698790	-0.918235	-2.061531
O	2.792001	1.681661	-2.708540
H	2.154747	2.316294	-2.271933
H	3.095988	1.113228	-1.945254
O	1.135303	-0.199293	-3.642660
H	0.299612	-0.078830	-3.127199
H	1.729229	0.561832	-3.332864
O	2.143766	-2.091798	-2.054311
H	1.349392	-2.187047	-1.472982
H	1.794421	-1.441273	-2.752210
O	1.337357	-2.480921	1.792131
H	2.023503	-1.749837	1.930841
H	0.846887	-2.203148	0.979077
O	3.127855	-0.102336	-0.620334
H	2.928835	-0.951837	-1.148848
H	2.194295	0.178648	-0.422161
O	3.121115	-0.509404	2.112551
H	2.494319	0.238681	2.333543
H	3.311899	-0.360902	1.143438
O	0.150001	3.702436	1.287289
H	0.581758	2.947208	1.782399
H	0.530193	3.616261	0.367661
O	1.135772	1.367517	2.362655
H	0.334016	0.963944	2.858718
H	0.934320	1.053227	1.439977
O	-1.641327	2.784823	-2.078206
H	-1.956979	2.840475	-1.115750
H	-1.549062	1.807113	-2.196984
O	-2.226270	2.721574	0.527833
H	-1.348735	3.082099	0.885361
H	-2.134607	1.740644	0.607776
O	-0.760686	-2.297542	3.419443
H	0.069510	-2.387569	2.846585
H	-1.508347	-2.495767	2.776262
O	-2.224031	-3.586066	-0.745991
H	-2.787447	-2.902784	-1.218931
H	-1.361231	-3.102216	-0.702919
O	0.868380	3.017648	-1.287727
H	0.780675	2.115587	-0.873553
H	-0.052566	3.081883	-1.720448
S	-0.626268	-0.323372	-0.503758
O	0.557856	0.595698	-0.154257
O	-0.151409	-1.769672	-0.427487
O	-1.758138	-0.073782	0.491276
O	-1.104844	-0.000145	-1.916581

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O	0.071458	-1.116108	3.169351
H	-0.328227	-0.708633	2.355121
H	0.764668	-1.745680	2.766873
O	-3.601624	-0.229012	0.927029
H	-2.613726	-0.098776	0.945275
H	-3.663251	-0.776824	0.072124
O	-3.248057	-1.672845	-1.274352
H	-2.745187	-2.394496	-0.768273
H	-2.506394	-1.104361	-1.593519
O	2.471601	2.183012	-2.711502
H	1.857393	2.683487	-2.113440
H	3.011339	1.616594	-2.096121
O	1.039776	0.119379	-3.677576
H	0.266625	0.070441	-3.063756
H	1.541218	0.935673	-3.355426
O	2.458819	-1.757216	-2.402419
H	1.792242	-1.958399	-1.701526
H	1.946170	-1.102152	-2.983547
O	1.899818	-2.546694	1.864846
H	2.687770	-1.912413	1.786721
H	1.420581	-2.377585	1.015394
O	3.585586	0.201699	-1.002388
H	3.345893	-0.602881	-1.575816
H	2.675184	0.402776	-0.651041
O	3.829962	-0.708057	1.638012
H	3.210078	-0.026828	2.039548
H	3.882463	-0.425701	0.682480
O	-0.992365	2.732749	1.466324
H	-0.448014	3.074695	0.703242
H	-0.889496	1.752976	1.386103
O	1.865681	0.935640	2.534715
H	1.256890	0.261194	2.949042
H	1.520499	1.001345	1.611576
O	-1.902385	2.478943	-1.964681
H	-2.536927	2.505334	-1.173996

H	-1.607329	1.534287	-1.954344
O	-3.413315	2.483387	0.249502
H	-2.591752	2.664962	0.798098
H	-3.629017	1.536349	0.477993
O	-2.543103	-2.301997	2.567595
H	-1.713670	-1.904155	2.935714
H	-3.023576	-1.537552	2.147686
O	-1.797866	-3.360200	0.203280
H	-0.930256	-2.925058	0.018908
H	-2.042995	-3.014783	1.119138
O	0.440556	3.196852	-0.908576
H	0.700216	2.274387	-0.639761
H	-0.445856	3.030760	-1.381733
S	-0.073945	-0.310415	-0.328060
O	1.091586	0.679411	-0.207579
O	0.453121	-1.737677	-0.338341
O	-0.954928	-0.063596	0.901799
O	-0.872670	-0.059528	-1.598482

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O	-0.679367	-0.874035	3.006642
H	-1.026532	-0.643825	2.102242
H	0.157931	-1.407091	2.767214
O	-3.994630	-1.200847	0.623561
H	-3.205965	-0.618049	0.514027
H	-3.616335	-1.851385	1.303553
O	-3.049265	-2.300022	-1.642584
H	-3.522733	-1.892667	-0.847923
H	-2.406211	-1.601404	-1.904183
O	2.806881	2.107856	-2.546430
H	2.090897	2.645538	-2.104990
H	3.184210	1.570819	-1.794536
O	1.480733	0.019409	-3.581235
H	0.612722	-0.006499	-3.109979
H	1.929379	0.854214	-3.225314
O	2.708496	-1.759635	-2.005329
H	1.925842	-1.973880	-1.440296
H	2.289004	-1.144197	-2.694563
O	1.486076	-2.131339	2.142143
H	2.200972	-1.414127	2.188583
H	1.195425	-2.092281	1.196753
O	3.380117	0.311333	-0.500852
H	3.314324	-0.541671	-1.055977
H	2.406363	0.472765	-0.360281
O	3.215434	-0.090430	2.228442
H	2.481196	0.559776	2.408036
H	3.425207	0.053598	1.261432
O	-0.286506	3.691739	1.395577
H	0.154592	2.951422	1.896007
H	0.153374	3.664641	0.498748
O	0.854806	1.369053	2.413485
H	0.258577	0.690296	2.847776
H	0.799641	1.105222	1.452821
O	-1.728738	2.504111	-2.093660
H	-2.084013	2.508965	-1.142678
H	-1.499146	1.549990	-2.214622
O	-2.415979	2.359996	0.480478
H	-1.659825	2.895640	0.890051
H	-2.098988	1.427481	0.572055
O	-2.664461	-2.848326	2.276930
H	-2.003862	-2.234874	2.689365
H	-2.174675	-3.226702	1.475065
O	-1.510819	-3.754033	0.028328
H	-2.124349	-3.315777	-0.643750
H	-0.716754	-3.169847	-0.062163
O	0.660431	3.173685	-1.159354
H	0.708332	2.251224	-0.782643
H	-0.226834	3.085452	-1.650619
S	-0.298244	-0.407271	-0.531579
O	0.748144	0.678338	-0.205578
O	0.373806	-1.768331	-0.389041
O	-1.431079	-0.253932	0.483322
O	-0.837554	-0.219166	-1.937596

SO_4 – 20 water molecules

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O	-1.050180	0.679070	-3.225196
H	-1.839250	0.122336	-2.975886
H	-0.567542	0.825796	-2.383389
O	-2.352209	3.080860	-2.423096
H	-1.599055	3.507718	-1.935505
H	-1.917967	2.343203	-2.904409
O	4.033018	-1.292768	-1.511617
H	4.049337	-1.303417	-0.529521
H	3.218602	-1.793725	-1.749270
O	-3.358356	1.521362	-0.501333
H	-2.522974	1.108261	-0.195285
H	-3.050912	2.198607	-1.169480

