Evaluating the preferential adsorption of N_2 from a binary mixture of N_2/O_2 on extra-framework cations of zeolites: A computational and experimental study

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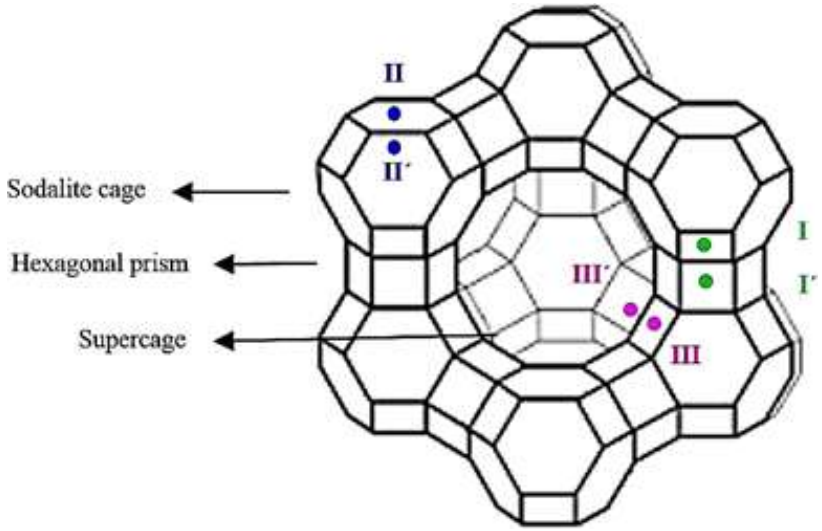
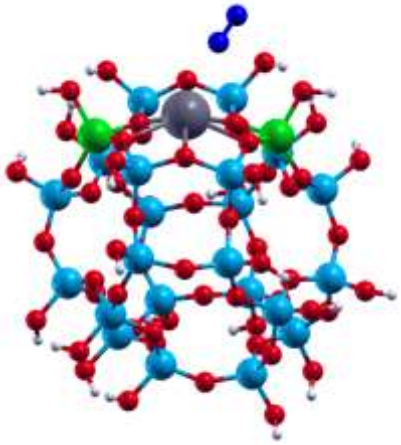
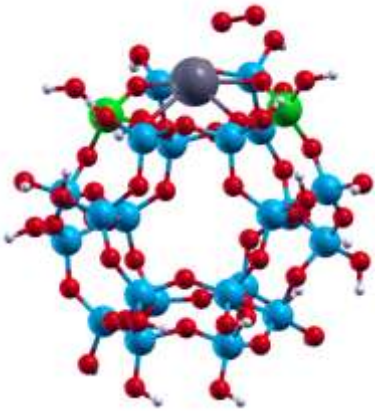


Figure S1. Possible coordination sites of the cation in an FAU zeolite.

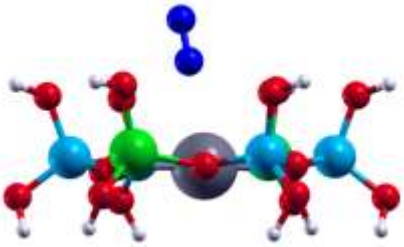
Figure S2. Three different possible configurations in which two silicon atoms can be replaced with aluminum atoms.



(a) Ca^{2+} - N_2 - cage



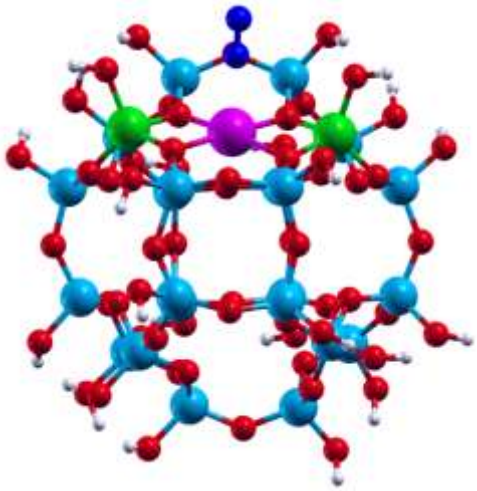
(b) Ca^{2+} - O_2 - cage



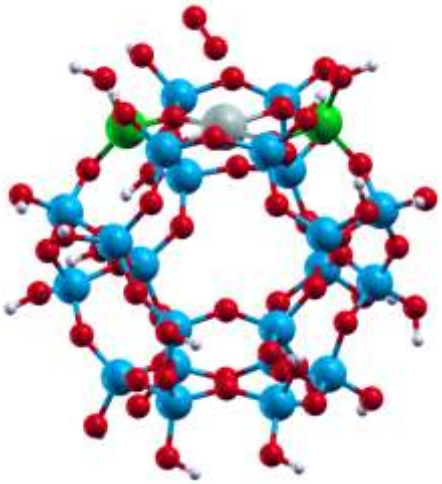
(c) Ca^{2+} - N_2 – A6

(d) Ca^{2+} - O_2 – A6

Figure S3. Optimized geometries of N_2 and O_2 molecules adsorbed on sodalite cage, and A6 cluster models exchanged with Ca^{2+}. The color code follows as silicon – light blue, oxygen – red, hydrogen – white, aluminum – green, nitrogen – dark blue, and calcium – grey.

