Formation of small clusters of NaCl dihydrate in the gas phase
Supporting Information

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1 First system, $NaCl(H_2O)$ CCSD(T)

(a) aug-cc-pVTZ

8			
Energy=-773.623146488698			
Cl	-1.418165	0.000302	-0.003335
Na	1.210321	-0.000139	-0.013770
O	0.636666	-2.239264	0.009700
H	0.565072	-3.196065	0.018944
H	-0.277901	-1.881619	0.010397
O	0.637077	2.239007	0.009103
H	0.565720	3.195714	0.025126
H	-0.277567	1.881523	0.010240
8			
Energy=-773.619815466247			
Cl	-0.060886	-1.752276	-0.006110
Na	1.550200	0.157826	0.002705
O	-1.872214	0.720798	-0.048760
H	-2.505670	0.662514	0.672339
H	-1.440901	-0.167085	-0.074177
O	0.388617	2.125842	0.020236
H	0.326863	3.022931	-0.314822
H	-0.531680	1.762256	0.016724

(b) 6-311++G(d,p)

8			
Energy=-773.589745318345			
Cl	-1.451655	0.000727	-0.012451
Na	1.108187	-0.000212	-0.025074
O	0.640283	-2.250129	0.011483
H	0.649353	-3.209219	0.023416
H	-0.295890	-1.973854	0.014021
O	0.640983	2.249757	0.009582
H	0.650182	3.208624	0.030862
H	-0.295225	1.973481	0.013510
8			
Energy=-773.585528530864			
Cl	-0.065469	-1.749245	-0.014324
Na	1.519527	0.127588	0.023671
O	-1.867580	0.748185	-0.026833
H	-2.538372	0.664341	0.655977
H	-1.462736	-0.145076	-0.078176
O	0.430276	2.129695	0.005099
H	0.403122	2.977921	-0.442924
H	-0.499544	1.807869	0.021882

2 Second system, $(NaCl)_2(H_2O)_4$ M06-2X/6-311++G(d,p)

16			
Energy=-1550.93564540			
Cl	-1.226208	-1.984793	0.001216
Na	-0.861859	0.000347	-1.627493
Cl	-1.222300	1.987039	0.000452
Na	-0.859462	0.001117	1.628223
O	1.839870	2.174576	-0.003657
H	2.300252	3.016974	-0.005101
H	0.877787	2.367287	-0.002323
O	1.835588	-2.178230	-0.000975
H	0.873229	-2.369434	0.000076
H	2.294680	-3.021315	-0.001272
O	1.382882	-0.002721	-1.748954
H	1.759617	-0.776318	-1.301397

H	1.761482	0.770840	-1.302932
O	1.385730	-0.000183	1.744515
H	1.762542	-0.774419	1.298140
H	1.763837	0.772688	1.296867

16

Energy=-1550.93037492

Cl	-1.535115	1.487420	-0.219818
Na	-1.256641	-1.044254	-0.051689
Cl	1.460462	-1.298311	-0.508033
Na	1.218872	1.263444	-0.071947
O	-0.179077	-1.588658	2.003871
H	-0.259447	-2.286407	2.658972
H	0.607095	-1.783120	1.455756
O	-1.042258	-2.899135	-1.325430
H	-1.362970	-3.391460	-2.083028
H	-0.086103	-2.772038	-1.439780
O	0.845029	3.005136	-1.451492
H	-0.119592	2.898309	-1.408332
H	1.050510	3.505510	-2.242310
O	0.573643	1.214932	2.142092
H	0.372930	0.303550	2.397839
H	-0.293063	1.596543	1.943474

16

Energy=-1550.93101241

Cl	1.187184	1.239185	1.001913
Na	-0.216195	0.182883	-0.981405
Cl	-0.452484	-2.258860	0.018395
Na	-0.595804	-0.476931	1.999573
O	-2.182876	0.618594	0.749225
H	-2.663969	0.167454	0.041635
H	-2.031032	1.515384	0.419810
O	-0.795536	2.497805	-0.853776
H	-0.848846	3.325128	-1.336646
H	-0.054089	2.565459	-0.218977
O	1.322205	-1.562360	2.661781
H	1.916694	-0.875960	2.331570
H	1.286954	-2.218960	1.953786
O	-2.295820	-0.703440	-1.754047
H	-1.983278	-1.549988	-1.375888
H	-2.830464	-0.902752	-2.525352

16

Energy=-1550.93116061

Cl	-1.058594	1.262484	1.802812
Na	-1.409101	-0.652042	0.058230
Cl	1.292146	-1.165420	-0.332184
Na	1.417674	0.646375	1.506818
O	-1.033351	0.497785	-1.871936
H	-0.157744	0.111063	-2.004758
H	-0.876966	1.439006	-1.698909
O	2.156320	2.022012	-0.132692
H	1.400824	2.545226	-0.447829
H	2.303298	1.345581	-0.804658
O	-0.427327	2.999853	-0.663115
H	-0.761070	2.637143	0.185259

H	-0.801074	3.879405	-0.760714
O	-1.208861	-2.895878	0.133374
H	-0.251242	-2.894998	-0.024955
H	-1.493399	-3.804268	0.241129

16

Energy=-1550.92860367

Cl	1.680421	-1.302702	-0.433489
Na	0.814638	0.862500	0.795215
Cl	-1.262744	1.485832	-0.706513
Na	-0.798185	-0.992463	-1.487609
O	-2.030424	-1.356167	0.445275
H	-2.341654	-0.440088	0.455925
H	-1.429498	-1.407947	1.201971
O	0.301100	-2.193317	-3.049679
H	1.138773	-2.198727	-2.561133
H	0.488504	-2.437780	-3.957159
O	0.564482	3.069242	1.192113
H	-0.184058	3.115857	0.574123
H	0.887564	3.961100	1.328603
O	0.271719	-1.005006	2.194417
H	0.433735	-1.297895	3.094694
H	0.849817	-1.522969	1.601333

16

Energy=-1550.92963721

Cl	-2.121750	-0.642034	0.508342
Na	-0.650109	1.355759	-0.345940
Cl	1.675531	0.515270	0.841644
Na	0.058511	-1.310126	1.693469
O	1.806383	-1.373538	-1.607448
H	2.627364	-1.528750	-2.081443
H	2.005519	-0.738830	-0.889011
O	-0.567256	0.070209	-2.237152
H	-1.248870	-0.526230	-1.899927
H	0.243911	-0.459329	-2.274153
O	0.342857	3.260986	0.348246
H	0.370021	4.194302	0.563707
H	1.123758	2.839679	0.736954
O	0.222900	-2.941786	0.127666
H	-0.675344	-2.832863	-0.208760
H	0.807111	-2.637957	-0.585736

16

Energy=-1550.92712677

Cl	-2.006438	0.601525	-0.406957
Na	-1.176468	-1.775076	0.218760
Cl	1.475122	-1.141383	-0.045012
Na	0.518880	1.377354	-0.109837
O	-0.544406	3.252367	-0.794060
H	-0.654205	4.174283	-1.029642
H	-1.412817	2.822128	-0.841608
O	-0.120691	-3.194344	1.620044
H	-0.011155	-4.088103	1.948249
H	0.757621	-2.858826	1.377417
O	2.653450	1.601478	0.599460
H	3.458547	2.074968	0.811997

H	2.858843	0.654486	0.561339
O	-0.951839	-2.012386	-2.069864
H	-1.340620	-1.142657	-2.234290
H	0.002316	-1.858479	-2.053336

16

Energy=-1550.92625616

Cl	-1.891851	0.459059	0.420864
Na	0.402351	1.719269	-0.100724
Cl	1.895023	-0.468301	-0.422959
Na	-0.400080	-1.725905	0.084991
O	-2.413100	-2.308486	-0.786986
H	-2.942058	-2.725411	-1.468306
H	-2.785485	-1.428214	-0.617060
O	-1.183534	3.197653	-0.752863
H	-1.910606	2.613089	-0.485571
H	-1.540570	4.077306	-0.880569
O	2.402600	2.292636	0.807176
H	2.774938	1.411625	0.640838
H	2.912901	2.700035	1.508318
O	1.180375	-3.229860	0.691539
H	1.910704	-2.646112	0.431966
H	1.530718	-4.114484	0.801891

16

Energy=-1550.92852657

Cl	0.147375	2.046401	0.860892
Na	-1.234466	-0.240486	0.761146
Cl	0.767289	-1.974132	0.809958
Na	1.502119	0.126754	-0.535847
O	-2.507208	1.412224	-0.364233
H	-3.361605	1.845491	-0.421420
H	-1.860657	2.063101	-0.026580
O	2.789361	1.980142	-0.734303
H	2.183442	2.500620	-0.181580
H	3.657977	2.379964	-0.667185
O	-1.924398	-2.165191	-0.473695
H	-1.092070	-2.555290	-0.132854
H	-2.571325	-2.869433	-0.553610
O	-0.480246	-0.085305	-1.718990
H	-0.977977	-0.914534	-1.752627
H	-1.146793	0.614174	-1.741488

16

Energy=-1550.92572876

Cl	1.621068	-0.722034	-0.346457
Na	0.345309	1.609040	0.108419
Cl	-2.047887	0.618725	0.609025
Na	-1.013548	-1.653020	0.083038
O	2.531448	2.067936	0.529011
H	3.290964	2.651430	0.554745
H	2.841678	1.180985	0.288940
O	0.267647	-2.676746	1.666394
H	0.286313	-2.673272	2.625318
H	1.074003	-2.227704	1.365520
O	-1.067106	3.128773	-0.831075
H	-1.366814	4.010855	-1.054299

H	-1.839098	2.613709	-0.542583
O	-0.412562	-2.389213	-1.983930
H	0.463080	-1.971935	-1.947042
H	-0.690588	-2.388990	-2.901344

16

Energy=-1550.92816927

Cl	0.934392	-1.774198	-0.677628
Na	0.739671	0.869102	-0.543725
Cl	-0.488693	3.035380	0.148234
Na	-1.359204	-1.174802	0.573514
O	2.371392	0.253586	1.062113
H	3.269017	0.468436	1.325812
H	2.365176	-0.656780	0.717596
O	-1.817967	0.542858	-0.835467
H	-2.279392	0.568885	-1.677142
H	-1.690320	1.479069	-0.550840
O	-1.571823	-3.367908	0.132930
H	-0.705101	-3.418566	-0.301719
H	-1.953232	-4.246851	0.140442
O	-0.360977	0.422442	1.810940
H	0.575908	0.377072	2.045911
H	-0.543578	1.370448	1.667939

16

Energy=-1550.92631998

Cl	-1.792773	1.616268	-0.479236
Na	0.835155	1.717075	-0.193150
Cl	1.166744	-0.960513	-0.026330
Na	-1.434461	-0.894595	-0.313374
O	-1.860331	-3.077971	-0.231277
H	-1.036050	-3.575154	-0.041642
H	-2.506650	-3.710596	-0.546896
O	2.672304	1.315190	-1.455197
H	3.161787	1.493301	-2.259357
H	2.634124	0.353508	-1.338448
O	0.626191	-4.032910	0.237376
H	0.948423	-4.382792	1.070835
H	1.049475	-3.160936	0.136112
O	0.108252	3.348577	1.194416
H	0.132425	3.849775	2.010267
H	-0.820540	3.149991	0.991624

16

Energy=-1550.92687214

Cl	-1.620125	-0.669138	-0.615420
Na	1.122079	-0.731094	-0.745361
Cl	1.434195	1.536192	0.537292
Na	-1.154736	1.615248	0.408750
O	0.630248	-2.808812	-1.607211
H	-0.250793	-2.651058	-1.966136
H	0.454938	-3.299608	-0.791205
O	-0.692308	3.646182	1.227415
H	-0.826272	4.551620	1.510440
H	0.263774	3.475009	1.201481
O	1.633861	-1.687824	1.241472
H	1.668484	-0.909213	1.808210

H	0.898508	-2.241761	1.540911
O	-0.682688	-3.186614	0.952979
H	-1.209663	-2.447737	0.590107
H	-1.298714	-3.795901	1.365760

16

Energy=-1550.92626065

Cl	-1.490760	-1.099270	0.400672
Na	-0.956992	1.398874	0.076258
Cl	1.780494	1.095254	-0.377974
Na	1.182200	-1.379463	-0.072217
O	0.109351	-2.722888	-1.662328
H	-0.731121	-2.342888	-1.349453
H	0.049632	-2.789726	-2.617749
O	0.059559	2.649308	1.679484
H	0.108674	2.752998	2.631394
H	0.943029	2.388692	1.371457
O	-0.543577	2.428222	-1.906653
H	-0.639104	3.236482	-2.413001
H	0.405711	2.229507	-1.851115
O	0.711256	-3.302129	1.135924
H	0.522253	-3.905515	0.408874
H	-0.158300	-2.964528	1.395996