O	-0.244239	3.911838	-0.953396
H	-0.606639	3.875129	-0.029479
H	0.177596	3.036159	-1.047380
O	-3.286890	-0.550031	-2.377881
H	-3.032257	-1.301806	-1.793999
H	-3.524335	0.155690	-1.734267
O	-0.970452	3.538192	1.620339
H	-0.329239	2.809519	1.726051
H	-1.841442	3.123609	1.852749
O	-0.261446	-3.931655	-0.998249
H	0.110136	-3.845054	-0.092149
H	0.367178	-3.417963	-1.556209
O	0.432846	-3.047067	1.604754
H	-0.499714	-2.987728	1.950313
H	0.568547	-2.195828	1.137252
O	-2.266355	-2.253515	-0.468967
H	-1.553468	-2.894357	-0.752053
H	-1.788433	-1.439273	-0.206140
O	-1.976701	-0.073725	3.065395
H	-1.106100	0.022500	3.538836
H	-1.710348	0.007385	2.124378
O	3.082300	1.186007	-2.015489
H	3.452836	0.278440	-1.838975
H	2.158266	1.157913	-1.689399
O	-3.325734	2.282824	2.204992
H	-3.534788	2.018083	1.282441
H	-2.986113	1.466756	2.632174
O	0.574787	0.288370	3.953776
H	1.153292	-0.510671	3.840444
H	0.755584	0.795270	3.138613
O	-2.168606	-2.774722	2.281220
H	-2.426386	-2.654792	1.339873
H	-2.230321	-1.872045	2.667410
O	2.194950	-1.837606	3.453530
H	1.613531	-2.416330	2.911013
H	2.848218	-1.501593	2.800709
O	1.501530	-2.134214	-2.111902
H	1.275582	-1.585132	-1.330833
H	1.422636	-1.508792	-2.886273
O	3.607125	-0.899035	1.229152
H	3.796082	0.073756	1.186693
H	2.689035	-0.915232	0.879097
O	3.574912	1.778375	0.735335
H	3.527903	1.737915	-0.245019
H	2.642872	1.847782	1.021494
O	1.439618	-0.262080	-4.009182
H	0.530331	0.103007	-3.898453
H	2.025603	0.397283	-3.588997
S	0.305681	0.487910	0.259408
O	0.799886	1.344810	1.389852
O	1.087541	-0.813216	0.220974
O	-1.160101	0.151651	0.431108
O	0.503474	1.208334	-1.055322

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O	-0.713993	0.649644	-3.223885
H	-1.603287	0.251377	-3.010195
H	-0.252101	0.615935	-2.358709
O	-1.418021	3.226080	-2.350031
H	-0.607654	3.513891	-1.874225
H	-1.134569	2.411438	-2.824929
O	3.571185	-1.297492	-0.487231
H	3.696926	-0.568968	0.178427
H	2.657895	-1.590671	-0.316456
O	-2.828582	1.910560	-0.421815
H	-2.165153	1.261126	-0.103495
H	-2.332941	2.477421	-1.073748
O	0.857229	3.501356	-0.725258
H	0.770327	2.526954	-0.809120
H	0.514254	3.650850	0.197143
O	-3.101663	-0.168042	-2.332029
H	-3.060453	-0.969476	-1.761282
H	-3.227864	0.564542	-1.690227
O	0.055034	3.392328	1.839938
H	0.481009	2.514688	1.874031
H	-0.901076	3.178550	2.002482
O	-1.022190	-4.169536	-1.130387
H	-0.641356	-4.209696	-0.226241
H	-0.334689	-3.697984	-1.661334
O	-0.183851	-3.574416	1.493658
H	-1.056806	-3.310588	1.895771
H	0.106989	-2.759314	1.030973
O	-2.686337	-2.163787	-0.429067
H	-2.105797	-2.909257	-0.752346
H	-2.066642	-1.478136	-0.102965
O	-2.271221	-0.053564	3.129343
H	-1.425296	-0.052600	3.655870
H	-1.924106	-0.050368	2.210544
O	2.983914	0.599347	-2.294420
H	3.341127	-0.157213	-1.752962
H	2.122507	0.743247	-1.850425
O	-2.539252	2.674478	2.271647

H	-2.817394	2.508607	1.343825
H	-2.565328	1.788458	2.692261
O	0.221997	0.023423	4.130179
H	0.639214	-0.852688	3.940395
H	0.512084	0.524396	3.344598
O	-2.592291	-2.739949	2.342906
H	-2.891193	-2.579489	1.421629
H	-2.578177	-1.843794	2.748521
O	1.567377	-2.166679	3.152945
H	0.991510	-2.846723	2.736534
H	1.926992	-1.700188	2.381823
O	0.914451	-2.610244	-2.210702
H	0.843969	-2.031061	-1.430276
H	1.063942	-2.002405	-2.978471
O	3.673453	0.826885	1.174337
H	3.698070	1.592337	0.544244
H	2.743477	0.823399	1.477120
O	3.606735	2.836147	-0.695695
H	3.553246	2.168367	-1.414186
H	2.703570	3.226387	-0.683603
O	1.430908	-0.797131	-4.185582
H	2.102423	-0.289787	-3.677479
H	0.605435	-0.279367	-4.041401
S	0.295623	0.030298	0.395788
O	0.934805	0.730268	1.563724
O	0.841151	-1.371421	0.259652
O	-1.205971	-0.042940	0.583368
O	0.593487	0.795829	-0.877047

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O	-1.489571	-0.291393	-2.868546
H	-1.810766	-1.085800	-2.371043
H	-0.911392	0.152002	-2.211091
O	-0.712094	3.449229	-1.466318
H	-1.048860	3.642002	-0.550355
H	-0.404916	2.523624	-1.354769
O	3.971784	-0.968058	-1.508682
H	3.946332	-0.690582	-0.561500
H	3.277639	-1.662446	-1.574271
O	-3.806962	1.042905	-0.282357
H	-2.973526	0.575401	-0.083009
H	-3.568205	1.571295	-1.086812
O	2.196644	3.480721	-1.732044
H	1.227769	3.623367	-1.739894
H	2.328746	2.621093	-2.192138
O	-2.921160	2.172853	-2.596286
H	-2.509069	1.322085	-2.860775
H	-2.161003	2.731433	-2.313202
O	-1.362898	3.535111	1.154546
H	-0.667261	2.886485	1.375379
H	-2.174974	3.092850	1.515143
O	-0.197670	-4.187798	-0.622685
H	0.096570	-3.996432	0.297983
H	0.508914	-3.757989	-1.156777
O	0.527939	-3.130446	1.845815
H	-0.402361	-3.131245	2.189138
H	0.578103	-2.273307	1.368608
O	-2.102006	-2.280996	-1.064188
H	-1.404210	-2.978445	-0.938906
H	-1.901826	-1.612365	-0.379922
O	-2.345119	-0.351168	3.146376
H	-1.457186	-0.356649	3.587252
H	-2.077328	-0.239222	2.208126
O	2.349608	0.872537	-2.538915
H	3.057917	0.265909	-2.177526
H	1.617492	0.812293	-1.889334
O	-3.507646	2.170769	2.163761
H	-3.752275	1.794609	1.280110
H	-3.171655	1.401702	2.665356
O	0.265125	-0.202265	3.835814
H	1.052719	-0.785658	3.711941
H	0.393822	0.486007	3.155324
O	-2.143548	-3.012161	2.335290
H	-2.501108	-2.997292	1.432783
H	-2.363249	-2.123505	2.701937
O	2.523481	-1.693620	3.273805
H	1.989688	-2.352243	2.781848
H	2.962082	-1.149348	2.588612
O	1.605965	-2.432442	-1.710713
H	1.249177	-1.832371	-1.023516
H	1.335059	-2.017933	-2.578080
O	3.423852	-0.067065	1.019112
H	3.334901	0.921290	0.942561
H	2.515475	-0.375705	0.812899
O	2.741928	2.551713	0.772616
H	2.569585	2.902424	-0.139451
H	1.859173	2.295548	1.100676
O	0.980518	-1.075941	-3.944893
H	0.051857	-0.807827	-3.758929
H	1.508575	-0.298562	-3.650046
S	-0.038030	0.318526	0.387557
O	0.342829	1.327917	1.432369