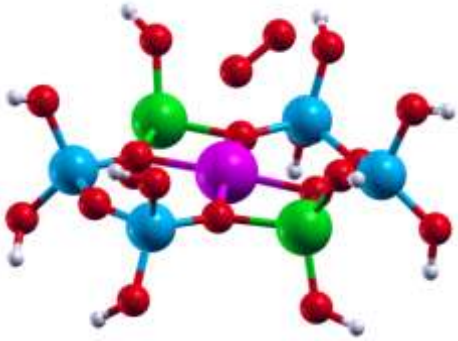


(a) Mg^{2+} - N_2 - cage



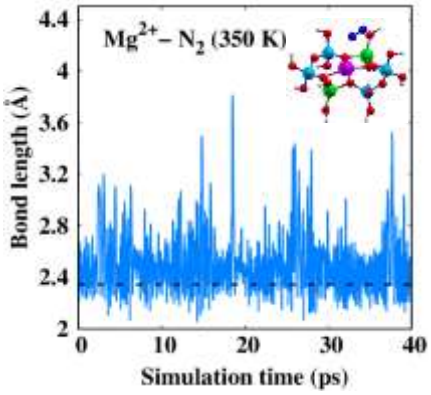
(b) Mg^{2+} - O_2 - cage

(c) Mg^{2+} - N_2 – A6

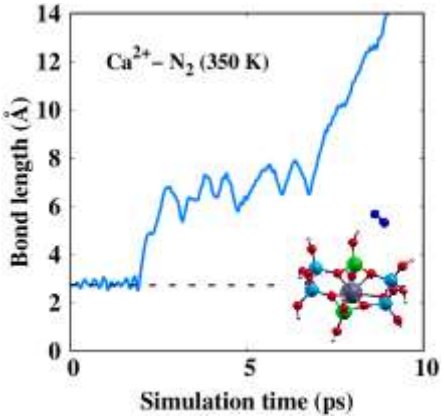


(d) Mg^{2+} - N_2 - cage

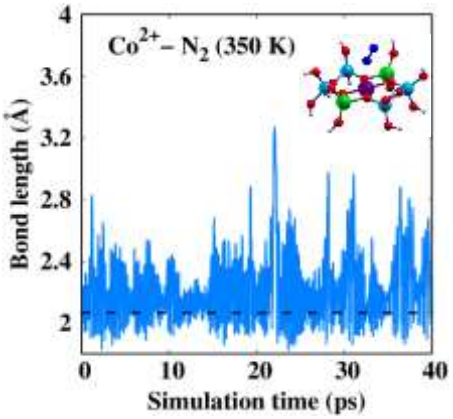
Figure S4. Optimized geometries of N_2 and O_2 molecules adsorbed on sodalite cage, and A6 cluster models exchanged with Mg^{2+}. The color code follows as silicon – light blue, oxygen – red, hydrogen – white, aluminum – green, nitrogen – dark blue, and magnesium – magenta.



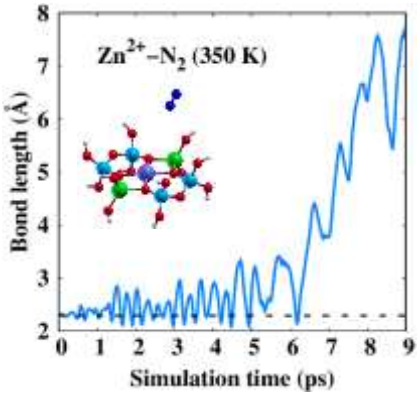
(a) Mg^{2+}- N_2 – 350 K



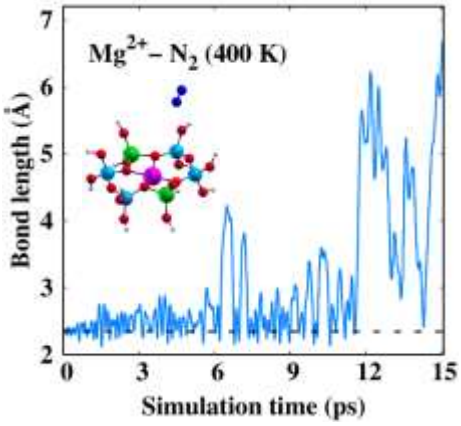
(b) Ca^{2+}- N_2 – 350 K



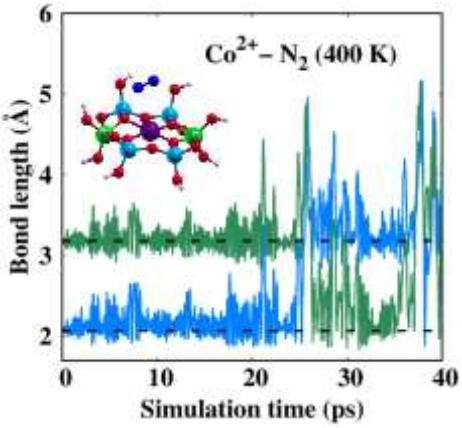
(c) Co^{2+}- N_2 – 350 K



(d) Zn^{2+}- N_2 – 350 K

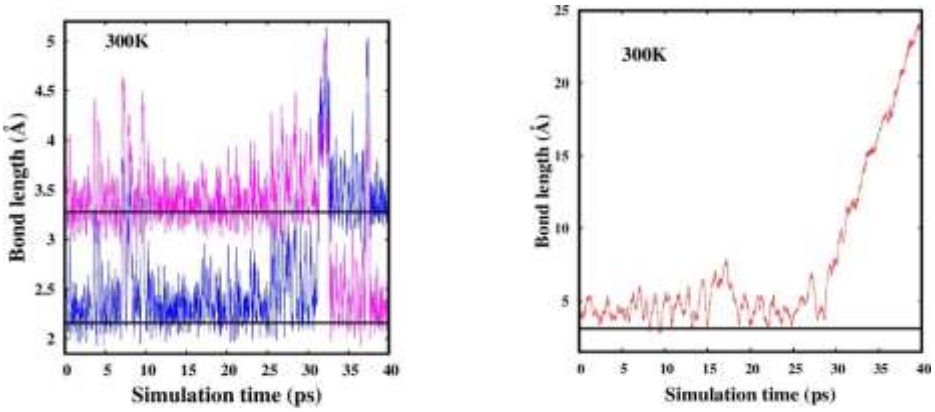


(e) Mg^{2+}- N_2 – 400 K



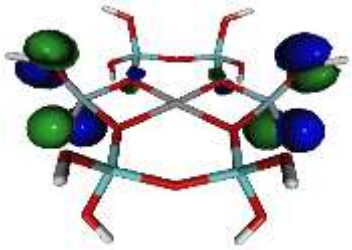
(f) Co^{2+}- N_2 – 400 K

Figure S5. Inter-atomic distances between the adsorbed N_2 molecule and the extra-framework cations for Mg^{2+}, Ca^{2+}, and Sr^{2+} at 350 K and 400 K as a function of time. The black line passing through graphs a, b, c, d and e is the optimized distance from the cation to one of the nitrogen atoms of the N_2 molecule. The black lines passing through graph f are the optimized distance from the Co^{2+} ion to both the nitrogen atoms of the N_2 molecule.