16

Energy=-1550.92484554

Cl	-1.553109	0.838383	0.545816
Na	-1.463170	-1.648300	0.091347
Cl	1.077156	-1.958644	-0.422757
Na	1.047295	0.726931	0.029359
O	2.806093	-0.059269	1.238192
H	2.666531	-0.984920	0.984593
H	3.538504	-0.023986	1.853978
O	-1.365515	3.652290	-0.826233
H	-1.651883	2.882612	-0.301389
H	-1.954044	3.675556	-1.583856
O	-1.366612	-3.819999	-0.462348
H	-0.409811	-3.776637	-0.624431
H	-1.663362	-4.709520	-0.656352
O	1.198896	2.756955	-0.917215
H	1.875324	3.416692	-1.076801
H	0.332454	3.210869	-0.971786

16

Energy=-1550.92518991

Cl	-1.694128	0.653851	-1.722959
Na	-0.538387	-1.404945	-0.460804
Cl	1.648250	0.343955	0.464067
Na	0.098144	2.100366	-0.717959
O	1.518231	-2.214180	-1.251396
H	1.843733	-2.419995	-2.130097
H	1.987570	-1.417543	-0.950830
O	0.408391	-2.429161	1.415644
H	0.927258	-1.652995	1.670722
H	1.035735	-2.981844	0.936724
O	1.685637	3.404243	0.183944
H	2.105356	4.216178	0.470951

H	2.163219	2.659730	0.582957
O	-2.460518	-2.295144	-1.310733
H	-3.249503	-2.801838	-1.113409
H	-2.743337	-1.448145	-1.688864

16

Energy=-1550.92597281

Cl	-1.353077	1.804400	-0.643585
Na	1.178461	1.313146	0.167690
Cl	2.068817	-1.012333	-0.353214
Na	-0.057544	-1.775212	0.864518
O	-0.489871	0.282055	1.777897
H	-1.052903	0.798260	1.154013
H	-0.688594	0.604600	2.660179
O	0.862628	3.503387	0.623877
H	1.180473	4.406983	0.654067
H	-0.018100	3.510326	0.213669
O	-1.623092	-3.318215	0.368470
H	-2.015938	-4.190905	0.339719
H	-1.788985	-2.880512	-0.481266
O	-1.033040	-1.272259	-1.268692
H	-0.144868	-1.219609	-1.650592
H	-1.367831	-0.358161	-1.294051

16

Energy=-1550.92550288

Cl	1.865414	0.305907	0.845309
Na	0.866090	-1.958107	0.284694
Cl	-1.461136	-1.100555	-0.523528
Na	-0.226352	1.232316	-0.784097
O	-1.125796	1.158869	1.768545
H	-0.193512	0.964303	1.945966
H	-1.494219	0.331079	1.424896
O	-1.409488	3.039929	-0.138934
H	-2.046489	3.741754	-0.271969
H	-1.550905	2.658104	0.744687
O	1.706513	1.613103	-1.935224
H	2.266786	1.320216	-1.198503
H	2.185113	2.296297	-2.407307
O	-0.118547	-3.864916	-0.340168
H	-0.934053	-3.413096	-0.612103
H	-0.230199	-4.803128	-0.498572

16

Energy=-1550.92633600

Cl	-1.850158	0.626203	-0.538340
Na	-0.090383	-0.937032	0.795739
Cl	1.998813	-0.104090	-0.835631
Na	0.370148	1.787697	-1.201941
O	0.903897	0.734789	2.044611
H	1.731215	0.697932	1.544924
H	0.540722	1.610526	1.856757
O	-0.393137	2.966476	0.671195
H	-0.634187	3.839973	0.989238
H	-1.214797	2.446411	0.564757
O	-0.400986	-2.166560	-1.409478
H	-1.079198	-1.511164	-1.622531

H	0.441892	-1.754101	-1.653593
O	-0.493883	-3.132231	1.108797
H	-0.579326	-3.964963	1.572706
H	-0.547522	-3.298399	0.155072

16

Energy=-1550.92620243

Cl	1.271902	-2.093563	1.020625
Na	1.106652	0.328622	-0.061365
Cl	-1.416556	0.826715	0.538756
Na	-1.262324	-1.750823	0.942114
O	1.074850	-1.312003	-1.858942
H	1.348077	-1.923467	-1.144574
H	1.612448	-1.501234	-2.632162
O	1.811538	2.432284	-0.304680
H	1.085125	3.060511	-0.103240
H	2.530331	2.940951	-0.681593
O	-0.446581	3.797927	0.296430
H	-0.997258	2.997394	0.364311
H	-0.594772	4.282464	1.111745
O	-1.708091	-1.752506	-1.302440
H	-0.847186	-1.709278	-1.747017
H	-2.024110	-0.838948	-1.319841

16

Energy=-1550.92759180

Cl	1.335726	-1.265307	-0.631582
Na	1.934448	1.059521	0.183577
Cl	0.045624	2.539857	-0.773584
Na	-1.045800	0.168028	-0.836032
O	-1.318287	-0.071319	1.414330
H	-0.669073	0.445967	1.908049
H	-1.172291	-0.999063	1.650649
O	-0.675035	-2.780503	1.128080
H	0.146139	-2.490504	0.679992
H	-0.476833	-3.596102	1.593561
O	-1.832656	-1.932985	-1.334679
H	-1.094912	-2.303354	-1.832097
H	-1.777330	-2.389530	-0.481219
O	0.765690	1.870902	2.058083
H	0.862442	2.381930	2.865300
H	0.306280	2.433197	1.399911

16

Energy=-1550.92460333

Cl	2.076046	-0.544171	-0.086770
Na	-0.203505	-1.472637	-0.887576
Cl	-1.643027	0.578409	-0.073547
Na	0.926874	1.731946	0.075121
O	-0.279373	-1.848088	1.661587
H	-0.871947	-1.084178	1.638525
H	0.614071	-1.479154	1.567749
O	-0.147470	2.795583	-1.614071
H	-0.330866	3.596109	-2.107705
H	-0.987902	2.329872	-1.479590
O	-0.171564	2.448825	1.927338
H	-0.156936	2.566734	2.878439

H	-0.997009	1.992993	1.699894
O	-0.794560	-3.574551	-0.366448
H	-0.694494	-3.375068	0.579050
H	-0.787029	-4.525395	-0.478133

16

Energy=-1550.92524057

Cl	-2.273725	-1.110166	-0.514177
Na	-1.153642	0.879758	0.652091
Cl	1.439282	-0.101530	0.532440
Na	0.024308	-2.111363	-0.462505
O	1.475456	2.778236	-0.666883
H	2.275270	3.195365	-0.994835
H	1.711379	1.865373	-0.413874
O	-0.013597	2.509145	1.815683
H	0.357114	3.048699	1.102983
H	0.740901	1.988898	2.117477
O	2.071015	-3.011700	-0.272942
H	2.479373	-2.213323	0.095491
H	2.749229	-3.683451	-0.360014
O	-1.156948	2.134736	-1.221856
H	-0.272638	2.473031	-1.425056
H	-1.420962	1.546032	-1.934986

16

Energy=-1550.92620919

Cl	1.439514	-1.151806	-0.672330
Na	1.133505	1.022559	0.715735
Cl	-1.151893	1.970203	-0.623219
Na	-0.975660	-0.488236	-1.265044
O	-0.627536	0.316557	2.032226
H	-1.230203	0.979133	1.665505
H	-0.974837	-0.518678	1.687277
O	-1.795206	-1.839411	0.393576
H	-2.681004	-2.135389	0.616893
H	-1.191229	-2.608370	0.526078
O	0.132883	-3.675721	0.529654
H	0.789678	-3.059335	0.151562
H	0.549547	-4.087470	1.289681
O	1.537648	3.190482	0.259717
H	2.146627	3.851403	-0.072603
H	0.695694	3.301177	-0.212475

16

Energy=-1550.92559352

Cl	1.699697	1.037485	-0.081713
Na	1.006688	-1.432481	0.049851
Cl	-1.699697	-1.037485	-0.081713
Na	-1.006688	1.432481	0.049851
O	-0.249826	2.809984	-1.670118
H	-0.382662	2.964507	-2.607681
H	0.625823	2.396657	-1.567655
O	0.206462	-3.249045	1.232925
H	-0.686120	-2.877638	1.286400
H	0.146403	-3.913193	0.537935
O	-0.206462	3.249045	1.232925
H	0.686120	2.877638	1.286400

H	-0.146403	3.913193	0.537935
O	0.249826	-2.809984	-1.670118
H	0.382662	-2.964507	-2.607681
H	-0.625823	-2.396657	-1.567655

16

Energy=-1550.92342682

Cl	1.400804	-0.265553	-0.379569
Na	-1.241524	-0.674022	-0.120429
Cl	-1.813641	1.858851	0.564411
Na	0.651068	2.194965	0.175799
O	1.602432	-3.287097	0.453469
H	2.126916	-3.375064	1.252584
H	1.786098	-2.391080	0.118492
O	2.779876	2.479762	-0.460418
H	2.913739	1.536819	-0.648213
H	3.562418	2.954512	-0.743788
O	-2.929396	-0.072535	-1.524051
H	-2.992859	0.818619	-1.143908
H	-3.564677	-0.140329	-2.237834
O	-1.080424	-2.843671	0.419092
H	-0.155663	-3.156020	0.492681
H	-1.631119	-3.619375	0.306121

16

Energy=-1550.92698081

Cl	-0.883735	-2.221109	0.138064
Na	-0.714612	-0.178792	1.641488
Cl	-1.498422	1.679454	0.025536
Na	-0.990072	-0.312318	-1.601652
O	1.171617	0.147172	-1.960451
H	1.702204	-0.517209	-1.478283
H	1.464986	0.998090	-1.609293
O	1.431582	2.403030	-0.166363
H	1.747290	3.308832	-0.213203
H	0.448408	2.432362	-0.167519
O	1.490941	0.475121	1.779698
H	1.608736	1.224439	1.157898
H	2.088289	0.633104	2.514948
O	2.259155	-1.652994	-0.159750
H	1.478807	-2.225967	-0.108373
H	2.168831	-1.086808	0.617233

16

Energy=-1550.92456219

Cl	-1.416810	-1.329536	-0.748689
Na	-1.186832	1.221842	-0.724541
Cl	1.418412	1.332197	-0.743663
Na	1.188238	-1.218911	-0.722941
O	-0.837388	-4.402084	-0.621557
H	-1.269975	-3.530097	-0.574453
H	-1.262675	-4.862282	-1.348447
O	1.666806	-3.384530	-0.628931
H	0.832191	-3.901593	-0.642470
H	2.359126	-3.974230	-0.327693
O	-1.665463	3.387343	-0.627752
H	-0.830734	3.904304	-0.638874

H	-2.358165	3.976485	-0.326234
O	0.838643	4.404618	-0.612955
H	1.266096	4.866605	-1.337451
H	1.271289	3.532633	-0.566398

16

Energy=-1550.92501470

Cl	-0.615690	2.465201	0.560906
Na	-1.556827	0.694630	-1.011994
Cl	0.017862	-2.026940	1.317935
Na	0.918227	0.335776	0.949119
O	1.329001	-2.525177	-1.434794
H	0.982636	-2.643687	-0.528268
H	1.116814	-3.323928	-1.920973
O	2.249872	1.902513	-0.234876
H	3.059237	2.416581	-0.201862
H	1.501046	2.515250	-0.097255
O	0.542928	0.038574	-1.471205
H	0.837208	-0.878504	-1.660071
H	1.296351	0.626298	-1.609475
O	-2.411787	-1.247588	-0.379492
H	-1.723072	-1.638760	0.203499
H	-3.247032	-1.621046	-0.093470

16

Energy=-1550.92366237

Cl	-2.622111	-0.747829	-0.259495
Na	-0.523928	-2.017745	0.384746
Cl	1.149674	0.140809	0.339319
Na	-1.174067	1.320825	-0.122891
O	-0.509616	3.437616	0.046243
H	-0.900645	4.290988	0.237882
H	0.437772	3.491703	0.294462
O	1.039906	-3.477037	1.176815
H	1.653290	-3.319369	1.897706
H	1.554962	-3.417524	0.360384
O	2.069461	3.105080	0.788308
H	2.856809	3.328369	0.287720
H	2.016010	2.132494	0.780036
O	1.132319	-2.418734	-1.348983
H	1.416898	-1.499984	-1.198768
H	1.045650	-2.541456	-2.296678