O	0.886074	-0.881473	0.457393
O	-1.462004	-0.143847	0.584071
O	0.105476	0.910115	-0.999803

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O	-0.663668	0.946706	-3.354354
H	-1.523064	0.475837	-3.166883
H	-0.271320	1.057327	-2.461354
O	-1.795245	3.534176	-3.207544
H	-1.653425	3.739225	-2.267431
H	-1.375160	2.657579	-3.328278
O	3.924341	-1.452910	-1.540672
H	3.955066	-1.518536	-0.561641
H	3.091992	-1.908329	-1.799783
O	-3.183655	1.619587	-0.338962
H	-2.475171	1.011696	-0.035844
H	-2.643092	2.438294	-0.489801
O	-1.268464	3.514706	-0.419527
H	-1.176331	3.643872	0.563082
H	-0.530908	2.909189	-0.638820
O	-3.015571	-0.054821	-2.577921
H	-2.905428	-0.858860	-2.020944
H	-3.239477	0.637531	-1.916868
O	-0.988458	3.374970	2.255866
H	-0.318436	2.671936	2.162302
H	-1.846193	2.893737	2.397914
O	-0.535534	-3.829514	-1.271112
H	-0.141879	-3.804539	-0.371029
H	0.116404	-3.328732	-1.813414
O	0.313857	-3.089338	1.328477
H	-0.613684	-2.992946	1.683624
H	0.509835	-2.227795	0.905204
O	-2.420204	-2.011307	-0.652386
H	-1.772668	-2.702094	-0.968555
H	-1.851699	-1.299069	-0.293113
O	-1.880110	-0.217055	3.149108
H	-1.027225	-0.095345	3.651844
H	-1.584414	-0.086705	2.221841
O	3.132069	1.119108	-1.876957
H	3.407286	0.173006	-1.732717
H	2.202450	1.182953	-1.578948
O	-3.343470	2.044275	2.456465
H	-3.500667	1.869302	1.503542
H	-2.990522	1.200301	2.816368
O	0.634684	0.210805	4.045245
H	1.117404	-0.639126	3.864475
H	0.814948	0.717668	3.229851
O	-2.231062	-2.776796	2.105158
H	-2.552835	-2.546411	1.207275
H	-2.236779	-1.926106	2.600738
O	1.984551	-2.027453	3.337585
H	1.411325	-2.553439	2.736335
H	2.703484	-1.714676	2.745569
O	1.335940	-2.099007	-2.267889
H	1.161570	-1.537418	-1.483682
H	1.415177	-1.453200	-3.024406
O	3.576937	-1.115378	1.225149
H	3.827992	-0.155483	1.227718
H	2.670939	-1.050378	0.850193
O	3.689240	1.580520	0.874230
H	3.631793	1.584962	-0.106354
H	2.762337	1.687977	1.164443
O	1.713469	-0.181787	-4.094703
H	0.828130	0.247516	-4.008873
H	2.306264	0.401973	-3.580000
S	0.349255	0.500943	0.315903
O	0.879123	1.254350	1.500820
O	1.139247	-0.776764	0.103179
O	-1.100355	0.113019	0.544241
O	0.470171	1.356840	-0.925173

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O	-0.668713	0.444572	-3.871000
H	-1.523250	0.014083	-3.612651
H	-0.346639	0.816580	-3.026776
O	-1.579887	3.425716	-1.217125
H	-1.372600	3.677842	-0.289085
H	-0.825280	2.858317	-1.467005
O	3.972371	-1.376226	-1.673081
H	3.988460	-1.321390	-0.692707
H	3.183286	-1.928610	-1.875325
O	-3.373769	1.452168	-0.884498
H	-2.633833	0.922748	-0.518971
H	-2.872390	2.273252	-1.134020
O	-1.017251	3.557486	1.538062
H	-1.890537	3.093861	1.672271
H	-0.373935	2.837586	1.367289
O	-3.068954	-0.478199	-2.929475
H	-2.907221	-1.214915	-2.299366
H	-3.323363	0.262475	-2.336843
O	-0.634366	2.978535	4.315042
H	-0.187657	2.119646	4.194163