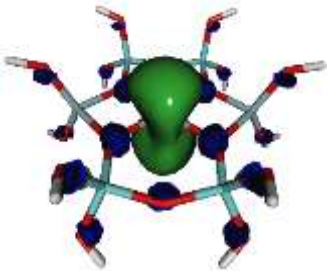


(a) N_2 (b) O_2

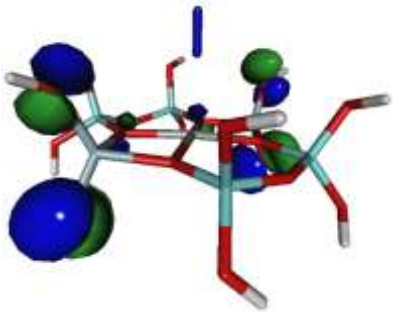
Figure S6. Inter-atomic distances between the adsorbed N_2 molecule and the extra-framework cations for Li^+ at 300 K as a function of time. The black lines passing through graph a are the optimized distance from the Li^+ ion to both the nitrogen atoms of the N_2 molecule.



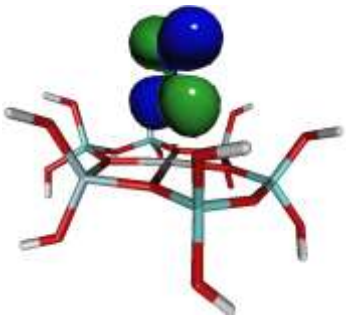
(a) Mg^{2+}- HOMO



(b) Mg^{2+}- LUMO



(c) Mg^{2+}- N_2 - HOMO



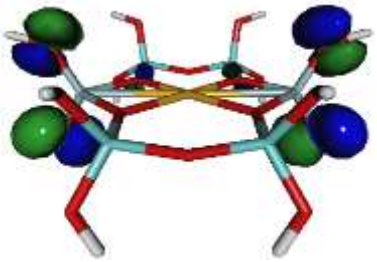
(d) Mg^{2+}- N_2 - LUMO

Figure S7.

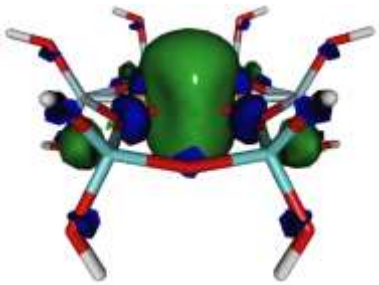
(a) Highest Occupied Molecular Orbital (HOMO) of Mg^{2+} exchanged A6 cluster model.

(b) Lowest Occupied Molecular Orbital (LUMO) of Mg^{2+} exchanged A6 cluster model.

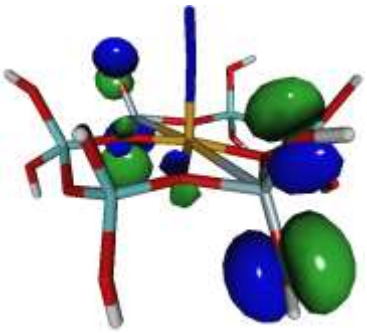
(c and d) HOMO and LUMO after adsorption of N_2 molecule on Mg^{2+} exchanged A6 cluster model.



(e) Zn^{2+}- HOMO



(f) Zn^{2+}- LUMO



(g) Zn^{2+} - N_2 - HOMO

(h) Zn^{2+} - N_2 - LUMO

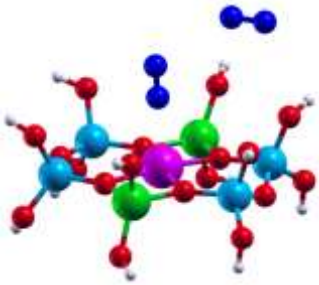
Figure S8.

(e and f) HOMO and LUMO of Zn^{2+} exchanged A6 cluster model.

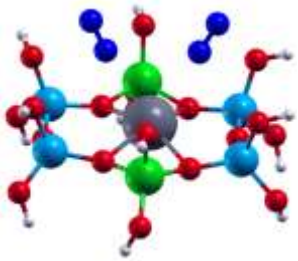
(g and h) HOMO and LUMO after adsorption of N_2 molecule on Zn^{2+} exchanged A6 cluster model.

Cations	Adsorption Energies (kJ/mol)		Löwdin Charges (e)	
	1^{st} N_2 molecule	2^{nd} N_2 molecule	1^{st} N_2 molecule	2^{nd} N_2 molecule
Mg^{2+}	-44.634	-12.340	0.289	0.011
Ca^{2+}	-44.896	-18.904	0.205	0.196
Co^{2+}	-42.796	-21.004	0.322	0.026
Zn^{2+}	-41.483	-12.340	0.272	0.010

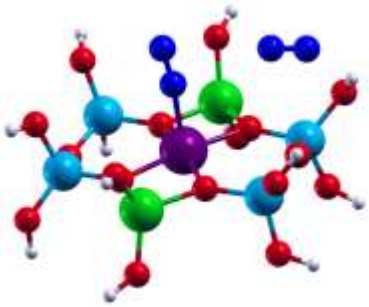
Table T1. Adsorption energies (in kJ/mol) and Löwdin charges (in e) of 1^{st} and 2^{nd} N_2 molecules adsorbed on Mg^{2+}, Ca^{2+}, Co^{2+}, and Zn^{2+} exchanged A6 cluster model.