16

Energy=-1550.92462068

Cl	1.403609	0.798341	-0.572401
Na	-1.198513	0.359685	0.270113
Cl	-1.487631	-1.992092	-0.859494
Na	1.067240	-1.672301	-1.039661
O	-1.759243	2.519317	0.419849
H	-2.224317	3.042972	1.074168
H	-1.065777	3.096728	0.037953
O	0.727245	-2.971577	0.894087
H	-0.196173	-3.029370	0.571651
H	0.949162	-3.805239	1.315888
O	0.394439	3.771164	-0.662869
H	0.430399	4.145300	-1.545981

H 0.947843 2.970906 -0.691613
O 0.068019 -0.369308 2.080294
H 0.847823 0.138658 1.819671
H 0.335285 -1.291773 1.967739
16
Energy=-1550.92396008
Cl 0.985883 -0.005240 -0.005918
Na -1.067986 -1.695235 -0.005960
Cl -2.934018 0.009875 -0.008886
Na -1.054911 1.700740 -0.009163
O 0.064802 3.620499 -0.028686
H 1.028601 3.464491 -0.114890
H -0.056398 4.540333 0.209800
O 0.036970 -3.623392 0.017775
H -0.090959 -4.542951 -0.218177
H 1.001779 -3.474890 0.106004
O 2.598746 2.695046 -0.234768
H 2.336869 1.765506 -0.114790
H 3.131141 2.714129 -1.033098
O 2.577467 -2.716617 0.228137
H 2.322693 -1.785079 0.108219
H 3.108440 -2.740666 1.027275
16
Energy=-1550.92574236
Cl -0.671081 2.371197 -0.963120
Na -1.028523 -0.144759 -0.703363
Cl 1.570164 -0.879117 -0.293212
Na 1.524535 1.651528 0.203726
O -0.327207 -2.985465 1.162867
H -0.616116 -3.195482 0.264911
H 0.561293 -2.619260 1.031042
O -0.728891 -2.277594 -1.674350
H 0.229937 -2.106269 -1.634512
H -0.915204 -2.687465 -2.522883
O 0.146218 1.658109 2.032321
H -0.275963 0.787556 2.088109
H -0.510681 2.196460 1.568166
O -1.554265 -0.640030 1.490287
H -2.363606 -0.634282 2.007114
H -1.172787 -1.548565 1.550614
16
Energy=-1550.92476385
Cl 1.997181 0.202449 1.180670
Na 1.186002 -2.017282 0.138317
Cl -1.333402 -2.007365 -0.041752
Na -0.703043 0.394219 -0.852337
O 0.617389 2.268679 -0.747153
H -0.026411 2.935759 -0.484817
H 1.187306 2.103249 0.019567
O -1.129835 0.625734 1.734983
H -0.179445 0.611840 1.933445
H -1.376995 -0.306326 1.624917
O 1.413450 -0.535891 -1.695031
H 1.703346 -0.459999 -2.607717

H	1.948297	0.080111	-1.164522
O	-2.173082	2.141114	-0.221621
H	-2.030457	1.790323	0.678182
H	-3.094163	2.400235	-0.285639

16

Energy=-1550.92338634

Cl	-1.386134	-1.186731	0.725188
Na	-1.451005	1.161715	-0.243582
Cl	-0.119648	3.347614	-0.237549
Na	1.159605	-0.637957	0.398998
O	0.636599	0.711463	-1.427880
H	0.841095	0.468305	-2.334476
H	0.726011	1.684290	-1.349457
O	1.876023	-2.581331	-0.430159
H	2.647440	-3.021925	-0.788234
H	1.108297	-3.177282	-0.565301
O	-0.509584	-3.825552	-0.692366
H	-0.825085	-4.607904	-0.234471
H	-1.010660	-3.078185	-0.314581
O	1.455406	1.313069	1.470495
H	1.503626	1.541007	2.401697
H	1.084555	2.102641	1.022930

16

Energy=-1550.92404745

Cl	-1.495826	0.983122	-0.328234
Na	0.737625	2.344429	-0.200331
Cl	2.282858	0.339718	-0.270553
Na	0.135768	-0.974178	-1.057450
O	-0.598156	-3.045127	-1.509377
H	-1.382668	-3.346254	-1.970647
H	-0.544288	-3.562968	-0.681094
O	-0.372603	-3.944142	1.031893
H	0.221801	-4.556708	1.468330
H	-0.186730	-3.059223	1.392466
O	0.081084	-1.258420	1.373055
H	0.923153	-0.776296	1.331471
H	-0.609463	-0.578579	1.372332
O	-0.794974	3.975055	-0.144090
H	-1.154142	4.862331	-0.104884
H	-1.536407	3.350695	-0.199933

16

Energy=-1550.92380339

Cl	2.261010	0.800544	0.294425
Na	0.817803	-1.220234	-0.307712
Cl	-1.167497	0.139738	-1.579057
Na	0.370890	2.096983	-0.844351
O	-0.324011	2.472526	1.284145
H	0.465434	2.059885	1.660991
H	-1.064462	1.898853	1.534174
O	0.964159	-3.440973	0.118661
H	1.521643	-4.199173	0.297885
H	0.170831	-3.509314	0.666108
O	-1.231510	-2.040164	0.785478
H	-1.590935	-1.348077	1.360401

H	-1.700710	-1.892987	-0.047133
O	-2.395947	0.525268	1.237431
H	-2.231249	0.507880	0.271736
H	-3.327867	0.725891	1.357367

16

Energy=-1550.92303305

Cl	-1.859734	-0.644934	0.568288
Na	0.727044	-0.978689	0.842263
Cl	0.499853	2.750162	-0.519742
Na	-1.756179	1.782883	-0.011340
O	-0.453196	-2.375949	-1.752239
H	0.030698	-1.558151	-1.939826
H	-1.228980	-2.068788	-1.260079
O	1.620154	0.896967	1.716916
H	1.986161	1.281726	2.514653
H	1.402615	1.639391	1.119814
O	1.204865	-3.099639	0.246519
H	1.246368	-3.995411	0.582841
H	0.619079	-3.106953	-0.540873
O	1.284428	-0.154204	-1.280852
H	1.062920	0.799020	-1.235216
H	2.184464	-0.195293	-1.615951

16

Energy=-1550.92302665

Cl	-0.499827	-2.748210	0.516244
Na	1.756769	-1.779380	0.016630
Cl	1.858159	0.647215	-0.564213
Na	-0.725956	0.980194	-0.844289
O	-1.613464	-0.896185	-1.722991
H	-1.397705	-1.638454	-1.125207
H	-1.974250	-1.281315	-2.523054
O	-1.293926	0.153855	1.274481
H	-2.193781	0.197864	1.609602
H	-1.075445	-0.800352	1.227768
O	-1.197817	3.101957	-0.245404
H	-1.225846	3.996551	-0.586663
H	-0.615398	3.105622	0.544483
O	0.449522	2.368535	1.758953
H	-0.038198	1.552118	1.943028
H	1.224315	2.059423	1.266113

16

Energy=-1550.92303706

Cl	0.509765	-2.750146	0.514838
Na	0.713454	0.976371	-0.844964
Cl	-1.866376	0.634293	-0.550200
Na	-1.755266	-1.792628	0.030421
O	-0.445491	2.376982	1.753112
H	-1.225086	2.067979	1.268464
H	0.040217	1.560045	1.939467
O	1.613117	-0.890911	-1.723323
H	1.980841	-1.271998	-2.522034
H	1.400304	-1.635292	-1.127288
O	1.291796	0.155759	1.275724
H	1.076085	-0.798921	1.230197

H	2.194482	0.202248	1.602485
O	1.191976	3.097721	-0.261811
H	1.249450	3.995149	-0.591093
H	0.614591	3.108576	0.531458

16

Energy=-1550.92368107

Cl	1.061692	-2.526380	0.426967
Na	1.189290	-0.001463	0.211084
Cl	0.427428	2.427784	0.730183
Na	-1.216506	-2.097203	-0.519209
O	-2.389096	1.622172	0.081466
H	-3.047331	2.315773	-0.003237
H	-1.553837	2.046584	0.398793
O	1.580521	1.246297	-1.800161
H	1.354035	2.018128	-1.244857
H	2.298640	1.499266	-2.384227
O	-2.458339	-0.977816	0.978629
H	-2.290346	-1.069028	1.919395
H	-2.566174	-0.023819	0.808782
O	-0.837912	-0.097698	-1.469969
H	-0.142475	0.326272	-1.993300
H	-1.432522	0.613523	-1.176531

16

Energy=-1550.92143705

Cl	-0.138671	-3.384953	-0.470396
Na	-0.729736	-1.441689	1.081190
Cl	-1.120139	2.573158	-0.479670
Na	0.964206	0.849637	-0.226140
O	1.692540	-1.207464	0.430458
H	2.501576	-1.492963	0.861930
H	1.332357	-2.007503	-0.032346
O	-0.807638	-0.430800	-0.990769
H	-0.865029	-1.249536	-1.506605
H	-1.369865	0.262895	-1.364873
O	1.916371	2.890537	-0.253507
H	1.046709	3.310400	-0.378858
H	2.589563	3.529476	-0.492092
O	-0.657434	0.685669	1.797686
H	-0.550109	1.132826	2.640721
H	-1.026464	1.365713	1.177912

16

Energy=-1550.92170921

Cl	-0.970801	2.351876	0.802204
Na	-1.890235	0.134611	-0.032335
Cl	-1.475322	-2.337817	0.289685
Na	0.886175	-1.471819	-0.067249
O	-0.138195	-0.059402	-1.695457
H	0.276778	0.806057	-1.882020
H	-0.405313	-0.444867	-2.534525
O	1.677923	0.642345	0.681063
H	1.856064	1.227886	-0.070865
H	0.974406	1.124518	1.151919
O	1.007602	2.388222	-1.465012
H	1.270511	3.174770	-1.948343

H	0.335315	2.656909	-0.793946
O	3.010198	-1.683633	0.682629
H	3.652428	-2.216897	1.153273
H	3.022886	-0.791228	1.057688

16

Energy=-1550.92081212

Cl	1.452788	1.627714	-0.382416
Na	-1.078316	1.308565	0.524816
Cl	0.754510	-2.680579	0.389944
Na	2.236038	-0.728957	-0.043883
O	-1.771718	-2.068548	-1.280559
H	-0.940371	-2.421753	-0.899236
H	-2.177207	-2.784430	-1.775297
O	-1.482448	0.691270	-1.623151
H	-1.591782	-0.270662	-1.712495
H	-0.623884	0.903438	-2.006661
O	-1.657932	-0.749740	1.257144
H	-0.910616	-1.349963	1.412164
H	-2.133424	-1.197350	0.542785
O	-0.453297	3.319251	1.353021
H	0.426632	3.308767	0.946236
H	-0.622591	4.208675	1.667234

16

Energy=-1550.92056839

Cl	-2.075077	1.007553	-0.437578
Na	0.572656	1.276013	-0.570164
Cl	0.183119	-2.676180	0.416459
Na	-1.958755	-1.441983	0.073671
O	1.201943	-0.656941	-1.723825
H	1.006055	-1.394731	-1.108581
H	1.017189	-0.999243	-2.601738
O	2.906140	1.401842	-0.667969
H	2.916217	1.034972	0.226134
H	2.929096	0.617100	-1.229490
O	-0.117729	2.545262	1.348366
H	-1.036604	2.352024	1.097587
H	-0.096464	3.445501	1.680318
O	1.331807	0.112736	1.301839
H	1.084558	-0.826722	1.351949
H	0.842330	0.588991	1.981455

16

Energy=-1550.91961469

Cl	-1.060675	-0.333568	0.002830
Na	0.030072	-2.670046	0.662646
Cl	2.355664	-1.880263	1.174111
Na	1.430776	0.400258	0.512102
O	-0.234510	3.987210	-0.789147
H	-0.242848	4.259130	-1.708880
H	-1.080123	3.515712	-0.638491
O	-2.450817	2.467168	-0.407925
H	-3.067252	2.582481	0.318153
H	-2.125055	1.552493	-0.333448
O	1.783151	2.577870	0.288109
H	2.440102	3.177110	0.645308