H	-0.719697	3.323643	3.405683
O	-0.385474	-3.944796	-1.079219
H	-0.017728	-3.767070	-0.184922
H	0.269490	-3.516280	-1.677389
O	0.305852	-2.781943	1.409842
H	-0.646611	-2.733411	1.699667
H	0.457175	-1.983732	0.863693
O	-2.362309	-2.163371	-0.792058
H	-1.675365	-2.862279	-0.987934
H	-1.839029	-1.374855	-0.539056
O	-2.079318	0.032809	2.716038
H	-1.215481	0.149638	3.195285
H	-1.784863	0.083359	1.780348
O	3.040786	1.059602	-2.395424
H	3.368106	0.165936	-2.099306
H	2.110229	1.122621	-2.100097
O	-3.372983	2.309986	1.874488
H	-3.592433	1.996222	0.970947
H	-3.056018	1.502239	2.340225
O	0.451088	0.459526	3.511943
H	1.067093	-0.324339	3.563405
H	0.672635	0.850474	2.639929
O	-2.324614	-2.636839	1.967841
H	-2.569957	-2.518617	1.023032
H	-2.397876	-1.736701	2.357235
O	2.090684	-1.623227	3.261662
H	1.488235	-2.183339	2.720708
H	2.746584	-1.303287	2.601293
O	1.471862	-2.331727	-2.304608
H	1.219263	-1.680515	-1.616219
H	1.519940	-1.785584	-3.140364
O	3.492832	-0.774402	1.006636
H	3.704131	0.189571	0.907034
H	2.599152	-0.801538	0.599637
O	3.515088	1.863879	0.326366
H	3.481514	1.762229	-0.648951
H	2.578784	1.970246	0.585480
O	1.741704	-0.645670	-4.348427
H	0.822546	-0.271898	-4.303765
H	2.293856	0.040383	-3.922586
S	0.239562	0.583563	-0.146343
O	0.733378	1.459224	0.977772
O	1.060929	-0.690316	-0.190816
O	-1.201065	0.185955	0.111048
O	0.372091	1.318687	-1.453400
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O	-1.071916	0.782895	-3.176746
H	-1.857476	0.187584	-2.899138
H	-0.563753	0.932207	-2.336873
O	-2.466539	3.084837	-2.433843
H	-1.722263	3.506122	-1.884289
H	-1.985706	2.341456	-2.892801
O	4.065595	-1.393014	-1.466232
H	4.047711	-1.346463	-0.468632
H	3.207300	-1.857217	-1.692901
O	-3.354397	1.530925	-0.518885
H	-2.466028	1.205095	-0.219235
H	-3.099192	2.228702	-1.228269
O	-0.473158	3.910672	-0.902616
H	-0.789107	3.803456	0.055939
H	0.074118	3.099863	-1.031394
O	-3.218687	-0.514081	-2.346343
H	-2.905160	-1.252279	-1.745038
H	-3.458154	0.199457	-1.685161
O	-1.064007	3.510934	1.657284
H	-0.362742	2.826811	1.765132
H	-1.924409	3.019492	1.864990
O	-0.234619	-3.866977	-0.861080
H	0.116630	-3.729654	0.065378
H	0.418725	-3.368208	-1.431605
O	0.396102	-2.987893	1.667209
H	-0.578526	-2.931485	1.983576
H	0.535662	-2.115408	1.216436
O	-2.159100	-2.131572	-0.460389
H	-1.433055	-2.813785	-0.707638
H	-1.665323	-1.311238	-0.204312
O	-1.957159	-0.150102	2.924707
H	-1.051704	-0.072032	3.396148
H	-1.681298	-0.012366	1.979925
O	3.167256	1.067205	-2.032425
H	3.510871	0.132395	-1.831960
H	2.234658	1.077042	-1.696081
O	-3.326180	2.181099	2.177643
H	-3.533004	1.950939	1.229528
H	-2.956460	1.338347	2.559550
O	0.498980	0.146379	3.819394
H	1.120421	-0.647722	3.701597
H	0.743410	0.723799	3.055789
O	-2.161585	-2.752396	2.220489
H	-2.375394	-2.597611	1.256272
H	-2.188604	-1.821372	2.599104

O	2.180122	-1.895672	3.423773
H	1.571532	-2.460376	2.866119
H	2.828837	-1.539216	2.757814
O	1.514271	-2.160755	-2.042568
H	1.272904	-1.591958	-1.264601
H	1.380984	-1.532461	-2.836970
O	3.599889	-0.881435	1.219938
H	3.795764	0.108756	1.133191
H	2.666471	-0.886302	0.877087
O	3.686054	1.734378	0.644261
H	3.608063	1.635401	-0.347710
H	2.754269	1.877141	0.936817
O	1.321089	-0.329619	-3.928672
H	0.424722	0.095172	-3.785186
H	1.965257	0.310630	-3.540945
S	0.365701	0.588477	0.240293
O	0.880631	1.452123	1.374306
O	1.086867	-0.766625	0.236769
O	-1.130346	0.300156	0.384865
O	0.606468	1.285696	-1.095410

65

O	-0.821653	0.717566	-3.092071
H	-1.744793	0.326558	-2.882340
H	-0.324273	0.637045	-2.237136
O	-1.464821	3.244584	-2.226225
H	-0.631926	3.494476	-1.725461
H	-1.189066	2.420571	-2.723263
O	3.920015	-0.914292	-0.368262
H	3.966026	-0.065650	0.188373
H	3.051358	-1.288526	-0.089822
O	-2.728767	1.826412	-0.409196
H	-2.012180	1.204710	-0.120434
H	-2.258129	2.457753	-1.066329
O	0.759638	3.466549	-0.697937
H	0.756358	2.476515	-0.794872
H	0.435518	3.559581	0.267413
O	-3.235674	-0.048603	-2.370083
H	-3.116212	-0.875815	-1.813020
H	-3.281738	0.662217	-1.669190
O	-0.029881	3.315450	1.813763
H	0.409057	2.433117	1.891294
H	-1.009641	3.087473	1.952016
O	-1.045926	-3.986403	-1.084367
H	-0.715578	-4.012995	-0.145047
H	-0.280904	-3.536726	-1.577033
O	-0.294170	-3.401938	1.544453
H	-1.228929	-3.068552	1.801027
H	0.164014	-2.616761	1.144503
O	-2.636714	-1.981549	-0.588469
H	-2.059533	-2.786848	-0.870033
H	-1.964825	-1.336022	-0.248167
O	-2.166213	-0.049941	2.960954
H	-1.320109	-0.182965	3.517867
H	-1.761548	-0.059129	2.052508
O	2.973404	0.475747	-2.430765
H	3.472266	-0.130252	-1.784038
H	2.141568	0.603132	-1.900676
O	-2.575583	2.603109	2.205897
H	-2.803325	2.405999	1.252678
H	-2.509532	1.693169	2.612213
O	0.219675	-0.343605	4.033883
H	0.514679	-1.309504	3.974681
H	0.674433	0.077910	3.264363
O	-2.745827	-2.591970	2.082030
H	-2.937252	-2.377735	1.123897
H	-2.662461	-1.690824	2.511225
O	1.054190	-2.878733	3.790750
H	0.550843	-3.211038	2.982592
H	1.962543	-2.755100	3.449550
O	1.048673	-2.722157	-2.103955
H	1.154207	-2.174324	-1.290255
H	1.018854	-2.046869	-2.859590
O	3.788850	1.378150	0.990930
H	3.677572	2.022788	0.216781
H	2.863937	1.245154	1.312260
O	3.448218	2.929237	-1.165479
H	3.343013	2.146353	-1.774605
H	2.516644	3.263590	-1.037645
O	1.170177	-0.894892	-4.036784
H	1.928694	-0.403232	-3.615309
H	0.385337	-0.303901	-3.848207
S	0.522259	0.010005	0.404927
O	1.094081	0.779832	1.584638
O	1.148263	-1.374577	0.334711
O	-0.999772	-0.112877	0.538573
O	0.789648	0.773191	-0.898238