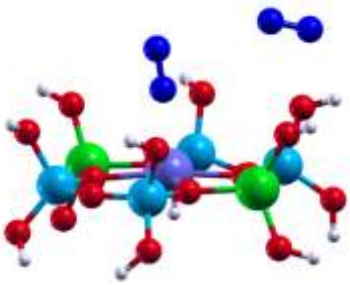
(a) Mg^{2+}- 2 N_2 molecule



(b) Ca^{2+}- 2 N_2 molecule



(c) Co^{2+}- 2 N_2 molecule



(d) Zn^{2+}- 2 N_2 molecule

Figure S9. Optimized geometries of 2 N_2 molecules adsorbed on Mg^{2+}, Ca^{2+}, $Co^{2+}$and Zn^{2+} exchanged A6 cluster model. The color code follows as silicon – light blue, oxygen – red, hydrogen – white, aluminum – green, nitrogen – dark blue, magnesium – magenta, calcium – grey, cobalt – purple, and zinc - violet.

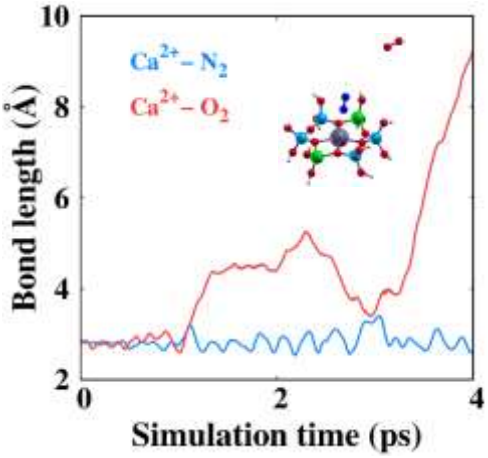


Figure S10. Inter-atomic distances between the adsorbed N_2 and O_2 molecules and the extra-framework cations for Ca^{2+} at 300 K as a function of time.

Optimized coordinates of N_2 molecule adsorbed on various cation in the sodalite cage.

1. **Mg^{2+}**

O	1.403067	4.061688	7.884554
O	7.922302	4.187677	0.862018
O	8.166550	4.469136	8.187322
O	1.808983	5.010436	1.174937
O	8.011202	0.689698	4.724890
O	0.716225	8.087409	4.849415
O	8.048323	8.022829	4.375725
O	0.850610	0.742632	4.306500
O	3.848282	7.481030	1.165720
O	3.934922	1.361076	7.890362
O	4.833470	8.073227	8.150260
O	5.035631	1.911388	1.437351
O	5.911587	0.091204	3.201418
O	5.906576	8.705969	2.946583
O	2.905042	0.034563	5.865867
O	3.012125	8.338930	6.219257
O	3.395387	1.057382	3.398403
O	3.022873	8.038884	3.510942
O	5.523153	0.708361	5.814332
O	5.657116	8.173775	5.592189
O	3.370520	5.795920	-0.818951
O	3.505699	5.696438	8.328263
O	5.953074	3.243008	-0.703159
O	5.727484	3.305515	8.385292
O	3.311461	3.171117	-0.183341
O	3.318300	3.324739	9.581057
O	5.683055	5.639906	0.556236
O	6.118736	5.928488	9.037169
O	0.874342	3.180226	5.421617
O	8.130902	3.059975	5.913265
O	0.971581	5.807247	3.459513
O	7.967192	5.636038	3.136675
O	0.422565	2.888583	2.776322
O	7.992872	2.906581	3.196130
O	0.378655	5.769166	6.117855
O	8.125356	5.783777	5.855902
Si	2.421188	4.539525	-0.295933
Si	2.447165	4.606194	9.013242
Si	6.727452	4.597827	-0.177720
Si	6.754806	4.405631	9.030697
Si	0.145073	2.242617	4.247432
Si	8.596672	2.213717	4.573774
Si	0.112225	6.551294	4.690814
Si	8.577040	6.488641	4.425541
Si	4.600937	0.624732	2.359704
Si	4.554005	8.732017	6.674139
Si	4.716101	2.303937	-0.138981
Si	4.537413	2.344846	9.050493

Si	4.568781	6.684598	-0.092803
Si	4.647157	6.673708	8.985969
Si	2.368558	0.147884	4.320176
Si	2.234144	8.722135	4.813629
Si	6.519419	-0.006005	4.729236
Si	6.618804	8.858048	4.404701
Si	0.390888	4.191966	6.615453
Si	8.498047	4.262320	2.390327
O	1.130082	4.300160	-1.289923
O	1.583458	5.306516	10.227169
O	7.317064	5.428019	-1.490520
O	7.054124	3.879459	10.579788
O	-1.470263	2.096499	4.549363
O	10.259214	2.199001	4.538582
O	-1.479085	6.576613	4.296588
O	10.240217	6.419269	4.273587
O	4.085378	-0.553035	1.299465
O	3.537204	10.366582	2.103815
O	4.646731	-1.210914	7.532341
O	4.723669	10.389165	6.777710
O	4.597569	0.982282	-1.104476
O	5.137038	1.445205	10.289429
O	5.249606	7.760298	-1.128357
O	4.104934	7.014423	10.524497
O	2.403069	-1.351057	3.576235
O	2.266785	10.365201	4.647740
O	6.644398	-1.590354	5.214177
O	6.958598	10.426511	4.792254
O	-1.145198	3.681220	7.010847
O	10.347104	4.492288	6.566127
O	-1.156325	5.256820	1.786859
O	10.164984	4.217456	2.382216
H	1.278739	3.680868	-2.027031
H	2.119506	5.930595	10.758651
H	7.762101	4.896237	-2.175157
H	7.605187	4.456621	11.138246
H	-1.725421	2.421739	5.439885
H	10.603122	2.628413	3.721709
H	-1.639788	6.208320	3.387351
H	10.670011	6.090123	5.094123
H	3.464191	-1.185380	1.724414
H	4.090828	11.089590	1.762038
H	5.293164	-1.751493	7.034194
H	3.931480	10.868515	6.458472
H	4.330921	0.180469	-0.600195
H	5.773829	1.937446	10.846003
H	6.037457	7.406880	-1.590776
H	4.555004	7.739382	10.994153
H	1.909924	-2.062830	4.023258
H	2.563484	10.635761	3.736594
H	7.202069	-2.173106	4.667882
H	6.403767	10.760001	5.530152