H 1.082697 3.136943 -0.116339
O -2.024222 -3.273743 0.010049
H -2.306137 -2.374292 -0.215925
H -2.728128 -3.876711 -0.232288
16
Energy=-1550.92165446
Cl 0.004117 2.306667 -1.023994
Na -0.693023 1.491111 1.334065
Cl -1.808889 -0.706829 0.711336
Na -0.774088 -0.079119 -1.624358
O 0.183893 -3.082615 0.628819
H -0.564854 -2.476052 0.786438
H -0.021211 -3.900949 1.086522
O 0.727723 -1.729366 -1.833944
H 1.466659 -1.393339 -1.294543
H 0.470137 -2.519468 -1.338726
O 1.617378 1.604951 1.430821
H 2.375998 1.993728 1.873629
H 1.567721 1.989559 0.532823
O 2.203529 -1.088198 0.418240
H 1.995512 -0.274540 0.894199
H 1.665122 -1.788934 0.813502
16
Energy=-1550.92035234
Cl -1.957747 1.900034 -0.382895
Na 0.417880 2.336731 0.477346
Cl 2.291462 0.769566 -0.142366
Na 0.675796 -1.012867 0.800325
O -1.173586 -3.271598 -1.413960
H -2.070769 -3.466148 -1.690308
H -1.012086 -2.330083 -1.606811
O 0.164761 -3.187179 0.924453
H 0.604115 -3.994619 1.195046
H -0.385481 -3.411392 0.145466
O -0.619080 0.571252 1.918912
H -1.360007 0.861490 1.337353
H -0.963445 0.529615 2.814526
O -0.407354 -0.647954 -1.273284
H 0.392146 -0.246031 -1.642874
H -1.034307 0.097912 -1.167985
16
Energy=-1550.92053212
Cl 2.049070 -1.555823 0.000341
Na -0.110964 -2.776957 0.000244
Cl -2.216687 -1.401275 -0.000137
Na 1.090818 0.824054 -0.000291
O -0.699026 0.821514 -1.525150
H -1.299722 0.114766 -1.206875
H -0.604007 0.681422 -2.470779
O 1.537545 3.013415 0.000267
H 2.171460 3.730574 0.002922
H 0.634627 3.391556 0.000498
O -0.698682 0.820947 1.525037
H -0.603087 0.680216 2.470516

H	-1.299479	0.114323	1.206637
O	-1.140594	3.201474	0.000745
H	-1.269685	2.610232	-0.754263
H	-1.269307	2.609685	0.755395

16

Energy=-1550.91971511

Cl	0.818455	2.219644	1.119561
Na	-1.281026	1.352567	-0.199316
Cl	1.276802	-2.591029	-0.115898
Na	1.548959	-0.175384	0.631745
O	-1.770131	-2.712305	0.425773
H	-0.800069	-2.798554	0.321058
H	-2.158947	-3.442157	-0.059955
O	-2.573944	-0.176783	0.757883
H	-2.342970	-1.117036	0.583489
H	-2.978421	-0.169011	1.627410
O	0.088330	-0.074931	-1.324414
H	0.343210	0.376632	-2.135627
H	0.311178	-1.022009	-1.393081
O	-0.138926	2.667295	-1.762579
H	-0.197604	3.470896	-2.283423
H	0.474087	2.848023	-1.025173

16

Energy=-1550.92006711

Cl	-1.363069	2.086509	0.019222
Na	-2.375329	-0.029461	0.884849
Cl	-1.219183	-2.232437	0.715169
Na	1.179008	-1.390089	0.181076
O	2.320486	0.119619	1.379592
H	2.605474	0.196419	2.291514
H	2.196668	1.029296	1.046360
O	1.685694	2.509513	0.192791
H	2.010284	3.411124	0.247620
H	0.707206	2.558219	0.232307
O	0.880907	-2.573123	-1.789722
H	0.710762	-1.754187	-2.271758
H	0.010051	-2.907095	-1.539313
O	0.823890	0.280795	-1.407469
H	1.474878	0.993429	-1.385390
H	-0.005963	0.743324	-1.190784

16

Energy=-1550.91998864

Cl	-0.364528	2.590390	-0.433657
Na	1.895380	1.530640	-0.531969
Cl	2.322321	-0.891584	-0.107382
Na	-0.101318	-1.819824	-0.212735
O	-1.763170	1.092731	1.883219
H	-2.301693	1.583666	2.508137
H	-1.318526	1.751997	1.310120
O	-0.168681	-1.219528	1.985143
H	-0.673534	-0.409871	2.164589
H	0.762728	-0.974859	2.044565
O	-1.665400	-2.718185	-1.576763
H	-2.173324	-1.893870	-1.604080

H	-2.036372	-3.328658	-2.214219
O	-1.807723	-0.221643	-0.628825
H	-2.166154	0.003433	0.243453
H	-1.449417	0.631834	-0.931625

16

Energy=-1550.92020129

Cl	-1.633331	0.113878	0.094684
Na	-1.485372	-2.396493	-0.262002
Cl	0.945519	-2.850794	-0.131998
Na	1.106652	-0.305293	0.283849
O	-0.313183	2.570583	-1.500286
H	-0.942879	1.844021	-1.377200
H	-0.446962	3.106244	-0.706479
O	1.953634	1.097282	-1.341447
H	2.401801	0.889522	-2.163775
H	1.212819	1.703651	-1.556768
O	1.546433	1.630762	1.409621
H	2.086650	2.057501	0.735910
H	0.782363	2.212325	1.547399
O	-0.958945	2.911534	1.292461
H	-1.415376	2.064899	1.132772
H	-1.505274	3.415439	1.900460

16

Energy=-1550.92020126

Cl	-0.948170	-2.850989	-0.127547
Na	-1.107411	-0.304868	0.286975
Cl	1.632531	0.112122	0.097451
Na	1.483057	-2.398654	-0.256106
O	-1.546908	1.635851	1.405206
H	-0.782310	2.217111	1.541400
H	-2.086187	2.060700	0.729543
O	-1.952651	1.091727	-1.344190
H	-2.399180	0.880314	-2.166497
H	-1.212137	1.698009	-1.560658
O	0.959101	2.914730	1.284273
H	1.415335	2.067368	1.127857
H	1.504962	3.420234	1.891327
O	0.314742	2.564077	-1.507152
H	0.448455	3.103408	-0.715807
H	0.943431	1.837346	-1.380180

16

Energy=-1550.91967787

Cl	1.592332	1.685353	0.763483
Na	1.159405	0.566719	-1.522782
Cl	-1.392447	0.733132	-1.621655
Na	-0.980777	1.744546	0.726666
O	-1.732967	0.192645	2.175525
H	-1.424881	0.024364	3.068279
H	-1.637187	-0.646084	1.684726
O	0.699346	-3.772800	0.422423
H	0.706345	-4.730115	0.391414
H	-0.224800	-3.480890	0.407481
O	-1.224317	-1.776310	0.298245
H	-1.784624	-1.404308	-0.399383

H	-0.346672	-1.421771	0.065478
O	1.525531	-1.248358	-0.212799
H	1.853232	-0.735707	0.542312
H	1.634743	-2.196144	-0.028906
16			
Energy=-1550.91972270			
Cl	1.695164	-1.625728	0.775281
Na	1.107788	-0.675999	-1.553605
Cl	-1.440498	-0.885152	-1.487447
Na	-0.873429	-1.682002	0.913801
O	-1.244326	1.784263	0.184845
H	-1.831410	1.353857	-0.454746
H	-0.375681	1.411910	-0.054005
O	0.669288	3.794672	0.097380
H	0.667563	4.731663	-0.103040
H	-0.252847	3.496942	0.120959
O	1.491390	1.234775	-0.387675
H	1.866549	0.772946	0.378406
H	1.585890	2.193910	-0.261828
O	-1.653199	-0.031218	2.227360
H	-1.594922	0.766031	1.666482
H	-1.432048	0.239458	3.120146

3 Third system, $(NaCl)_4(H_2O)_8$ M06-2X/6-311++G(d,p)

32			
Energy=-3101.92343900			
Cl	-0.577934	-1.116208	1.775686
Na	1.483334	0.511235	1.630633
Cl	1.944413	0.517589	-1.025103
Na	-0.392756	-1.181043	-1.016191
Cl	-0.000724	2.684480	1.662009
Na	-2.051283	1.067898	1.116852
Cl	-1.785286	1.146241	-1.510792
Na	0.306103	2.610866	-1.035021
O	-1.242525	-4.082919	0.647688
H	-1.174978	-3.450765	1.378182
H	-0.353751	-4.053897	0.262337
O	-3.681558	-0.522510	0.930755
H	-3.485601	-1.178025	1.608204
H	-3.398016	-0.962048	0.110749
O	3.816791	-1.882341	-0.710003
H	3.411085	-1.055270	-1.038528
H	4.628466	-2.018675	-1.204862
O	2.927597	-1.242437	1.826569
H	3.492010	-1.516898	1.083083
H	3.074022	-1.864523	2.543018
O	-2.435889	-2.288174	-0.982716
H	-2.867256	-2.575709	-1.791539
H	-2.186031	-3.090586	-0.474549
O	1.155773	-2.830456	-0.213895

H	1.237068	-2.354399	0.627689
H	2.049592	-2.831084	-0.585148
O	-0.008964	-0.847231	-3.309420
H	0.819131	-0.371623	-3.168374
H	-0.682246	-0.152389	-3.317022
O	0.546999	4.805519	-0.528683
H	0.330281	5.715319	-0.739265
H	0.389649	4.677656	0.419334

32

Energy=-3101.91927882

Cl	-1.580275	-1.902101	1.066625
Na	-2.129516	1.949474	0.363222
Cl	-1.344450	0.592933	-1.801344
Na	-1.184012	-2.072815	-1.572785
Cl	-0.148284	3.656872	0.087434
Na	0.419534	-0.098279	0.213111
Cl	2.590297	0.816431	-1.487907
Na	0.627461	2.358331	-2.019733
O	0.928209	-3.836116	0.690889
H	0.175741	-3.381655	1.105669
H	1.695744	-3.614184	1.247629
O	-0.793665	0.954445	1.943350
H	-0.198703	1.457116	2.522980
H	-1.069420	0.141767	2.388648
O	-3.683389	0.450268	1.017347
H	-3.180261	-0.385280	1.055223
H	-4.578113	0.209409	0.769690
O	2.373681	0.192470	1.515655
H	2.213891	0.993866	2.042326
H	2.805871	0.497795	0.695659
O	1.330792	2.579353	2.580315
H	1.638177	3.248104	3.197490
H	1.011674	3.059315	1.784635
O	2.908574	-2.485585	2.046630
H	3.808066	-2.630273	2.345546
H	2.796798	-1.522107	1.952602
O	1.036192	-1.857896	-1.228533
H	1.768122	-1.333065	-1.591850
H	1.381599	-2.583516	-0.683019
O	-0.810910	-4.327273	-1.437029
H	-1.450240	-4.980071	-1.142060
H	-0.069677	-4.401053	-0.811496

32

Energy=-3101.91741921

Cl	1.615584	-3.069617	-0.239925
Na	0.222909	-1.762970	-2.105863
Cl	-0.782293	2.919599	-0.848928
Na	1.787027	2.652829	-0.565202
Cl	1.739785	0.340367	-1.789938
Na	-0.698256	0.349355	-0.221568
Cl	2.926848	1.732289	1.558937
Na	2.525599	-0.702312	0.512289
O	-2.644918	0.437331	1.094702
H	-2.676517	1.343124	1.472157

H	-2.472398	-0.187179	1.816833
O	-1.288774	0.018735	-2.572396
H	-0.959228	0.912496	-2.741027
H	-2.244282	0.090246	-2.420213
O	-3.719615	-0.375020	-1.218046
H	-3.558673	0.042384	-0.344425
H	-4.657094	-0.299621	-1.408104
O	-1.557121	-1.432716	2.955079
H	-1.310581	-2.296405	2.563553
H	-1.772190	-1.589769	3.877526
O	0.530012	-0.093637	1.658684
H	-0.047702	-0.452926	2.349001
H	1.044178	0.652094	2.020081
O	-1.501962	-1.928470	-0.603033
H	-1.476279	-2.616350	0.080835
H	-2.428478	-1.729304	-0.810330
O	-2.578640	3.066157	1.683540
H	-2.181081	3.556990	2.405836
H	-2.042496	3.269135	0.892594
O	-0.760566	-3.599350	1.519245
H	-0.866476	-4.544616	1.655027
H	0.115695	-3.481625	1.069387

32

Energy=-3101.91654000

Cl	-0.580447	0.495148	1.675572
Na	0.519545	-0.860494	-0.416989
Cl	-1.955528	-0.586969	-1.570487
Na	-1.793720	1.789791	-0.476150
Cl	-0.057120	3.708514	-0.937134
Na	1.887707	1.336987	1.106942
Cl	-0.112624	-3.319927	0.494225
Na	-2.057028	-1.683851	1.036148
O	2.159151	3.539898	1.182613
H	2.637010	4.309967	1.493801
H	1.503171	3.849327	0.524148
O	1.509573	1.100626	-1.174673
H	1.107265	1.943785	-1.457627
H	2.155006	0.805742	-1.832494
O	3.098016	-0.923582	-2.218244
H	3.823227	-1.143405	-2.807908
H	2.350520	-1.505856	-2.457437
O	-2.390045	3.207648	1.250837
H	-1.929323	2.728381	1.950890
H	-1.761205	3.878039	0.949474
O	-4.144791	-1.855625	0.206455
H	-4.910920	-2.425837	0.120060
H	-3.909020	-1.543610	-0.681433
O	2.671964	-0.749774	0.598145
H	2.784270	-1.555307	1.147055
H	3.155407	-0.893708	-0.229928
O	0.714987	-2.265643	-2.370068
H	-0.132026	-1.916035	-2.684765
H	0.478351	-2.984156	-1.758173
O	2.644654	-3.096718	1.930761