65

O	-1.562062	-0.452290	-2.772699
H	-1.890141	-1.220358	-2.213949
H	-0.961939	0.031415	-2.144800

O	-0.726527	3.411752	-1.414757
H	-1.059110	3.576152	-0.466893
H	-0.403663	2.476734	-1.324445
O	3.958445	-0.800854	-1.606383
H	3.954291	-0.616065	-0.620048
H	3.281420	-1.531138	-1.693731
O	-3.798724	0.960268	-0.283271
H	-2.952984	0.490378	-0.093878
H	-3.543966	1.496932	-1.101691
O	2.183251	3.454720	-1.545634
H	1.200753	3.597480	-1.527835
H	2.293844	2.637988	-2.109854
O	-2.888211	2.073730	-2.535048
H	-2.470241	1.208330	-2.782358
H	-2.122837	2.642066	-2.230595
O	-1.354859	3.532533	1.165013
H	-0.633231	2.894014	1.376460
H	-2.167981	3.035750	1.513458
O	-0.092064	-4.092786	-0.689335
H	0.163632	-3.914979	0.261603
H	0.622909	-3.608244	-1.195539
O	0.403473	-3.109904	1.828266
H	-0.581773	-3.077713	2.078161
H	0.523307	-2.258782	1.329072
O	-2.127443	-2.381428	-0.838217
H	-1.350133	-3.041567	-0.829419
H	-1.813745	-1.640821	-0.260901
O	-2.258522	-0.357745	3.094539
H	-1.353839	-0.256916	3.548843
H	-1.976749	-0.229442	2.150047
O	2.287888	0.951417	-2.670435
H	3.020298	0.356763	-2.275501
H	1.557405	0.864760	-2.003563
O	-3.430716	2.129960	2.095232
H	-3.684964	1.733692	1.201499
H	-3.080872	1.351689	2.598970
O	0.233024	0.115871	3.882938
H	0.968882	-0.557987	3.718552
H	0.345325	0.728821	3.118496
O	-2.223758	-2.942337	2.183228
H	-2.501092	-2.833342	1.243684
H	-2.355648	-2.035076	2.593236
O	2.212181	-1.626842	3.341812
H	1.672950	-2.313596	2.863583
H	2.760455	-1.203188	2.635909
O	1.697236	-2.360701	-1.787700
H	1.359762	-1.770764	-1.065586
H	1.340734	-1.929349	-2.645807
O	3.513024	-0.242545	1.041794
H	3.430149	0.767024	0.971477
H	2.586527	-0.515585	0.812123
O	2.917654	2.358990	0.818327
H	2.696307	2.764474	-0.080109
H	2.019409	2.155647	1.172620
O	0.861227	-1.064013	-3.916693
H	-0.081599	-0.856978	-3.655671
H	1.368890	-0.241403	-3.662334
S	0.013030	0.314796	0.337241
O	0.385074	1.357728	1.368258
O	0.956310	-0.887087	0.415267
O	-1.415693	-0.171036	0.563913
O	0.108956	0.881203	-1.081514

65

O	-0.860708	0.932881	-3.208651
H	-1.738612	0.457897	-2.982588
H	-0.438618	1.079995	-2.323558
O	-2.051503	3.467590	-3.274067
H	-1.794265	3.742686	-2.364576
H	-1.621514	2.575353	-3.343783
O	4.060285	-1.346312	-1.447337
H	4.029636	-1.372825	-0.448296
H	3.219292	-1.817077	-1.717980
O	-3.109481	1.786513	-0.376129
H	-2.422423	1.150994	-0.040618
H	-2.504992	2.561326	-0.609290
O	-1.138670	3.603090	-0.622882
H	-1.067585	3.697530	0.394704
H	-0.408023	2.967660	-0.821159
O	-3.163803	-0.060428	-2.430632
H	-2.952010	-0.856037	-1.859853
H	-3.313955	0.663681	-1.758172
O	-0.911660	3.485089	1.987657
H	-0.217009	2.783890	1.968461
H	-1.757725	2.975818	2.217995
O	-0.426051	-3.723364	-1.177346
H	-0.088447	-3.701232	-0.236635
H	0.286029	-3.227101	-1.677099
O	0.249574	-3.116571	1.432140
H	-0.726108	-3.041880	1.736419
H	0.445185	-2.217265	1.063025
O	-2.306550	-1.957198	-0.653590

H	-1.609187	-2.644280	-0.956158
H	-1.765081	-1.214636	-0.281890
O	-1.979499	-0.351291	3.002934
H	-1.069617	-0.345465	3.472413
H	-1.689103	-0.174005	2.068280
O	3.155413	1.130195	-1.881025
H	3.488180	0.183062	-1.716525
H	2.223244	1.147463	-1.546596
O	-3.158815	2.112885	2.427666
H	-3.364733	1.981556	1.463141
H	-2.846030	1.216789	2.736793
O	0.493656	-0.194952	3.883437
H	1.084753	-0.998620	3.697230
H	0.754443	0.436165	3.169637
O	-2.313059	-2.841298	1.975184
H	-2.525503	-2.571255	1.037346
H	-2.309617	-1.967277	2.469118
O	2.067696	-2.276499	3.302105
H	1.440226	-2.749453	2.683912
H	2.744046	-1.880336	2.689705
O	1.524551	-2.090987	-2.123472
H	1.290296	-1.545906	-1.327271
H	1.460685	-1.418560	-2.892049
O	3.566983	-1.050487	1.253718
H	3.780934	-0.060353	1.240893
H	2.635794	-1.010732	0.906840
O	3.694781	1.594624	0.850193
H	3.613999	1.584010	-0.144827
H	2.765960	1.740863	1.151114
O	1.500360	-0.174128	-3.921424
H	0.593665	0.235501	-3.782417
H	2.120150	0.437613	-3.451382
S	0.361999	0.536844	0.352744
O	0.890389	1.313100	1.543219
O	1.091248	-0.806867	0.221938
O	-1.126796	0.216969	0.520970
O	0.564410	1.345608	-0.923847
65			
O	-0.908275	0.491666	-3.733932
H	-1.745448	0.021607	-3.415243
H	-0.539023	0.877769	-2.903625
O	-1.409976	3.575331	-1.241123
H	-1.283466	3.726042	-0.256593
H	-0.652458	2.985884	-1.467581
O	4.033367	-1.394669	-1.566186
H	3.981284	-1.288784	-0.575496
H	3.217837	-1.928701	-1.794806
O	-3.252320	1.656511	-0.955050
H	-2.530964	1.081258	-0.586516
H	-2.692263	2.466084	-1.196236
O	-1.104579	3.511319	1.484825
H	-1.982890	3.007537	1.622870
H	-0.430175	2.801747	1.330381
O	-3.207039	-0.491230	-2.781514
H	-2.960773	-1.197056	-2.117790
H	-3.391841	0.304822	-2.213823
O	-0.626618	2.915077	4.259794
H	-0.198879	2.038092	4.108186
H	-0.763738	3.256441	3.343144
O	-0.289754	-3.897233	-1.033628
H	0.055536	-3.710561	-0.115914
H	0.395549	-3.460940	-1.619798
O	0.361460	-2.829923	1.443029
H	-0.629700	-2.790879	1.705433
H	0.497612	-2.004259	0.912286
O	-2.245356	-2.147704	-0.810201
H	-1.513469	-2.837751	-1.003749
H	-1.745391	-1.332185	-0.550576
O	-2.075234	-0.069977	2.576903
H	-1.190024	0.085084	3.054466
H	-1.779188	0.008077	1.630528
O	3.078039	0.972587	-2.371198
H	3.409457	0.064508	-2.057999
H	2.135982	1.036152	-2.075981
O	-3.383355	2.219193	1.783826
H	-3.542649	1.991496	0.825446
H	-3.044503	1.370231	2.187884
O	0.378284	0.422077	3.426528
H	1.012865	-0.379636	3.483138
H	0.634804	0.833292	2.559979
O	-2.224370	-2.692383	1.896344
H	-2.448657	-2.553986	0.931808
H	-2.296555	-1.769084	2.279090
O	2.013376	-1.624097	3.264038
H	1.435084	-2.212459	2.695420
H	2.683411	-1.279464	2.610336
O	1.563860	-2.343127	-2.242074
H	1.276837	-1.698787	-1.543093
H	1.476252	-1.781096	-3.097126
O	3.470088	-0.709067	1.065627
H	3.661550	0.272739	0.903888