H	-1.661799	4.273508	7.587010
H	10.729663	3.660597	6.210602
H	-1.829821	4.685289	1.379328
H	10.542687	5.034102	2.787443
Al	0.389316	4.545371	2.253098
Al	4.266717	8.785742	2.385303
Mg	2.338775	6.643310	2.259420
Si	8.682453	4.438057	6.634219
Si	4.268685	0.206264	6.784823
N	-0.048336	8.696052	0.766435
N	0.725954	8.041529	1.231976

2. Ca^{2+}

O	0.873213	4.558009	8.177881
O	8.148833	4.548718	0.781766
O	7.967381	4.224929	8.097762
O	1.253687	4.835141	0.873668
O	7.972103	0.711818	4.369427
O	0.767390	8.279858	4.519464
O	8.155645	8.058879	4.541865
O	1.133893	0.879453	4.762955
O	4.165421	8.051128	0.809578
O	3.850353	1.140641	7.635539
O	4.626358	8.065487	8.099123
O	5.356369	1.612721	1.596752
O	5.848388	-0.445939	3.229820
O	6.069054	8.694908	3.004250
O	3.196888	-0.556052	5.697398
O	3.022625	8.316887	5.973635
O	3.498741	0.886349	3.417646
O	3.089045	8.315485	3.229693
O	5.691583	0.465919	5.795041
O	5.721194	8.177534	5.649446
O	3.215812	5.958635	-0.275221
O	3.326014	5.680144	8.369110
O	6.056194	3.318722	-0.364725
O	5.448160	3.241503	8.176720
O	3.648313	3.531465	0.810761
O	2.922024	3.126561	9.107248
O	5.836370	5.907235	0.447481
O	5.980917	5.853377	8.772519
O	0.930330	3.346949	5.773376
O	8.005423	3.021329	5.700010
O	0.867097	5.935209	3.270367
O	8.097056	5.742791	3.180547
O	0.713444	2.921910	3.092842
O	8.074942	3.018968	2.974270
O	0.579477	6.047741	5.994608
O	8.118184	5.736818	5.901038
Si	2.547751	4.418868	-0.041413
Si	2.246454	4.624305	9.070699

Si	6.838563	4.757687	-0.172780
Si	6.507434	4.290666	8.852049
Si	0.366332	2.331433	4.573203
Si	8.555825	2.237225	4.355447
Si	0.168356	6.727393	4.550172
Si	8.655687	6.513712	4.541636
Si	4.671017	0.343623	2.393108
Si	4.499099	8.724228	6.598431
Si	4.816453	2.470445	0.306376
Si	4.264432	2.236097	8.782762
Si	4.651239	6.859006	-0.202386
Si	4.538369	6.642622	8.907515
Si	2.444695	0.014169	4.349201
Si	2.315556	8.869669	4.586374
Si	6.651875	-0.221502	4.661518
Si	6.710013	8.869988	4.490167
Si	0.273921	4.563466	6.660778
Si	8.648463	4.438381	2.340677
O	2.165079	3.711820	-1.472802
O	1.837842	5.134130	10.581183
O	7.274584	5.332393	-1.668878
O	6.668801	3.803029	10.435997
O	-1.258664	2.086085	4.772182
O	10.220036	2.207621	4.432183
O	-1.471569	6.734556	4.349279
O	10.323563	6.418678	4.469644
O	4.012089	-0.629402	1.213405
O	3.958802	10.700173	2.239617
O	4.878672	-1.353211	7.653101
O	4.626486	10.382452	6.725886
O	4.176207	1.496830	-0.877266
O	4.807617	1.439808	10.116267
O	5.069295	7.428668	-1.683560
O	4.225595	6.976231	10.514149
O	2.049817	-1.282867	3.370436
O	2.379623	10.526427	4.594307
O	7.098435	-1.698694	5.264928
O	6.999842	10.450413	4.880001
O	-1.373952	4.289582	6.688490
O	10.238251	4.277970	6.607699
O	-1.428590	4.846615	2.237950
O	10.310978	4.361789	2.405500
H	2.619559	2.853564	-1.623424
H	2.477446	5.778388	10.951306
H	7.758439	4.717556	-2.249893
H	7.101544	4.433859	11.039328
H	-1.635962	2.644624	5.487470
H	10.625227	2.684693	3.672078
H	-1.719622	6.111199	3.610554
H	10.702088	6.018140	5.283152
H	3.268613	-1.168684	1.565264
H	4.608433	11.398799	2.049667

H	5.569939	-1.913047	7.249050
H	3.863790	10.840202	6.308628
H	3.963464	0.596625	-0.539093
H	5.406547	1.980819	10.670823
H	5.816214	6.942654	-2.093648
H	4.352027	7.905507	10.778183
H	1.499429	-1.975392	3.779354
H	2.828457	10.854449	3.765074
H	7.597868	-2.281319	4.664884
H	6.416162	10.771139	5.600816
H	-1.915410	5.090812	6.551561
H	10.602207	3.474471	6.173396
H	-2.050966	4.099873	2.181501
H	10.681998	5.140719	2.884526
Al	0.299463	4.452284	2.367687
Al	4.505159	9.014912	2.309950
Ca	1.953165	7.135105	1.534682
Si	8.573277	4.301127	6.579160
Si	4.415715	-0.083996	6.715565
N	-1.708133	8.155379	1.139257
N	-0.605211	7.979697	1.141843