H	1.771208	-3.375589	1.596396
H	2.642502	-3.275613	2.873547

32

Energy=-3101.91635533

Cl	-1.969283	-2.481773	1.228760
Na	-1.892392	-1.833272	-1.290680
Cl	-1.760069	0.750020	-0.885864
Na	-1.820079	0.066491	1.756054
Cl	2.319870	0.076163	-1.210449
Na	0.633527	1.809140	0.047820
Cl	0.763936	0.555352	2.365910
Na	2.255066	-1.185523	1.201046
O	-1.006777	3.490401	0.366804
H	-0.738816	4.289087	-0.120785
H	-1.620229	3.018321	-0.216220
O	1.001257	-3.083161	0.994424
H	0.051353	-2.914725	1.209775
H	1.193457	-3.964038	1.327316
O	-1.756439	-3.066177	-3.181201
H	-2.039828	-3.621576	-3.908014
H	-0.795419	-3.145068	-3.085799
O	-1.947676	2.178971	2.692057
H	-1.115779	2.109286	3.177412
H	-1.765529	2.862461	2.027695
O	0.531677	2.432464	-2.322657
H	-0.277919	1.898498	-2.357615
H	1.255169	1.809706	-2.489947
O	0.180073	5.050745	-1.537196
H	0.403931	4.258992	-2.054428
H	0.126206	5.789415	-2.145598
O	0.362613	-2.375385	-1.695708
H	0.935864	-1.592817	-1.782620
H	0.692216	-2.820443	-0.898537
O	4.400845	-1.425319	0.506367
H	5.336698	-1.404121	0.713625
H	4.268680	-0.913153	-0.306803

32

Energy=-3101.91538906

Cl	-1.193291	0.266110	1.850899
Na	1.140430	1.413554	1.429629
Cl	-1.889721	-1.520171	-1.632375
Na	-1.747118	0.935819	-0.701055
Cl	1.111936	1.005021	-1.352390
Na	0.799035	-1.574708	-1.652971
Cl	1.059033	-2.975193	0.566771
Na	-1.473625	-2.197431	0.888655
O	-1.311812	2.275378	-2.663322
H	-0.411038	1.899867	-2.647999
H	-1.718299	2.016387	-3.495190
O	0.413947	-3.648020	-2.585486
H	0.596995	-4.143241	-1.776516
H	-0.546938	-3.549307	-2.609765
O	2.270928	-0.451380	1.999448
H	1.855108	-1.242330	1.606001

H 3.187721 -0.695356 2.141669
O -2.607374 2.710036 0.406332
H -2.294138 3.603387 0.217138
H -2.341820 2.490311 1.308375
O -1.106508 4.533607 -1.057944
H -1.210458 3.881794 -1.774941
H -1.081045 5.403861 -1.462152
O 0.653013 3.633155 1.012772
H 1.556624 3.821462 0.730683
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O 3.126593 2.496649 0.464345
H 4.077102 2.403613 0.558236
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O -1.021938 -2.747104 3.079209
H -0.124276 -3.063751 2.916395
H -0.920170 -1.829731 3.366198
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Cl 0.555457 -3.579927 -0.816869
Na -1.174898 -1.607827 -1.247669
Cl 0.648757 0.240235 -1.942941
Na 2.130132 -1.554652 -0.620937
Cl -0.472869 3.708052 0.243949
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O -3.088978 -2.427399 1.967642
H -3.024472 -1.494862 1.689639
H -3.762451 -2.476787 2.650352
O -1.440855 2.580657 -2.636904
H -0.872260 1.803655 -2.758154
H -0.826789 3.254100 -2.313680
O 2.552748 1.898153 -0.036876
H 2.225947 1.860956 -0.947529
H 2.698051 2.843280 0.179789
O 1.275409 -0.740785 1.415461
H 0.659772 -1.426937 1.785236
H 2.071863 -0.753366 1.956111
O 3.897134 -0.417874 0.254083
H 4.852897 -0.410238 0.177258
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H -1.217144 -2.717847 2.212257
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O 2.503803 4.499637 0.704552
H 2.841907 5.327654 0.357778
H 1.532654 4.549614 0.654468
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H -1.992337 -3.989087 -0.679723
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Cl 0.971212 -2.656066 1.134170
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Cl	-1.404712	-0.993759	-1.543340
Na	-1.624083	-2.632287	0.463211
Cl	-0.644717	1.392876	1.394674
Na	-1.452237	1.733046	-1.169805
Cl	1.135486	2.026560	-1.811506
Na	1.773867	2.595832	0.623385
O	0.989701	3.862960	2.320367
H	1.173883	4.378578	3.107011
H	0.189765	3.343531	2.489673
O	-2.582483	-1.097166	1.803508
H	-2.815760	-1.099599	2.733965
H	-2.111231	-0.259141	1.654266
O	1.421783	-0.336916	3.262582
H	0.622610	0.144032	3.004765
H	1.260398	-1.237613	2.940795
O	3.060657	-1.486423	-0.763366
H	2.712236	-2.256971	-0.284072
H	3.511478	-1.806685	-1.547492
O	-1.486462	1.438517	-3.594302
H	-0.610146	1.820229	-3.729422
H	-1.317374	0.497252	-3.440206
O	2.698258	0.609334	1.059747
H	3.291901	-0.011721	0.618551
H	2.433045	0.217017	1.920750
O	-1.290062	-4.754341	1.192693
H	-1.448509	-5.699036	1.198274
H	-0.347908	-4.609465	1.369480
O	-3.674508	1.399862	-1.727976
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H	-3.654244	0.445600	-1.583133

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Energy=-3101.91375905

Cl	-1.713288	-2.734658	-0.075319
Na	-2.536850	-0.619220	1.228274
Cl	-2.126485	1.154496	-0.859435
Na	-0.770157	-0.954160	-1.706655
Cl	-0.174861	-0.158060	2.286758
Na	0.565249	-2.552434	1.228915
Cl	1.578001	0.454064	-1.582011
Na	0.240745	1.709267	0.475286
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H	0.998173	4.300290	1.308381
H	0.894672	3.516678	2.658483
O	1.768912	-3.052557	-0.607122
H	1.384590	-2.979094	-1.489682
H	2.618190	-2.589312	-0.639811
O	0.728484	-2.013064	-3.149719
H	1.349992	-1.267042	-3.139113
H	0.747132	-2.408179	-4.024598
O	3.835146	-1.155311	-0.178522
H	4.738583	-0.934980	-0.416126
H	3.260134	-0.484506	-0.594936
O	0.135425	3.290131	-1.463721
H	-0.756115	2.939895	-1.613141

H	0.726822	2.670555	-1.915618
O	2.517711	-1.893877	2.225964
H	2.164073	-1.087044	2.620481
H	3.148948	-1.603033	1.550757
O	-4.311137	0.774848	1.311053
H	-4.044540	1.328474	0.562577
H	-4.963673	1.260569	1.817200
O	0.763934	5.526730	0.012394
H	1.378587	6.153445	-0.372496
H	0.536885	4.888282	-0.686338

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Energy=-3101.91361014

Cl	-3.058602	0.376109	-1.650929
Na	-2.128815	1.945276	0.213240
Cl	2.624940	-0.623324	0.023120
Na	1.356720	1.553934	0.952437
Cl	0.169105	2.648936	-1.222878
Na	-0.853912	0.917221	-2.840573
Cl	-0.890498	0.342099	1.955686
Na	-0.155904	-3.658622	0.276938
O	0.778586	-2.416032	1.896008
H	0.237344	-1.735263	2.319055
H	1.498364	-1.902100	1.488969
O	0.425419	-5.633605	-0.635099
H	0.485011	-6.586358	-0.707736
H	1.133156	-5.238908	-1.164673
O	3.218779	2.553214	-0.011915
H	2.753281	2.895003	-0.784742
H	3.608196	1.716129	-0.296032
O	0.342276	-0.861392	-2.129418
H	-0.276790	-1.205384	-1.457132
H	1.102035	-0.554508	-1.597695
O	-1.472147	3.933140	1.179876
H	-0.924116	4.221979	0.439036
H	-0.833951	3.760967	1.887184
O	-1.467010	-1.891909	-0.204320
H	-2.235613	-1.521228	-0.674565
H	-1.320548	-1.248219	0.515966
O	0.595294	2.808595	2.859982
H	1.062389	3.162161	3.621023
H	0.059502	2.056103	3.159868
O	1.566073	-3.304942	-1.327013
H	2.231306	-2.746583	-0.889751
H	1.208166	-2.709802	-2.003431

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Energy=-3101.91355246

Cl	-1.926672	-2.475175	1.056991
Na	0.557252	-2.048281	1.607222
Cl	0.467489	0.521925	1.657503
Na	-2.068704	0.194850	0.683276
Cl	-2.034450	2.889817	-0.264477
Na	0.509808	2.814309	0.306639
Cl	1.674798	-2.599984	-0.681176
Na	-0.955345	-2.510439	-1.347057

O	-1.017757	-0.249991	-1.431544
H	-0.171383	0.151407	-1.161768
H	-1.315828	0.349440	-2.136160
O	-4.121035	1.078838	1.075379
H	-4.872550	1.096862	1.669305
H	-3.942398	1.985375	0.785221
O	3.222858	-0.064224	-1.593672
H	3.931069	-0.326459	-2.187004
H	2.771585	-0.893315	-1.327764
O	-1.264274	2.012569	-3.078851
H	-1.713558	2.362989	-3.851023
H	-1.633913	2.476555	-2.295441
O	1.067302	1.687132	-1.594503
H	0.602218	1.883800	-2.420591
H	1.886273	1.205341	-1.797588
O	3.479559	1.339026	0.877683
H	2.714458	0.913433	1.294144
H	3.577749	0.881139	0.029037
O	-0.158040	-4.250204	-2.571695
H	-0.320439	-5.178434	-2.748717
H	0.732759	-4.179825	-2.195729
O	2.446444	3.817075	0.848866
H	3.022584	3.022732	0.873729
H	2.796301	4.443258	1.483532

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Energy=-3101.91334537

Cl	1.673232	1.625918	-2.018095
Na	2.822295	-0.547821	-1.326409
Cl	-1.530101	2.939023	-0.204438
Na	0.960632	3.414561	-0.335579
Cl	0.685263	-2.058021	-1.414697
Na	-0.613333	0.537046	-1.064483
Cl	3.150176	-0.490275	1.220027
Na	0.779300	-1.675302	1.308036
O	0.601207	-4.016345	1.030061
H	0.598838	-3.855118	0.072243
H	1.219003	-4.735677	1.179709
O	-1.500462	-2.154033	1.509787
H	-2.076379	-1.597930	2.068037
H	-1.636875	-3.081785	1.722930
O	-0.185669	0.364675	1.285288
H	-1.048446	0.484277	1.722000
H	0.313003	1.182340	1.433480
O	-1.987593	-2.552026	-2.996834
H	-2.048913	-2.494882	-3.952480
H	-1.042172	-2.564076	-2.775446
O	-2.454941	-0.870992	-0.860863
H	-2.137040	-1.462534	-0.156265
H	-2.511144	-1.429175	-1.658498
O	1.914294	2.343860	1.429792
H	2.163553	2.603601	2.321150
H	2.428992	1.522917	1.252895
O	-3.994764	1.040958	0.459602
H	-3.492087	1.840179	0.228452

H	-3.701455	0.382185	-0.192628
O	-2.711680	0.055621	2.490597
H	-3.296068	0.468057	1.787391
H	-3.008606	0.390997	3.339343

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Energy=-3101.91168862

Cl	1.895509	2.033260	-1.600092
Na	2.572394	0.811539	0.620470
Cl	0.147141	-0.222969	0.729371
Na	-2.204500	-1.339317	0.276461
Cl	-1.836415	-1.554284	-2.284792
Na	0.018531	0.214868	-1.943511
Cl	-1.443341	2.798896	2.268749
Na	0.010977	2.671262	0.125351
O	-0.184858	-3.829352	-0.818655
H	-0.876481	-3.887800	-0.143391
H	-0.560370	-3.235253	-1.492151
O	3.618902	-1.120413	0.225420
H	3.072099	-1.926655	0.307599
H	4.223700	-1.283265	-0.501020
O	-3.061508	0.716705	0.777422
H	-3.960774	1.013813	0.943928
H	-2.499657	1.275498	1.376497
O	1.617157	2.357178	2.039080
H	1.932676	3.156964	2.469098
H	0.731919	2.197606	2.426364
O	2.092426	-3.415493	0.453093
H	1.272700	-3.497733	-0.102125
H	2.542188	-4.261733	0.381383
O	-1.875037	-3.281590	1.439321
H	-1.055585	-3.158510	1.989240
H	-2.460051	-3.865468	1.927067
O	0.415040	-2.744557	2.640758
H	0.413515	-1.789380	2.481744
H	1.117802	-3.063734	2.049791
O	-1.596987	1.842990	-1.327545
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Energy=-3101.91152588