H 2.565977 -0.757655 0.655842
O 3.552892 1.846978 0.272565
H 3.494973 1.687773 -0.711550
H 2.612918 2.005085 0.528644
O 1.433029 -0.665873 -4.239875
H 0.508193 -0.265647 -4.116069
H 2.043404 0.011463 -3.860047
S 0.267029 0.609239 -0.172412
O 0.756213 1.509899 0.954484
O 1.061589 -0.700513 -0.165152
O -1.203705 0.236409 0.039919
O 0.442129 1.324838 -1.499444

CO_3 – 1 water molecule

7

O 0.195107 0.622135 -1.013821
C 0.513069 0.949343 0.211472
O 0.235274 0.122462 1.184553
O 1.085474 2.063906 0.451843
O -0.906195 -1.665289 -0.375578
H -0.555017 -1.211695 0.446644
H -0.567712 -0.880863 -0.905113
7

O -0.210790 -0.670875 0.986873
C 0.143820 -1.068317 -0.207098
O 0.158370 -0.205434 -1.189034
O 0.474071 -2.283628 -0.409435
O -0.218103 1.878959 0.374877
H -0.057918 1.327337 -0.447426
H -0.289450 1.021958 0.891242
7

O -0.209680 1.129563 0.372224
C -0.054035 0.053224 1.098450
O 0.158779 -1.092797 0.507176
O -0.108884 0.121001 2.371197
O 0.096234 -0.090818 -1.929789
H -0.054254 0.626577 -1.243063
H 0.171840 -0.746750 -1.176196
7

O 1.116050 -0.216131 -0.414291
C 0.568848 0.934460 -0.120007
O -0.655272 0.963819 0.336225
O 1.223739 2.017867 -0.278004
O -0.997613 -1.642682 0.213809
H -1.180324 -0.667135 0.354715
H -0.075427 -1.390198 -0.092446
7

O 0.874841 0.154287 -0.826368
C 0.332207 1.044435 -0.037125
O -0.741198 0.729813 0.638926
O 0.846574 2.206408 0.075983
O -0.546726 -1.844304 0.105608
H 0.101103 -1.313885 -0.449605
H -0.866800 -0.976754 0.492582
7

O 0.178548 0.618225 -1.027528
C 0.505661 0.941917 0.209364
O 0.218670 0.111624 1.193379
O 1.097480 2.056051 0.452403
O -0.898801 -1.672375 -0.374408
H -0.542720 -1.190058 0.451616
H -0.558837 -0.865385 -0.904826
7

O -0.125230 -0.645578 1.018575
C 0.164707 -1.057755 -0.201486
O 0.249559 -0.175989 -1.178906
O 0.363604 -2.305549 -0.433642
O -0.292501 1.878494 0.359656
H -0.066194 1.304041 -0.453457
H -0.293945 1.002336 0.889260
7

O -0.205981 1.140925 0.355196
C -0.052046 0.053094 1.086826
O 0.165137 -1.102674 0.489191
O -0.113682 0.120108 2.368336
O 0.092448 -0.091815 -1.930412
H -0.056868 0.627779 -1.217559
H 0.170991 -0.747417 -1.151577
7

O 1.115554 -0.234000 -0.423574
C 0.562976 0.924936 -0.120316

O -0.676853 0.952672 0.331014
O 1.225010 2.016582 -0.264006
O -1.000383 -1.642313 0.215663
H -1.162602 -0.641641 0.355487
H -0.063702 -1.376236 -0.094269
7

O 0.945237 0.114824 -0.750486
C 0.346874 1.033477 -0.016311
O -0.682838 0.691892 0.734840
O 0.764123 2.248351 -0.031243
O -0.609141 -1.837671 0.036243
H 0.105271 -1.294479 -0.455242
H -0.869526 -0.956394 0.482200

CO_3 – 2 water molecules

10

O -0.083229 -0.526959 -0.019957
C 0.131578 0.768802 0.026901
O -0.375147 1.533696 -0.876022
O 0.846276 1.265470 0.975610
O -1.790181 -0.380195 -2.060521
H -1.409370 0.518344 -1.857753
H -1.228966 -0.776710 -1.344497
O 1.535450 -1.074260 2.019929
H 1.467832 -0.092145 1.864969
H 0.905757 -1.236044 1.271341
10

O 0.144173 -0.496301 0.071240
C -0.231392 0.751012 -0.102960
O -1.107748 1.037979 -1.003166
O 0.280588 1.679100 0.627876
O -1.429746 -1.461856 -1.845465
H -0.764134 -1.464643 -1.110382
H -1.521924 -0.472979 -1.760173
O 1.866097 0.043021 2.033101
H 1.418276 0.872929 1.714011
H 1.345808 -0.488261 1.375919
10

O -0.006204 -0.541938 0.026634
C -0.038398 0.772628 0.000172
O -0.860201 1.373859 -0.788369
O 0.750514 1.449015 0.761382
O -1.484783 -0.802409 -2.180291
H -1.467815 0.146090 -1.874292
H -0.932542 -1.063147 -1.398648
O 1.562621 -0.655101 2.177197
H 1.480644 0.283626 1.853779
H 0.996161 -0.962622 1.422436
10

O -0.383333 -0.085991 0.406704
C 0.505298 0.113439 -0.536312
O 0.194516 -0.097102 -1.770739
O 1.692198 0.520589 -0.233438
O -2.352971 -0.608434 -1.392731
H -1.459395 -0.458093 -1.819209
H -1.945216 -0.494558 -0.499799
O 1.416316 0.405567 2.385059
H 0.538055 0.176809 1.994100
H 1.794533 0.527775 1.466365
10

O -0.246562 0.317277 0.349940
C 0.362335 -0.465238 -0.512317
O 0.946239 0.048233 -1.539918
O 0.371254 -1.740429 -0.325843
O 0.226986 2.554508 -1.035597
H -0.114748 1.973809 -0.308086
H 0.638980 1.760891 -1.476644
O -0.909542 -1.677977 2.003026
H -0.835830 -0.752424 1.652979
H -0.439112 -2.018650 1.192459
10

O -0.089228 -0.537217 -0.018117
C 0.128796 0.770458 0.026899
O -0.457214 1.552139 -0.828627
O 0.925699 1.262365 0.925694
O -1.746624 -0.392747 -2.087477
H -1.402830 0.521725 -1.819353
H -1.196968 -0.787542 -1.341740
O 1.498821 -1.083018 2.034986
H 1.480882 -0.089973 1.839974
H 0.858666 -1.216189 1.267761
10

O 0.156973 -0.516926 0.072645
C -0.222790 0.742308 -0.098072
O -1.101474 1.035094 -1.007714
O 0.287631 1.676739 0.645485
O -1.430396 -1.464057 -1.837584
H -0.753073 -1.449212 -1.092735
H -1.516232 -0.459135 -1.745619
O 1.856984 0.043105 2.025465
H 1.391884 0.877846 1.690238
H 1.330495 -0.485762 1.347892
10