3. Sr^{2+}

Si	2.030581	0.431288	3.764842
Si	-0.399637	2.178929	4.464538
Si	-2.187835	-0.455188	4.798155
Si	0.264198	-2.010575	3.511420
Si	4.672757	2.193887	-0.463687
Si	4.481137	0.500529	2.157310
Si	3.776051	-1.965666	0.358808
Si	3.836480	-0.230761	-2.119968
Si	-2.105097	4.436013	-0.182011
Si	-0.132332	3.889235	2.070728
Si	2.184117	3.988552	0.137974
Si	0.295474	4.638286	-2.149336
Si	-4.698299	-2.282970	0.145947
Si	-3.662965	1.878484	-0.012226
Si	-4.421093	-0.202618	-2.131570
Si	2.320311	-4.569726	0.331222
Si	-2.090496	-3.985667	-0.447810
Si	0.472888	-3.864298	-2.103033
Si	-0.146573	2.101626	-3.858651
Si	2.156979	0.353581	-4.683518
Si	0.394890	-2.193109	-4.542575
Si	-1.959948	-0.333050	-3.765825
O	1.150824	1.599007	4.514188
O	-1.457272	0.994630	4.905911
O	-1.097199	-1.686256	4.451712
O	0.978979	-0.622013	3.034028
O	5.060838	1.469042	0.963279
O	4.269202	-1.053816	1.633889

O	3.166680	-0.961802	-0.813188
O	4.750307	1.072291	-1.671319
O	-1.311766	4.685370	1.258270
O	0.981228	3.285200	1.005104
O	1.562380	4.874183	-1.112897
O	-1.126395	4.975492	-1.402372
O	-4.828658	-1.716024	1.685140
O	-3.316893	0.647837	0.998409
O	-4.221410	1.278928	-1.460883
O	-5.112974	-1.236230	-1.030267
O	1.218829	-5.271055	1.309951
O	-1.752620	-4.810045	0.935686
O	-0.741735	-3.332635	-1.103986
O	1.726436	-4.425453	-1.221248
O	1.132306	1.642814	-4.803657
O	1.367423	-1.012808	-5.154331
O	-1.153223	-1.629861	-4.368168
O	-0.868379	0.779151	-3.205758
O	3.012437	1.118568	2.640081
O	-0.792805	2.646934	2.929575
O	-3.331830	-0.680577	3.653062
O	-0.332632	-2.880502	2.273056
O	3.163258	2.829331	-0.471891
O	2.639364	-3.022296	0.892100
O	2.655141	0.276131	-3.124898
O	-2.350951	2.815717	-0.388367
O	0.394124	3.084117	-2.670899
O	-3.113668	-2.798930	0.112495
O	-2.949313	-0.857212	-2.559782
O	0.995902	-2.627242	-3.054229
O	3.007647	-0.371827	4.845232
O	-0.570954	3.385023	5.568627
O	-2.907475	-0.821979	6.247163
O	1.379008	-2.794892	4.471149
O	5.728088	3.436778	-0.729254
O	5.587728	0.532728	3.374083
O	5.031760	-2.864599	-0.271633
O	4.847241	-1.367252	-2.801314
O	-3.486846	5.318323	-0.233653
O	0.601324	4.886594	3.183936
O	2.952445	5.012300	1.201918
O	0.416263	5.600482	-3.491633
O	-5.559064	-3.703809	-0.033442
O	-5.575773	1.106015	2.622025
O	-4.797469	2.922019	0.629971
O	-5.447783	-0.145466	-3.415240
O	3.693853	-5.476058	0.301943
O	-0.966022	-5.106342	3.554670
O	-2.778809	-4.916892	-1.639411
O	-0.133315	-5.033941	-3.130790
O	-1.301229	2.815064	-4.824647
O	3.498049	0.551505	-5.628567

O	0.415113	-3.449383	-5.602073
O	-2.938601	0.370932	-4.918846
H	2.733133	-1.302922	5.001947
H	-0.134325	4.209053	5.265941
H	-2.458320	-0.447357	7.026626
H	1.088514	-3.664719	4.807200
H	6.650385	3.250593	-0.476317
H	5.225575	0.147558	4.198631
H	5.290554	-2.589518	-1.179781
H	5.310430	-1.093596	-3.614869
H	-4.238220	4.803033	0.144463
H	1.467416	5.236903	2.884889
H	3.725144	5.493353	0.852073
H	0.061989	6.500993	-3.375630
H	-6.467769	-3.590079	-0.368236
H	-6.190077	1.020832	3.367542
H	-5.287447	2.512595	1.390148
H	-4.973761	0.125285	-4.231892
H	4.467061	-4.937627	0.025268
H	-1.002238	-6.041771	3.820142
H	-3.703959	-5.187409	-1.484916
H	-1.043452	-5.326135	-2.909603
H	-1.081304	3.698782	-5.175205
H	3.382629	0.298182	-6.562281
H	0.186288	-4.291389	-5.151330
H	-2.636659	1.265508	-5.194867
Al	-4.305005	-0.056783	2.269682
Sr	-2.886338	-3.184695	2.859575
Al	-0.268112	-4.654364	1.948251
N	-4.764883	-3.252035	5.101582
N	-5.466817	-3.032283	5.942348

4. Co^{2+}

Si	1.891701	0.079135	3.712649
Si	-0.280919	2.146977	4.457968
Si	-2.146103	-0.296219	4.881299
Si	-0.089121	-2.170709	3.910329
Si	4.753878	2.333312	-0.273487
Si	4.386027	0.312719	2.078413
Si	3.740344	-1.868399	-0.049928
Si	4.197274	0.114726	-2.263953
Si	-2.164789	4.453630	-0.427152
Si	-0.239083	3.722652	1.923734
Si	2.169849	3.978542	0.121258
Si	0.385371	4.757505	-2.193807
Si	-4.710491	-2.326021	0.402381
Si	-3.730391	1.968373	-0.347230
Si	-4.346751	-0.439583	-2.149858
Si	2.061901	-4.330342	0.405983
Si	-2.298347	-4.414812	-0.062506
Si	0.081279	-3.938219	-1.928542