Cl	-1.312745	1.269071	-1.481133
Na	-0.359391	-1.148472	-1.923430
Cl	-1.686557	-2.227456	0.150689
Na	-2.600925	0.149127	0.634566
Cl	1.124744	-0.634422	2.828807
Na	0.869938	-2.470198	1.017718
Cl	2.116585	-1.146812	-0.878488
Na	2.092263	0.877289	0.884790
O	0.517183	5.067857	0.331331
H	0.498817	4.220876	0.807753
H	1.228591	5.582690	0.717210
O	0.498937	-3.189069	-2.634282
H	1.419105	-2.917877	-2.516331
H	0.362575	-3.828259	-1.921076

O	0.311573	2.367488	1.006062
H	-0.329486	2.042796	1.659295
H	-0.107369	2.168575	0.147472
O	0.220847	-4.532742	0.001382
H	0.278773	-5.473093	0.190968
H	-0.713823	-4.272542	0.069101
O	-4.134115	1.544351	-0.254746
H	-3.579556	1.850170	-0.988346
H	-5.017652	1.889498	-0.389903
O	2.930037	2.030645	-0.859036
H	2.290273	2.610195	-1.323571
H	3.130657	1.320908	-1.478529
O	0.979473	3.582084	-1.997529
H	0.175894	3.064633	-2.136121
H	0.747702	4.274452	-1.356009
O	-1.528456	0.791325	2.544805
H	-0.743878	0.220771	2.736035
H	-1.886389	1.043759	3.400477

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Energy=-3101.91145420

Cl	-1.595282	-0.164099	-1.247232
Na	1.167697	-0.760407	-1.132433
Cl	1.542606	-0.426907	1.566007
Na	1.887617	2.062049	1.028468
Cl	1.824702	1.809041	-1.641066
Na	-0.680182	2.269369	-1.242934
Cl	1.075825	-3.333918	-1.312932
Na	-0.692693	-3.680461	0.661096
O	-0.359703	2.512591	1.143015
H	-0.852157	1.841450	1.654645
H	-0.940332	3.283190	1.095730
O	-2.092530	0.779611	2.553210
H	-2.171060	0.828918	3.509326
H	-1.901147	-0.158618	2.334145
O	-1.283679	-1.595219	1.492149
H	-0.361124	-1.288143	1.627009
H	-1.505677	-1.224032	0.615001
O	3.567002	3.426196	0.356232
H	3.478306	3.190171	-0.579519
H	4.473748	3.702859	0.498990
O	-2.064690	-3.417091	-1.172945
H	-1.281971	-3.473708	-1.743565
H	-2.402261	-2.529504	-1.347516
O	-3.659839	1.697050	0.375691
H	-3.368695	0.993284	-0.225035
H	-3.336169	1.410243	1.244243
O	1.294945	-3.675626	1.825105
H	1.776781	-3.717148	0.984650
H	1.555038	-2.816951	2.184582
O	-2.266120	3.758139	-0.507539
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H	-2.938435	3.109891	-0.178849

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Energy=-3101.90952130

Cl	2.778475	1.036673	0.088602
Na	1.538480	2.855843	-1.298114
Cl	-0.028201	3.807380	0.547558
Na	0.657992	1.477475	1.621925
Cl	-1.148281	-2.519844	-0.944668
Na	0.938713	-0.832562	-0.959215
Cl	-0.204688	1.183711	-2.223889
Na	-1.830598	2.071998	-0.363593
O	-3.012633	0.250647	-0.868078
H	-2.368471	-0.255468	-1.387678
H	-3.592780	-0.422489	-0.488250
O	-1.691790	1.429827	1.911344
H	-2.078462	0.559808	2.138288
H	-2.064908	2.085087	2.507401
O	-2.461739	-1.155129	2.304248
H	-3.066533	-1.591721	1.669961
H	-2.461787	-1.687151	3.103687
O	2.102837	-2.376615	0.299551
H	3.059014	-2.273174	0.454832
H	1.888933	-3.321455	0.184854
O	0.858078	-4.779678	-0.128491
H	0.084182	-4.256503	-0.408543
H	1.010287	-5.415642	-0.830775
O	-3.884751	-2.223223	0.254167
H	-4.583218	-2.867571	0.118824
H	-3.083287	-2.542142	-0.224028
O	4.676169	-1.447109	0.568531
H	4.337369	-0.549670	0.412882
H	5.257748	-1.383571	1.328697
O	0.288208	-0.719807	1.514155
H	0.944943	-1.423441	1.351338
H	-0.581849	-1.146842	1.535073

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Energy=-3101.90885236

Cl	-2.317866	2.437626	0.017595
Na	-2.331862	-0.081338	-0.764228
Cl	-0.525318	-4.120949	-0.375615
Na	0.531103	-1.753137	-0.670037
Cl	-0.170838	0.109885	-2.339256
Na	0.230044	2.147397	-0.822170
Cl	0.945255	1.574237	1.813963
Na	-0.820677	3.442381	1.821116
O	-2.623922	-2.136264	-1.676117
H	-2.191483	-2.900058	-1.253322
H	-2.235290	-2.101717	-2.556913
O	1.619731	-3.486022	2.006709
H	1.314378	-4.060940	1.289526
H	0.814755	-3.343360	2.524634
O	3.879734	1.156321	0.471160
H	3.567882	1.375906	1.357854
H	3.593022	0.234506	0.357913
O	0.559360	4.486158	0.335901
H	1.444502	4.139904	0.117716
H	0.421660	5.256768	-0.221241

O	-0.981038	-0.841838	0.945565
H	-1.156793	-1.542838	1.600669
H	-0.585508	-0.093502	1.421988
O	2.434114	2.910936	-0.925520
H	2.915349	3.101609	-1.735281
H	2.985121	2.245745	-0.436271
O	-1.223606	-3.172108	2.422156
H	-1.915569	-3.560980	2.962825
H	-1.191974	-3.676316	1.579109
O	2.248335	-1.132422	0.759419
H	2.234591	-1.946895	1.304213
H	1.805690	-0.451297	1.290730

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Energy=-3101.90824366

Cl	2.038161	0.796224	-1.468343
Na	-0.085347	2.240712	-1.877278
Cl	0.732094	2.529944	2.073933
Na	2.740385	1.353241	0.960386
Cl	-1.032362	-3.342710	-0.090559
Na	-2.850468	-1.635735	0.280727
Cl	-1.886878	0.392631	-1.034022
Na	0.409568	-1.128703	-0.423023
O	-1.291919	1.782823	-3.755779
H	-1.101909	1.479239	-4.645832
H	-1.835470	1.101885	-3.333143
O	-2.789089	-0.682154	2.316250
H	-2.701546	0.305167	2.238773
H	-3.181703	-0.870321	3.171863
O	2.891428	-0.735350	1.759587
H	2.952157	-1.388874	1.042067
H	2.026416	-0.914634	2.157485
O	2.459720	-2.236094	-0.557015
H	2.380297	-3.199960	-0.709817
H	2.878449	-1.827942	-1.322533
O	-0.349368	3.938878	-0.455266
H	0.013866	3.680321	0.414153
H	-0.982094	4.641039	-0.292041
O	-2.384353	1.865950	1.775716
H	-2.263809	1.749545	0.819421
H	-1.538253	2.230225	2.082510
O	1.678390	-4.819382	-0.672307
H	0.762213	-4.582725	-0.439624
H	1.615485	-5.501028	-1.344319
O	0.095900	-0.566568	1.813656
H	-0.749777	-0.893728	2.151856
H	0.094055	0.395135	1.969885

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Energy=-3101.90790514

Cl	2.094809	1.031934	-0.968918
Na	1.449574	-1.571080	-1.287558
Cl	0.766525	-2.790854	0.939330
Na	-1.743114	-1.912681	0.337941
Cl	-1.500635	2.714640	-0.473531
Na	0.749269	2.702277	0.906683

Cl	-1.005094	-1.045645	-2.165020
Na	-0.169158	1.392998	-2.212055
O	-3.765226	0.561815	-1.509926
H	-3.039777	0.112026	-1.969020
H	-3.384334	1.403699	-1.220360
O	-2.051719	-3.631915	1.837149
H	-2.480572	-3.816157	2.674692
H	-1.103762	-3.790259	1.960968
O	3.487058	-2.341547	-0.603838
H	4.190421	-1.781099	-0.264419
H	3.167972	-2.855425	0.151043
O	-4.003625	-1.308206	0.405686
H	-4.123017	-0.621194	-0.285937
H	-4.790287	-1.857106	0.402522
O	2.673489	3.760089	0.373499
H	3.058233	3.104764	-0.225685
H	3.367255	4.373105	0.622952
O	-1.853231	0.167756	1.396742
H	-1.821293	0.936892	0.798001
H	-2.786981	0.043998	1.609929
O	2.674503	-0.430354	1.947938
H	2.159258	-1.245612	1.832746
H	2.680565	-0.031304	1.066219
O	0.496613	1.226340	2.552093
H	-0.294708	0.680315	2.428325
H	1.253490	0.613905	2.578353

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Energy=-3101.90790189

Cl	0.298076	1.732086	-2.274861
Na	-0.424516	0.967548	0.416580
Cl	-2.137911	-3.482317	-0.767351
Na	-2.659049	-1.140663	0.139155
Cl	2.318149	0.935971	0.621712
Na	1.720907	-0.388972	-1.628123
Cl	-0.618556	3.449986	1.225347
Na	1.353562	3.226261	-0.404941
O	-2.460121	0.853217	-0.838258
H	-1.904946	1.053808	-1.609580
H	-2.936419	1.685301	-0.621832
O	-0.148186	-1.178589	-0.540182
H	-0.636515	-1.920473	-0.949691
H	0.290199	-1.586931	0.232272
O	0.688371	-4.366784	0.008379
H	0.852603	-5.312290	-0.043352
H	-0.241053	-4.236905	-0.291149
O	-1.400788	-0.531690	2.001688
H	-0.706695	-1.200760	2.175721
H	-1.610962	-0.114277	2.841970
O	0.675360	-2.319451	1.888000
H	1.612973	-2.121572	2.064142
H	0.651778	-3.226839	1.538608
O	3.378594	-1.654471	1.812123
H	3.247689	-0.708796	1.594295
H	4.128514	-1.709898	2.409400

O	-3.508071	3.126361	0.138583
H	-2.677572	3.437433	0.550196
H	-3.895566	3.886559	-0.300340
O	2.592676	-2.367411	-0.856169
H	2.004812	-3.126646	-0.711990
H	3.079363	-2.266045	-0.024482

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Energy=-3101.90695942

Cl	-2.144450	-2.059365	1.593418
Na	-1.385867	-3.928182	0.111598
Cl	0.325839	-3.394942	-1.638709
Na	1.837873	-1.472404	-0.689396
Cl	-0.942812	2.553178	1.384448
Na	-0.534791	3.024507	-1.239587
Cl	1.185227	0.998078	-1.562391
Na	-1.081602	0.121991	0.139361
O	-2.382043	1.797089	-1.714991
H	-2.995002	1.618983	-0.983955
H	-2.344776	0.959908	-2.198427
O	0.816775	4.653540	-0.310304
H	0.337009	4.695194	0.527498
H	1.664683	4.264449	-0.059602
O	2.873249	0.304141	2.561904
H	3.126309	0.445903	3.476448
H	2.709251	1.187830	2.145712
O	2.159529	2.388414	1.105276
H	2.105775	1.937960	0.243291
H	1.218848	2.460588	1.366315
O	-3.385072	0.751225	0.687571
H	-3.569005	-0.099312	1.108320
H	-3.055097	1.341864	1.379678
O	3.786417	-1.095538	0.379772
H	3.646138	-0.672642	1.245895
H	4.615458	-0.752738	0.041147
O	-1.329930	-0.730365	-2.097992
H	-1.161299	-1.678951	-2.202311
H	-0.499373	-0.316520	-2.381492
O	0.739228	-0.987713	1.272136
H	0.049683	-1.472174	1.754301
H	1.316351	-0.557805	1.926035