O 0.019551 -0.544778 0.007773
C -0.027999 0.780924 -0.006397
O -0.721193 1.392354 -0.918181
O 0.618577 1.460301 0.891416
O -1.562598 -0.824024 -2.107822
H -1.411177 0.151249 -1.879266
H -0.974049 -1.069607 -1.328930
O 1.616359 -0.671038 2.119269
H 1.399986 0.288212 1.878259
H 1.042544 -0.963593 1.343879
10

O -0.368451 -0.082782 0.393538
C 0.530901 0.118200 -0.560488
O 0.191235 -0.014466 -1.806302
O 1.745967 0.447236 -0.243132
O -2.334492 -0.641264 -1.302159
H -1.468336 -0.437194 -1.786309
H -1.850963 -0.490605 -0.432091
O 1.316953 0.414841 2.374779
H 0.466176 0.179006 1.887811
H 1.771010 0.507028 1.474353
10

O -0.255648 0.329915 0.360938
C 0.358688 -0.460530 -0.508506
O 0.901360 0.047495 -1.573074
O 0.415356 -1.739778 -0.292310
O 0.246311 2.549979 -1.012678
H -0.096393 1.944947 -0.284092
H 0.620428 1.730794 -1.477860
O -0.930874 -1.673307 1.983714
H -0.852358 -0.735901 1.627800
H -0.406870 -1.993615 1.176068

CO_3 – 4 water molecules

16

O -0.398661 -0.228526 -1.114792
C -0.269612 0.440042 -0.001480
O 0.937759 0.632175 0.464707
O -1.289668 0.874231 0.633504
O 2.171457 0.125251 -1.886931
H 1.219644 -0.111830 -1.964131
H 2.076995 0.376225 -0.939034
O -3.019090 0.221648 -1.401828
H -2.756167 0.579932 -0.524573
H -2.102099 -0.094904 -1.592574
O 1.108747 -2.112756 0.336609
H 1.318277 -1.218869 0.679191
H 0.583621 -1.790549 -0.424032
O 0.246181 0.737263 3.015594
H -0.604405 0.824268 2.540801
H 0.777018 0.746400 2.178968
16

O -0.349466 -1.098070 0.131211
C -0.134938 0.090515 -0.365996
O -0.080633 1.110824 0.440689
O 0.024178 0.244145 -1.629309
O 0.125533 -2.404424 -2.183574
H 0.148827 -1.433878 -2.348778
H -0.095639 -2.280976 -1.231606
O -1.994691 -0.119291 2.041699
H -1.543443 -0.776848 1.463532
H -1.427058 0.622158 1.743958
O 1.033332 2.755755 -1.449702
H 0.743599 1.912699 -1.870668
H 0.685248 2.483871 -0.569471
O 1.235268 -0.448429 2.284387
H 0.905110 0.374887 1.861208
H 0.724776 -1.032939 1.682418
16

O -0.774464 0.739527 0.545329
C -0.509469 0.033737 -0.516249
O -0.834585 -1.216677 -0.561269

O 0.138529 0.563483 -1.500075
O 1.739000 -1.560192 -1.179305
H 1.469158 -0.665181 -1.505945
H 0.808606 -1.810938 -0.942873
O -0.182917 3.102470 -0.700664
H 0.086606 2.321087 -1.244749
H -0.478407 2.531931 0.043617
O 1.737341 -0.316231 1.410724
H 1.824204 -0.805773 0.567399
H 0.870313 0.125739 1.289680
O -2.243032 -1.200866 1.742085
H -1.834976 -0.311485 1.638918
H -1.815908 -1.530630 0.913375
16

O -0.369320 -1.088989 -0.007907
C 0.356387 -0.014634 0.140436
O -0.238052 1.139838 0.247447
O 1.637760 -0.093734 0.175286
O 1.749487 -2.802043 0.233770
H 2.081090 -1.874376 0.240313
H 0.815236 -2.509790 0.121804
O -2.080304 0.388561 -1.635721
H -1.565360 0.989877 -1.051854
H -1.711073 -0.423226 -1.228199
O 2.008830 2.480237 -0.533286
H 2.231639 1.547597 -0.305808
H 1.070315 2.372787 -0.259850
O -2.347708 -0.069515 1.565170
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H -1.824582 -0.730324 1.056036
16

O -0.115011 0.915699 0.743145
C 0.282434 -0.167866 0.139828
O -0.530220 -0.768060 -0.683878
O 1.458896 -0.636938 0.353680
O 1.310004 -2.669343 -1.400532
H 1.667793 -2.059604 -0.710993
H 0.443480 -2.205485 -1.421757
O -1.512127 1.709650 -1.439786
H -1.395339 0.740964 -1.526149
H -1.067553 1.747352 -0.561333
O 2.384875 1.582693 1.591078
H 2.402248 0.682187 1.191892
H 1.414738 1.674124 1.449135
O -2.649260 -0.286543 0.927018
H -2.098993 -0.666913 0.202661
H -1.995964 0.408084 1.145989
16

O -0.396904 -0.396216 -1.030526
C -0.269040 0.173431 0.148737
O 0.900699 0.128102 0.747842
O -1.273359 0.764590 0.704862
O 2.137160 0.349071 -1.693195
H 1.208018 0.009040 -1.807857
H 2.058968 0.339249 -0.702694
O -2.995407 0.266894 -1.337315
H -2.676034 0.609438 -0.457400
H -2.093264 -0.113610 -1.539193
O 1.288184 -2.400785 -0.197178
H 1.429801 -1.572996 0.339321
H 0.627974 -1.952454 -0.788360
O 0.063069 1.454887 2.959838
H -0.689710 1.371558 2.309718
H 0.679847 0.969801 2.343402
16

O -0.202843 -1.146242 0.159772
C 0.068914 0.039909 -0.340225
O 0.078519 1.078398 0.466208
O 0.321585 0.180966 -1.599337
O -0.062557 -2.429308 -2.223149
H 0.143983 -1.461675 -2.350982
H -0.188156 -2.296049 -1.242157
O -1.987034 -0.016378 1.887356
H -1.509715 -0.731520 1.386075
H -1.340627 0.677918 1.588665
O 0.745390 2.852835 -1.469154
H 0.672035 1.938437 -1.862419
H 0.496068 2.506344 -0.566776
O 1.176408 -0.483060 2.427802
H 0.883722 0.349613 1.969445
H 0.704310 -1.060187 1.768876
16

O -0.442366 0.895769 0.620322
C 0.024205 0.117031 -0.332161
O 0.301928 -1.135995 -0.043503
O 0.206542 0.573905 -1.526248
O 1.236276 -1.739687 -2.508371

H 0.921732 -0.793568 -2.498934
H 0.981828 -1.856453 -1.549688
O -0.621084 3.091618 -0.954536
H -0.273760 2.322523 -1.487359
H -0.685828 2.523542 -0.136335
O 1.199731 -0.337324 2.420989
H 1.035214 -0.948171 1.653643
H 0.581852 0.350615 2.053401
O -1.833433 -1.223187 1.658083
H -1.545139 -0.278812 1.537444
H -1.087697 -1.561805 1.093252
16