Si	-0.114674	2.187446	-3.881918
Si	2.313804	0.473675	-4.695534
Si	0.463503	-2.100772	-4.272064
Si	-1.901962	-0.210643	-3.756803
O	1.165729	1.348060	4.468547
O	-1.457851	1.169428	5.099052
O	-1.084365	-1.541990	5.087569
O	0.712949	-0.946715	3.160604
O	4.952866	1.557529	1.159995
O	4.447284	-1.093985	1.221283
O	3.300627	-0.730381	-1.177791
O	5.074270	1.306692	-1.526899
O	-1.529881	4.296342	1.097680
O	0.920606	3.206729	0.860297
O	1.621462	4.931988	-1.110700
O	-1.040856	5.094116	-1.448459
O	-4.471124	-1.391237	1.766275
O	-3.103239	0.931739	0.747169
O	-4.415098	1.100849	-1.586700
O	-4.854050	-1.508567	-0.980311
O	1.086264	-4.704683	1.633445
O	-1.746181	-5.250110	1.201301
O	-1.206318	-3.571316	-0.943273
O	1.291405	-4.594314	-1.057143
O	1.130023	1.620060	-4.803812
O	1.656690	-1.026506	-4.606405
O	-1.015374	-1.382168	-4.487291
O	-0.895384	0.947547	-3.138455
O	2.806474	0.653690	2.477831
O	-0.734425	2.487186	2.896420
O	-2.672261	-0.499312	3.307973
O	-1.042194	-2.971674	2.782230
O	3.221143	2.884189	-0.486089
O	2.437339	-2.701940	0.476170
O	3.230151	0.821941	-3.377542
O	-2.583621	2.958206	-1.009001
O	0.471698	3.219213	-2.759869
O	-3.283116	-3.203699	0.635394
O	-2.797780	-0.876370	-2.542135
O	0.602638	-2.578846	-2.691425
O	2.905516	-0.724889	4.762572
O	-0.213010	3.484391	5.403339
O	-3.462080	-0.447191	5.862260
O	1.000776	-3.186676	4.599687
O	5.749506	3.653414	-0.292665
O	5.352703	0.229995	3.403791
O	4.810360	-2.954296	-0.717160
O	5.246470	-1.001992	-2.918962
O	-3.438464	5.490478	-0.389977
O	0.402613	4.886117	2.934570
O	2.841743	4.949059	1.297789
O	0.561885	5.771472	-3.485354

O	-5.976717	-3.354997	0.590945
O	-5.037033	1.448644	2.781007
O	-4.868355	2.982093	0.334255
O	-5.401977	-0.653757	-3.392444
O	3.423155	-5.256634	0.458511
O	-0.487292	-5.436468	3.969310
O	-3.184132	-5.312318	-1.138447
O	-0.422802	-4.986480	-3.128038
O	-1.250323	2.877336	-4.887482
O	3.318820	0.559986	-6.000983
O	0.636488	-3.354357	-5.320527
O	-2.987106	0.461403	-4.825041
H	2.635170	-1.643438	4.976790
H	0.083356	4.267914	4.887082
H	-3.405936	0.024334	6.713316
H	0.660823	-4.123973	4.663569
H	6.620227	3.512284	0.121800
H	4.906291	-0.220587	4.153150
H	5.253980	-2.623764	-1.528250
H	5.848634	-0.678920	-3.613893
H	-4.245057	5.029390	-0.069298
H	1.280414	5.219589	2.641232
H	3.680411	5.390182	1.065286
H	0.216033	6.671918	-3.347293
H	-6.677226	-3.274179	-0.081991
H	-5.574154	1.281429	3.572641
H	-5.174482	2.679584	1.224009
H	-5.068722	-0.235928	-4.214845
H	4.160721	-4.860198	-0.053559
H	-0.134192	-6.338509	4.061052
H	-3.686613	-6.046089	-0.737473
H	-1.253869	-5.463867	-2.941057
H	-0.955995	3.655276	-5.396769
H	2.994478	0.102379	-6.797370
H	0.235038	-4.179102	-4.969350
H	-2.718814	1.353073	-5.140105
Al	-3.854434	0.314868	2.186234
Co	-2.826290	-2.254348	2.389750
Al	-0.496627	-4.723296	2.349993
N	-4.081726	-4.103420	4.575961
N	-3.685058	-3.440456	3.764040

5. Ni^{2+}

O	0.784076	4.705246	8.318819
O	8.026789	4.207823	0.725063
O	7.963320	4.350372	8.058613
O	2.324444	4.896025	1.539043
O	8.135345	0.634833	4.475261
O	0.629510	8.204789	4.726211
O	7.904297	7.973216	4.361285
O	1.187506	0.865626	5.034031

O	3.926640	7.364088	1.347382
O	3.951239	1.149248	7.627379
O	4.607690	8.122081	8.131283
O	4.915313	1.938343	1.455626
O	5.926980	0.072154	3.093286
O	5.834117	8.962721	3.007467
O	3.320091	-0.594021	5.713718
O	2.864479	8.565586	6.174265
O	3.434034	1.010778	3.517077
O	3.010620	8.083951	3.512789
O	5.780277	0.492270	5.781298
O	5.521063	8.243051	5.598321
O	3.392864	5.825577	-0.744900
O	3.260866	5.773888	8.406585
O	5.969309	3.174968	-0.685600
O	5.426218	3.350113	8.167168
O	3.299253	3.169193	-0.303615
O	2.850210	3.152823	8.901540
O	5.761024	5.597359	0.535584
O	5.955046	5.930804	8.784715
O	0.837302	3.355645	5.962746
O	8.089878	2.952043	5.778802
O	1.281136	5.812841	3.638537
O	7.953313	5.649023	3.007627
O	0.798739	2.855042	3.306795
O	8.058409	2.919900	3.054716
O	0.139892	5.982662	6.098250
O	7.967444	5.673975	5.736458
Si	2.497905	4.581350	-0.121255
Si	2.230640	4.660349	9.098455
Si	6.759409	4.549436	-0.255872
Si	6.512808	4.376796	8.830089
Si	0.375763	2.280227	4.774743
Si	8.644293	2.190135	4.419224
Si	0.152550	6.633280	4.595794
Si	8.469576	6.454563	4.363757
Si	4.554920	0.622066	2.368078
Si	4.424676	8.834347	6.666078
Si	4.685184	2.281517	-0.150880
Si	4.254389	2.311236	8.738405
Si	4.608321	6.651399	0.006767
Si	4.503015	6.700271	8.938443
Si	2.474896	0.048473	4.455882
Si	2.138368	8.854857	4.722134
Si	6.671898	-0.120778	4.550503
Si	6.557745	8.921432	4.467205
Si	0.091678	4.510079	6.853506
Si	8.550275	4.293586	2.272135
O	1.017809	4.480788	-0.806325
O	1.970623	5.017276	10.682069
O	7.258865	5.349904	-1.619684
O	6.724874	3.857420	10.398643