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Energy=-3101.90658386

Cl	-2.148600	-3.210146	-0.282566
Na	0.347923	-3.263277	-0.636300
Cl	-2.080883	1.805440	-1.614741
Na	0.315926	1.490322	-2.488237
Cl	0.734807	-0.997775	-1.813427
Na	-1.794312	-0.657757	-0.714362
Cl	1.595108	2.732604	-0.637054
Na	-0.875189	3.089680	0.389657
O	-2.684842	2.286758	1.662140
H	-2.351152	1.368782	1.673012
H	-3.509363	2.256696	1.169482
O	3.273297	-1.191296	1.622700

H	3.469343	-0.727685	0.762093
H	4.101814	-1.258325	2.104224
O	-1.080047	-2.503757	2.605381
H	-0.191325	-2.794323	2.362492
H	-1.651665	-2.944440	1.955188
O	-0.163443	3.117990	2.559243
H	-0.958330	2.897190	3.055990
H	0.481961	2.419813	2.741761
O	1.537119	-3.276670	1.316979
H	2.182148	-2.544741	1.443212
H	1.904872	-4.035309	1.777771
O	-1.207814	-0.040491	1.437931
H	-1.233646	-0.858170	1.982904
H	-0.291676	0.284843	1.550194
O	3.483371	0.096451	-0.646149
H	2.754477	-0.305642	-1.148384
H	3.261105	1.040385	-0.637770
O	1.355064	0.897313	1.898865
H	1.617981	1.406882	1.109869
H	2.028483	0.211023	2.021313

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Energy=-3101.90638091

Cl	0.220246	0.399550	1.773295
Na	-0.164300	2.817060	0.486938
Cl	2.361758	3.375422	0.132357
Na	2.661160	1.030291	1.104390
Cl	-2.012029	-1.906678	-0.376708
Na	0.350622	-0.825819	-0.670775
Cl	-2.704482	2.970185	0.864759
Na	-2.365035	0.386269	0.790057
O	2.683166	-0.032689	-0.867985
H	2.723915	0.529513	-1.659523
H	2.807877	-0.964235	-1.115919
O	0.896408	-5.070964	-1.347172
H	1.318827	-5.930348	-1.300224
H	0.213803	-5.056480	-0.653767
O	1.902185	-2.575110	-0.807299
H	1.691410	-3.437652	-1.209030
H	1.795428	-2.728346	0.153831
O	-0.900753	-4.521369	0.732775
H	-1.568192	-5.083899	1.133695
H	-1.382553	-3.749606	0.358199
O	2.172989	2.066540	-2.609308
H	2.337239	2.672444	-1.852176
H	2.541236	2.484627	-3.391450
O	-0.235609	1.311201	-1.423255
H	-1.146665	1.308110	-1.767661
H	0.373034	1.629877	-2.109046
O	-2.951601	1.128397	-1.480749
H	-3.304084	1.950079	-1.096979
H	-3.637384	0.686044	-1.987153
O	1.059967	-2.748805	1.787023
H	0.634718	-1.933749	2.087433
H	0.354511	-3.407779	1.691917

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Energy=-3101.90613659

Cl	-1.477319	-0.133042	2.258323
Na	0.608048	-1.648673	1.748258
Cl	2.279566	-0.640871	-0.156107
Na	0.572157	-1.942385	-1.790165
Cl	-0.673388	-3.250357	0.079055
Na	-2.712070	-1.763337	0.613327
Cl	-3.221555	-0.070446	-1.259787
Na	-1.775771	1.541062	0.213061
O	2.667719	4.842972	-0.340759
H	3.190695	5.338515	-0.971921
H	1.726541	4.990332	-0.559614
O	-0.522246	2.973778	1.522799
H	0.406201	2.736828	1.322137
H	-0.692517	2.632051	2.406903
O	-0.702867	-0.422342	-2.923664
H	-0.853237	-0.346567	-3.869588
H	-1.591799	-0.356801	-2.499851
O	1.915728	2.382747	0.452012
H	2.478387	3.136159	0.190946
H	2.416692	1.555022	0.414245
O	-0.138777	1.914789	-1.332851
H	-0.109621	1.221604	-2.008116
H	0.717190	1.910431	-0.864998
O	-0.046607	4.712695	-0.700156
H	-0.188509	3.893138	-1.196308
H	-0.388555	4.513900	0.181614
O	2.642204	-1.668673	2.764565
H	3.105402	-1.421767	3.566602
H	3.118285	-1.275654	2.019497
O	2.590346	-2.857898	-2.347433
H	2.906951	-3.760329	-2.272152
H	3.061367	-2.340746	-1.677666

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Energy=-3101.90607951

Cl	-2.261878	-2.080778	-1.085175
Na	0.241370	-2.556733	-0.475393
Cl	0.559765	2.371071	-1.721566
Na	1.274864	3.137437	0.703674
Cl	-2.335230	1.325261	0.786213
Na	-1.124742	0.372267	-1.421973
Cl	-0.066842	-1.762013	2.112354
Na	-2.499964	-1.186726	1.319647
O	0.539536	1.380865	1.920970
H	-0.387907	1.308631	1.607360
H	0.578159	0.780617	2.675301
O	0.624902	-4.503876	0.988572
H	0.331646	-3.904320	1.700879
H	0.192031	-5.349378	1.126858
O	2.532659	-2.924632	-0.060569
H	2.339800	-3.754462	0.402098
H	3.304425	-3.063196	-0.615897
O	-0.776717	4.153355	0.580821

H	-0.848015	3.978100	-0.368764
H	-1.474965	3.597844	0.955183
O	2.489632	-0.156830	0.578085
H	1.661079	0.180256	0.963996
H	2.511798	-1.108552	0.756696
O	2.824709	0.259950	-2.166977
H	2.798615	0.162972	-1.197692
H	2.387235	1.115832	-2.310085
O	0.568997	-1.133813	-2.255718
H	1.435005	-0.668715	-2.384881
H	0.286401	-1.474727	-3.108895
O	3.440785	2.438452	0.643569
H	3.411416	1.471263	0.735194
H	4.006034	2.609604	-0.113840

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Energy=-3101.90543182

Cl	-2.648907	1.664000	-0.783825
Na	-0.538002	1.286283	-2.188779
Cl	1.526724	2.580198	-1.425935
Na	0.722007	2.649136	1.062613
Cl	0.116777	0.052952	1.655694
Na	-2.436498	-0.207996	1.071699
Cl	-0.017294	-4.156750	0.276282
Na	1.211929	-2.311052	1.491900
O	2.677671	2.011353	2.083379
H	2.347146	1.217794	2.518864
H	3.265158	1.677843	1.385644
O	2.688975	-1.658177	-0.023847
H	3.152161	-0.814288	-0.162071
H	2.673092	-2.137572	-0.865077
O	-4.601956	-0.690831	0.422859
H	-4.746616	0.059624	-0.165399
H	-4.220366	-1.378312	-0.141442
O	-1.263691	3.691868	1.132322
H	-1.546541	4.607560	1.091519
H	-1.854069	3.195574	0.534130
O	1.538215	-3.095501	-2.115542
H	1.041955	-3.623727	-1.447268
H	1.687392	-3.667100	-2.872487
O	3.801932	0.897683	-0.280324
H	3.143801	1.422702	-0.789420
H	4.660028	1.092263	-0.667287
O	-2.223347	-1.995044	-0.357315
H	-1.587349	-1.608765	-0.981314
H	-1.792074	-2.830016	-0.101209
O	0.073911	-0.790455	-1.584218
H	0.587967	-1.533160	-1.951805
H	0.470492	-0.613654	-0.714668

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Energy=-3101.90414500

Cl	1.532970	1.946621	-1.628624
Na	2.337729	1.289429	0.806454
Cl	0.410612	2.550447	1.922166
Na	-0.236762	3.455619	-0.442706

Cl	-2.519275	2.286633	-0.681689
Na	-1.006971	0.404755	0.639223
Cl	1.065558	-3.883117	0.349432
Na	-0.285540	-2.204515	-1.090770
O	-0.693742	-0.244745	-2.031054
H	-1.590786	0.046357	-2.242135
H	-0.101172	0.520153	-2.138925
O	3.480174	-0.244721	-0.496537
H	3.882574	-1.137342	-0.532190
H	3.441839	0.122465	-1.388202
O	-2.441614	1.118950	2.358655
H	-1.798055	1.711896	2.768606
H	-2.944273	1.691006	1.763541
O	-2.037249	-1.653623	0.207347
H	-2.213297	-2.316235	0.901433
H	-2.853498	-1.434110	-0.269913
O	-1.719596	-3.731032	1.912257
H	-0.845349	-4.009168	1.590727
H	-1.711136	-3.845857	2.864307
O	3.959683	-2.885538	-0.411066
H	4.673529	-3.502917	-0.240289
H	3.131222	-3.343837	-0.174979
O	-3.612975	-0.395015	-1.665387
H	-4.429338	-0.492509	-2.162111
H	-3.566912	0.537978	-1.378718
O	1.005137	-0.790944	0.546861
H	1.782968	-0.763090	-0.042617
H	1.079448	-1.650889	0.996195

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Energy=-3101.90209543

Cl	2.813325	-1.969123	0.612477
Na	1.612787	-2.645376	-1.528109
Cl	-0.791910	3.501907	-0.601161
Na	1.256015	1.821958	-1.014476
Cl	0.152406	-0.439055	-1.749155
Na	-2.176913	-0.036260	-0.559679
Cl	-1.924959	-2.273628	0.839148
Na	0.428715	-0.890695	1.014007
O	-3.264787	1.771223	-1.301376
H	-3.819621	2.024847	-2.040680
H	-2.609872	2.486035	-1.183648
O	-1.031749	-5.334597	0.770970
H	-1.734554	-5.976134	0.890850
H	-1.390492	-4.486851	1.079928
O	-0.206148	-3.909910	-1.455988
H	-0.899041	-3.280262	-1.208798
H	-0.349609	-4.634588	-0.822319
O	-0.987799	3.245618	2.402932
H	-1.647907	3.800791	2.825902
H	-0.949548	3.520624	1.457342
O	-1.321151	0.597997	1.544612
H	-1.296194	1.482008	1.951719
H	-1.860588	0.020218	2.098989
O	1.952452	0.965919	0.952775

H	2.629212	0.267125	0.980584
H	2.009961	1.506786	1.764333
O	1.628464	2.601304	3.107310
H	2.170892	3.351636	3.357102
H	0.722941	2.936723	2.990309
O	1.824570	3.666346	-2.223490
H	1.004731	4.141722	-2.022027
H	2.166018	4.012228	-3.049475

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Energy=-3101.90193286

Cl	3.448933	-0.166117	1.239442
Na	2.683057	-0.903420	-1.110055
Cl	0.756865	-2.590626	-1.077600
Na	-1.069578	-2.020762	0.763767
Cl	1.326296	1.277938	-1.753795
Na	-0.727184	2.885431	-1.747850
Cl	-0.895484	2.672253	1.030358
Na	1.467158	1.469445	0.871628
O	0.429148	-0.510796	1.813249
H	1.355388	-0.804219	1.892576
H	0.115601	-0.259667	2.694447
O	-2.581392	-3.621237	0.110448
H	-2.143458	-4.245405	-0.502978
H	-3.401762	-3.375403	-0.320917
O	-1.439295	-0.131309	-0.610274
H	-1.276065	0.585887	0.025366
H	-0.578471	-0.283254	-1.038304
O	-1.275334	0.874755	3.562629
H	-1.285195	1.550431	2.856818
H	-1.290297	1.348768	4.397150
O	-2.307811	-1.502709	2.586777
H	-2.181690	-0.674465	3.075526
H	-3.152934	-1.872609	2.845483
O	-0.837351	5.007099	-0.996949
H	-0.924470	4.809510	-0.053349
H	-0.917575	5.954996	-1.109274
O	-2.389314	1.574236	-2.538306
H	-2.599500	1.223650	-3.405259
H	-2.269881	0.806051	-1.947076
O	-1.090487	-5.028614	-1.692920
H	-0.637058	-5.860836	-1.544482
H	-0.393149	-4.347804	-1.716780

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Energy=-3101.90038497

Cl	2.068683	-2.176253	-1.686264
Na	1.316343	-3.083161	0.689976
Cl	-2.083257	1.298735	1.700665
Na	-1.002438	3.191861	0.253231
Cl	-2.415405	-2.062801	-1.015225
Na	-3.037703	0.316682	-0.467362
Cl	1.536710	2.455072	0.512844
Na	0.260352	0.186873	1.194899
O	2.353853	-0.850873	1.010147
H	2.528385	-1.031248	0.061984