O -0.400307 -1.106490 0.014969
C 0.347048 -0.024200 -0.004766
O -0.244295 1.149854 -0.024588
O 1.635815 -0.113412 -0.004602
O 1.692057 -2.822210 0.071391
H 2.030458 -1.884199 0.043625
H 0.746050 -2.502971 0.053733
O -2.205199 0.125578 -1.628572
H -1.663893 0.815145 -1.158670
H -1.765221 -0.614957 -1.131378
O 2.067315 2.562662 -0.065142
H 2.270048 1.586133 -0.044627
H 1.086167 2.380117 -0.047223
O -2.188381 0.177697 1.634388
H -1.656389 0.850716 1.131202
H -1.751275 -0.579463 1.160259
16

O -0.093748 0.960473 0.671136
C 0.324772 -0.122556 0.053066
O -0.518603 -0.774653 -0.717112
O 1.539561 -0.536046 0.197970
O 1.251911 -2.694523 -1.422580
H 1.693949 -2.051905 -0.800723
H 0.395903 -2.181575 -1.377523
O -1.600612 1.605449 -1.521397
H -1.407106 0.630168 -1.536106
H -1.160956 1.717665 -0.636111
O 2.300628 1.509217 1.808360
H 2.369024 0.669857 1.273666
H 1.337900 1.610974 1.564257
O -2.545962 -0.182298 1.028238
H -2.088867 -0.622701 0.262754
H -1.797795 0.462455 1.152105

CO_3 – 8 water molecules

28

O -1.124810 1.175349 -0.015479
C -0.053062 0.502312 -0.259211
O 0.128676 -0.641438 0.330748
O 0.856762 0.959662 -1.044511
O -1.492115 -0.984906 2.387497
H -1.235650 -0.097925 2.712820
H -0.871952 -1.013203 1.608145
O -1.076496 -2.257518 -1.375918
H -1.903018 -1.808618 -1.089491
H -0.479996 -1.865975 -0.697014
O 1.445633 -1.230232 -2.516707
H 0.580352 -1.651141 -2.346230
H 1.327498 -0.363193 -2.045781
O 2.501100 1.091597 1.192271
H 2.721348 0.168765 0.932578
H 2.019597 1.344986 0.375673
O 2.594327 -1.527084 0.097112
H 2.511644 -1.511540 -0.878525
H 1.653595 -1.276118 0.308628
O -0.181658 1.585893 2.542435
H 0.714881 1.309402 2.257633
H -0.658001 1.587288 1.679838
O -3.045996 -0.724988 0.060560
H -2.723114 -0.962013 0.958018
H -2.457487 0.060711 -0.076519
O -0.696087 3.054861 -1.956908
H 0.100397 2.487391 -1.913786
H -1.156370 2.587677 -1.227877
28

O -1.160311 1.126977 -0.056969
C -0.094479 0.468264 -0.373757
O 0.158663 -0.647868 0.242546
O 0.721844 0.910126 -1.258391
O -1.323968 -1.189302 2.350226
H -1.128586 -0.294607 2.703093
H -0.743981 -1.123327 1.543159
O -0.996722 -2.428576 -1.324750

H -1.825027 -1.970183 -1.059296
H -0.395528 -1.966593 -0.695516
O 1.594060 -1.362995 -2.454812
H 0.756372 -1.832376 -2.283006
H 1.370645 -0.466392 -2.086291
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H -0.828167 1.434373 1.665764
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H -2.437996 -0.047411 -0.073745
O -0.810138 3.211841 -1.761863
H -0.035065 2.635563 -1.906929
H -1.201753 2.637887 -1.067002
28

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H -0.744625 -1.121346 1.543828
O -0.988723 -2.434959 -1.321577
H -1.821892 -1.983495 -1.059939
H -0.393853 -1.964220 -0.692658
O 1.619384 -1.361726 -2.433528
H 0.783063 -1.835728 -2.269404
H 1.386733 -0.465147 -2.070111
O 2.269312 1.474748 1.045874
H 2.598239 0.563354 0.865153
H 1.792365 1.624504 0.205063
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H 2.684503 -1.306994 -0.693148
H 1.730225 -1.059684 0.409901
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H 0.551468 1.380531 2.235072
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O -2.976178 -0.880624 0.074036
H -2.605416 -1.117001 0.953629
H -2.442179 -0.060394 -0.079000
O -0.829112 3.204528 -1.773619
H -0.049176 2.636653 -1.923329
H -1.210268 2.628744 -1.074223
28

O -1.346835 0.775631 0.617992
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O 0.817438 0.885415 1.174272
O -0.203480 -2.776290 1.195974
H -1.147107 -2.504512 1.220351
H 0.087114 -2.128869 0.510756
O -1.808782 -1.028885 -2.088967
H -1.803698 -0.072418 -2.294349
H -1.047955 -1.019321 -1.446313
O 1.853145 1.805638 -1.272047
H 2.266782 0.912023 -1.252767
H 1.498683 1.823181 -0.359494
O 2.223323 -1.279760 1.956365
H 1.449638 -1.873174 1.889138
H 1.804370 -0.406429 1.732413
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H 2.832474 -1.028253 0.083999
H 1.669482 -0.840493 -0.812945
O -0.557678 3.307691 1.308376
H 0.198539 2.712372 1.481114
H -1.180854 2.586647 1.080527
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H -2.641645 -1.523557 -0.416700
H -2.352923 -0.636508 0.733452
O -1.060112 1.764462 -1.970605
H -0.083453 1.717705 -1.899379
H -1.335803 1.516348 -1.060536
28

O -1.198695 1.098999 -0.091808
C -0.116684 0.461767 -0.396117
O 0.160256 -0.643026 0.229563
O 0.693807 0.915030 -1.281128
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H -0.709045 -1.133953 1.546889
O -0.966944 -2.469387 -1.318501
H -1.806064 -2.032017 -1.051951
H -0.377846 -1.982234 -0.697192

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H 0.845664 -1.837111 -2.254512
H 1.413346 -0.451966 -2.051193
O 2.237887 1.531002 1.009245
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H 1.757338 1.652659 0.165585
O 2.720338 -1.144344 0.308872
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H 1.736850 -1.027646 0.428404
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H 0.517314 1.412912 2.210724
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H -2.572790 -1.166784 0.971297
H -2.445131 -0.114707 -0.072013
O -0.878176 3.217831 -1.753298
H -0.097262 2.661840 -1.935391
H -1.239648 2.623117 -1.058803
28

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H -1.587827 -2.092194 -0.867459
O 2.545958 -1.062885 -2.266149
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H 1.734960 -0.427283 -2.174263
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H 1.533486 2.164421 0.284066
O 2.427277 -0.858174 0.430885
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H 1.458178 -1.069184 0.292540
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H -2.554442 0.130113 0.259503
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H 0.713969 2.129212 -1.573079
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28

O -1.215658 0.798745 -0.465764
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O -0.028876 -1.137518 -0.468457
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H -2.812530 -1.977574 -0.326669
H -1.435706 -2.211258 -0.877310
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H 2.199299 -1.801840 -2.094517
H 1.759243 -0.331849 -2.167915
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H 1.518251 -0.940106 0.318774
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H -2.544348 -0.059786 0.258333
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H -0.471441 2.523166 -0.645142
28

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H 2.722554 -1.427286 -2.521080

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H 1.446820 2.141754 0.246446
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CO_3 – 12 water molecules

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CO_3 – 20 water molecules

64

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