H	2.985512	-0.173806	1.274188
O	0.243938	0.257328	-1.202821
H	0.535655	-0.589011	-1.597964
H	1.037690	0.813300	-1.139040
O	-0.689311	5.267326	-0.503292
H	0.269771	5.466464	-0.556767
H	-1.157626	6.051574	-0.791476
O	1.245146	-5.298786	1.141816
H	1.712592	-6.123919	1.275912
H	0.661893	-5.405543	0.371673
O	2.013407	5.360442	-0.556814
H	2.123463	4.436117	-0.269357
H	2.599121	5.878622	-0.000609
O	-0.565911	-1.970819	1.383484
H	-1.118234	-2.117654	2.157272
H	-1.188873	-2.027962	0.615939
O	-1.774556	1.872468	-1.626995
H	-1.858587	2.257316	-2.503086
H	-1.005578	1.248039	-1.664650
O	-0.136888	-4.285523	-0.922340
H	0.404485	-3.851612	-1.600609
H	-1.015959	-3.887217	-1.022163

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Energy=-3101.89984469

Cl	2.977412	-0.297690	0.451114
Na	1.566477	-2.411617	0.852034
Cl	0.189883	3.712219	1.739074
Na	0.244081	4.212667	-0.718786
Cl	-2.201067	-3.102137	-0.220051
Na	-1.335961	-0.646368	-0.558694
Cl	-0.179847	1.714016	-1.512236
Na	1.076524	1.338756	0.996521
O	-0.604022	-0.126715	1.579838
H	-0.595447	-0.942212	2.102273
H	-1.292625	0.477656	1.949616
O	-0.032847	-4.158881	-2.066277
H	-0.828395	-3.935005	-1.526209
H	-0.342332	-4.687174	-2.805307
O	-2.353886	1.788649	2.108837
H	-1.772266	2.566663	2.106739
H	-2.787277	1.771423	1.245138
O	0.652164	-1.630387	-1.164748
H	0.643148	-2.331974	-1.832336
H	1.409483	-1.044552	-1.318693
O	1.878799	-4.431294	-0.105620
H	1.266279	-4.547209	-0.854295
H	2.630133	-5.004377	-0.263680
O	0.922596	4.268232	-2.856918
H	1.533204	4.601266	-3.516629
H	0.795275	3.322097	-3.023090
O	-0.303206	-2.836674	2.128134
H	-0.993388	-3.060840	1.457861
H	-0.426278	-3.444886	2.860602
O	-3.022572	1.045200	-0.612103

H	-3.873870	1.003374	-1.054884
H	-2.430588	1.594405	-1.151679

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Energy=-3101.89928581

Cl	-3.059336	0.359853	-0.424025
Na	-0.632763	-0.563249	-0.714944
Cl	0.924256	-2.130039	-2.118058
Na	2.033013	-2.325238	0.341214
Cl	0.582608	1.808800	0.057143
Na	-2.011213	2.621469	0.055271
Cl	0.791955	-4.535175	0.994044
Na	-0.596871	-3.953322	-1.105050
O	-1.207851	-2.901012	2.580657
H	-1.610298	-3.146164	3.417272
H	-0.581769	-3.612642	2.323300
O	0.402599	-1.039365	1.362322
H	0.497430	-0.109965	1.610370
H	-0.171225	-1.480447	2.013649
O	-1.416762	4.768470	0.077809
H	-0.807054	4.839271	0.842888
H	-0.863594	5.030090	-0.669862
O	2.993012	-0.366872	-0.381131
H	2.760434	-0.483813	-1.312000
H	2.530580	0.444499	-0.124288
O	-2.053332	-2.583533	-0.077872
H	-2.741785	-1.915020	-0.232327
H	-1.981888	-2.668683	0.889490
O	0.965203	4.503338	-1.570613
H	0.945051	3.614944	-1.168511
H	1.150019	4.370392	-2.504177
O	0.544845	4.521896	1.960999
H	1.255231	5.120333	1.673870
H	0.839103	3.642448	1.690077
O	2.306089	5.990499	0.399940
H	3.248855	6.137889	0.308926
H	1.998795	5.583216	-0.426255

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Energy=-3101.89925503

Cl	3.194246	-0.008844	2.130020
Na	0.719732	1.538540	-0.542380
Cl	-0.684130	3.438484	0.725543
Na	-2.658384	2.111009	-0.160628
Cl	0.975273	-2.834656	-0.945682
Na	2.871677	-1.293649	-0.010661
Cl	-1.475002	0.556588	-1.907339
Na	-1.444919	-1.787668	-0.794738
O	1.010039	2.291388	-2.794371
H	0.099917	2.059838	-3.029706
H	1.114541	3.235454	-2.939272
O	2.084230	-0.051693	-1.746423
H	2.146112	0.684306	-2.372070
H	1.480594	-0.702651	-2.133251
O	-1.687913	-3.769753	2.242253
H	-0.913837	-4.131052	2.681208

H	-1.684659	-4.128847	1.341393
O	2.537010	2.554395	0.376937
H	2.125130	3.262876	0.884435
H	2.972334	1.970158	1.020932
O	-1.691430	-4.169594	-0.570226
H	-0.745106	-4.200776	-0.809134
H	-2.137746	-4.869273	-1.054745
O	-1.821570	-1.185681	1.366733
H	-1.764308	-2.008061	1.890575
H	-1.038541	-0.630902	1.581865
O	-3.741327	0.715859	1.208564
H	-3.165066	-0.060022	1.372179
H	-4.225515	0.873061	2.021422
O	0.228339	0.539257	1.576765
H	1.115073	0.353161	1.957681
H	-0.015131	1.443717	1.836097

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Energy=-3101.89920909

Cl	-0.924827	2.681052	-1.282325
Na	-1.109075	0.613509	0.376583
Cl	-1.744654	-3.768491	-0.196347
Na	0.660668	-3.541909	-0.900019
Cl	2.321672	-2.438983	0.712599
Na	0.852623	-1.190370	2.414685
Cl	0.885724	1.329837	2.000851
Na	1.262741	3.242718	0.298248
O	-3.625916	0.947625	-1.166313
H	-3.111614	0.215404	-1.539503
H	-3.107909	1.729463	-1.409632
O	0.956536	-1.971741	-2.588164
H	0.941487	-2.044826	-3.545966
H	1.713036	-1.392832	-2.361156
O	-3.194202	0.596507	1.466093
H	-3.610883	0.737130	0.586957
H	-3.567023	1.247368	2.064101
O	-1.282132	-1.439351	1.796051
H	-2.126460	-1.009069	1.996210
H	-1.500697	-2.247503	1.286117
O	2.991309	-0.445315	-1.509209
H	2.877110	-0.919032	-0.655799
H	3.917406	-0.560265	-1.742380
O	0.243413	5.227763	-0.007967
H	0.191096	6.182330	-0.067425
H	-0.460667	4.852665	-0.560655
O	2.232841	2.305251	-1.530876
H	2.523333	1.381317	-1.487998
H	1.393524	2.289975	-2.011195
O	-1.500989	-0.902272	-1.338790
H	-0.775525	-1.026947	-1.964620
H	-1.730323	-1.808763	-1.047003

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Energy=-3101.89838896

Cl	0.192580	1.136452	-1.189663
Na	1.214601	3.486472	-0.749319

Cl	-0.919590	-1.107179	1.725886
Na	1.144836	-2.599058	1.086269
Cl	-0.405538	4.019681	1.290515
Na	-0.935862	1.438020	1.314519
Cl	0.108688	-3.436536	-1.255665
Na	-1.263288	-1.178130	-1.045690
O	-3.345811	-0.266892	-1.136484
H	-3.614347	0.514354	-0.637723
H	-3.768284	-1.037823	-0.736463
O	-2.664902	2.213032	-0.120887
H	-2.059632	2.119538	-0.872032
H	-2.563538	3.130214	0.167485
O	2.286031	-1.210051	-0.343067
H	1.835852	-0.375423	-0.541560
H	2.126636	-1.753483	-1.126175
O	0.809276	5.869257	-0.809816
H	0.226341	5.704436	-0.045453
H	0.396457	6.553971	-1.341249
O	-2.880823	-2.839046	-0.114984
H	-2.331616	-3.553863	-0.463064
H	-2.498220	-2.632473	0.750607
O	2.286771	-4.467908	1.582824
H	3.148701	-4.638665	1.966044
H	2.147873	-5.148074	0.891289
O	1.716473	-6.034235	-0.562883
H	1.201396	-5.346814	-1.022511
H	1.173975	-6.825832	-0.581552
O	3.168276	4.571492	-0.410490
H	3.929223	4.553471	0.172895
H	2.771868	5.451190	-0.352526
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Energy=-3101.89830267			
Cl	-0.921766	-4.053260	-0.410194
Na	1.358598	-3.788588	0.761147
Cl	2.445457	3.404848	0.593841
Na	1.436884	1.315730	1.618408
Cl	1.417856	-1.233575	1.171820
Na	-0.542266	-1.466314	-0.843369
Cl	-0.190038	1.064388	-1.800978
Na	0.950698	3.365796	-1.479825
O	1.675624	-1.537751	-1.927537
H	1.557033	-0.794308	-2.530056
H	1.985670	-1.143045	-1.096896
O	-0.435416	4.620571	-0.245721
H	-1.315030	4.394890	0.098834
H	0.159483	4.653571	0.514944
O	2.170012	-4.232369	-1.326182
H	1.346774	-4.613428	-1.657228
H	2.227765	-3.380570	-1.786387
O	-2.779758	3.508221	0.798988
H	-3.096059	2.820429	0.161545
H	-3.553142	3.947204	1.159079
O	-3.141470	-3.055395	1.548321
H	-4.017706	-3.427986	1.430994

H	-2.539200	-3.599243	1.009276
O	-2.224478	-0.701731	0.548923
H	-2.643628	-1.466531	0.995893
H	-1.764938	-0.173979	1.218776
O	-3.266369	1.484119	-0.853538
H	-3.104418	0.645598	-0.383918
H	-2.590256	1.491781	-1.544240
O	-0.793591	1.601661	1.292080
H	-1.428403	2.311475	1.478327
H	-0.764170	1.556041	0.318663

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Energy=-3101.89597352

Cl	0.971160	-3.820242	-1.508027
Na	1.806619	-1.780302	-0.189452
Cl	-1.563928	3.389959	-0.550042
Na	-1.648485	2.018534	1.625764
Cl	-0.029465	-1.880045	1.880979
Na	-1.062476	-3.684044	0.270490
Cl	2.406538	2.524223	0.541732
Na	0.931344	4.133568	-0.759068
O	3.517557	-0.432802	0.388625
H	3.342553	0.524386	0.417198
H	4.385049	-0.558087	0.778595
O	-0.752831	-5.907169	-0.032381
H	-1.088708	-6.791521	-0.185330
H	-0.032831	-5.749778	-0.665508
O	-0.122747	5.805478	-1.815058
H	-1.016959	5.454183	-1.685704
H	-0.191294	6.613907	-2.325614
O	-1.903473	-2.478575	-1.457757
H	-1.134746	-2.679550	-2.012024
H	-2.174828	-1.578823	-1.690793
O	0.514772	0.175943	-0.448536
H	1.029012	0.985901	-0.276534
H	0.126332	-0.060648	0.410402
O	-2.505491	0.020573	1.150782
H	-2.523707	-0.060542	0.181611
H	-1.973342	-0.725229	1.469847
O	-2.002235	0.314989	-1.614061
H	-2.290156	1.224982	-1.760031
H	-1.051930	0.390549	-1.404294
O	0.240650	1.266076	2.530950
H	1.087621	1.621897	2.217442
H	0.369672	0.318916	2.693713

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Energy=-3101.89299196

Cl	-0.394865	-3.829774	0.750432
Na	1.549401	-2.983191	-0.664505
Cl	2.931850	2.779724	-0.490657
Na	2.596066	0.309648	0.029565
Cl	-3.009397	0.511842	-0.425329
Na	-0.816209	1.621501	-1.267959
Cl	0.558984	-0.705650	-1.308934
Na	-1.793993	-1.761713	-0.376253

O	3.174258	-1.936592	0.591514
H	4.062495	-2.218465	0.824496
H	2.611925	-2.006431	1.429364
O	-3.918332	2.468636	1.856764
H	-4.302737	1.937556	2.556942
H	-3.746028	1.850606	1.121366
O	0.059557	2.543471	0.633906
H	-0.519503	3.165437	1.130032
H	0.889354	2.995522	0.391386
O	-2.707571	-3.638843	-1.269200
H	-2.255025	-4.304432	-0.733339
H	-3.548329	-4.004482	-1.549531
O	1.498889	-2.010146	2.527084
H	1.160868	-1.098282	2.510429
H	0.763840	-2.599234	2.287899
O	-1.696871	4.008865	2.047709
H	-1.946399	4.918388	1.873839
H	-2.530201	3.492137	2.060377
O	0.561184	2.898687	-2.496480
H	1.411008	2.955913	-2.014419
H	0.761303	3.069273	-3.418094
O	1.407369	0.683565	2.022936
H	1.858047	1.229480	2.674588
H	0.759483	1.294515	1.595826