O	-1.248255	2.002248	4.865377
O	10.305834	2.271147	4.451278
O	-1.329204	6.473894	3.905826
O	10.139205	6.431683	4.289514
O	3.952494	-0.534600	1.330681
O	3.407556	10.327415	1.891366
O	5.022503	-1.314510	7.683043
O	4.705416	10.472224	6.810934
O	4.606186	0.930420	-1.075023
O	4.741051	1.617625	10.148149
O	5.220318	7.861774	-0.917870
O	4.158557	6.996959	10.542413
O	2.027927	-1.195419	3.433456
O	2.178321	10.469867	4.426388
O	6.885364	-1.727695	4.895957
O	7.062284	10.403767	4.985700
O	-1.482538	3.992058	7.012025
O	10.212448	4.464501	6.550259
O	-0.553608	4.815153	1.560001
O	10.216875	4.302457	2.315977
H	0.278752	4.711713	-0.186959
H	2.552376	5.729739	11.022078
H	7.512219	4.791862	-2.377156
H	7.508094	4.193198	10.870337
H	-1.683393	2.464915	5.613819
H	10.659953	2.717856	3.647913
H	-1.304992	6.222053	2.952700
H	10.544192	6.112557	5.126055
H	3.231678	-1.066646	1.737753
H	3.918043	11.052671	1.492373
H	5.590147	-1.965639	7.227567
H	3.914617	11.027304	6.670799
H	4.257751	0.158161	-0.575092
H	5.404266	2.145915	10.638634
H	6.013637	7.609733	-1.431146
H	4.785522	7.558539	11.032451
H	1.518357	-1.921855	3.836328
H	2.427905	10.683260	3.485826
H	7.323241	-2.262486	4.209467
H	6.441209	10.808467	5.628316
H	-2.115957	4.624124	7.397256
H	10.638526	3.673538	6.151308
H	-1.262876	4.144960	1.589024
H	10.554103	5.115986	2.760516
Al	0.876718	4.396679	2.538852
Al	4.230026	8.849459	2.368437
Ni	2.635570	6.534649	2.502889
Si	8.550846	4.347298	6.527544
Si	4.533004	-0.075073	6.719747
N	0.764975	8.561744	0.115035
N	0.558807	7.990004	1.055625

6. Cu^{2+}

Si	1.926436	0.085189	3.754947
Si	-0.260063	2.151925	4.465217
Si	-2.164511	-0.268173	4.860458
Si	-0.070106	-2.174826	3.930222
Si	4.764189	2.313253	-0.288824
Si	4.409111	0.325262	2.103488
Si	3.757854	-1.893431	0.020221
Si	4.135242	0.066133	-2.230518
Si	-2.157400	4.468487	-0.406730
Si	-0.210362	3.724356	1.924450
Si	2.188031	3.994986	0.105100
Si	0.377560	4.752655	-2.193762
Si	-4.737590	-2.296483	0.368898
Si	-3.759442	1.999772	-0.363904
Si	-4.391533	-0.396899	-2.166661
Si	2.089862	-4.366022	0.416800
Si	-2.271330	-4.351198	-0.110287
Si	0.131592	-3.907531	-1.932221
Si	-0.142202	2.183538	-3.871675
Si	2.277704	0.474874	-4.683294
Si	0.441496	-2.107190	-4.305926
Si	-1.930924	-0.220564	-3.754504
O	1.183292	1.347140	4.503490
O	-1.445173	1.180985	5.098760
O	-1.119337	-1.532293	5.049373
O	0.766496	-0.961158	3.205103
O	4.957066	1.554156	1.154491
O	4.467856	-1.100722	1.277715
O	3.279662	-0.771309	-1.106833
O	5.040563	1.258364	-1.529373
O	-1.512406	4.290359	1.111098
O	0.944816	3.220166	0.850597
O	1.634324	4.934201	-1.135626
O	-1.032287	5.109571	-1.427197
O	-4.507912	-1.390728	1.749701
O	-3.160543	0.945783	0.728189
O	-4.434298	1.152098	-1.622441
O	-4.928247	-1.441466	-0.989694
O	1.085853	-4.784484	1.608256
O	-1.776888	-5.185269	1.180521
O	-1.131234	-3.505781	-0.927386
O	1.352062	-4.560625	-1.072756
O	1.104670	1.631450	-4.801365
O	1.607093	-1.022460	-4.702219
O	-1.054725	-1.411402	-4.464639
O	-0.913902	0.931045	-3.140176
O	2.833132	0.664967	2.516693
O	-0.688673	2.481598	2.895218
O	-2.712842	-0.432212	3.294428

O	-0.981403	-2.974868	2.771368
O	3.246168	2.904307	-0.494011
O	2.476398	-2.745886	0.570898
O	3.121912	0.766686	-3.305881
O	-2.593561	2.983513	-1.001279
O	0.440935	3.206039	-2.739133
O	-3.293050	-3.148148	0.527964
O	-2.845977	-0.864890	-2.542478
O	0.657755	-2.568140	-2.727833
O	2.953110	-0.698078	4.808067
O	-0.198813	3.496204	5.401266
O	-3.466783	-0.409683	5.861076
O	0.977731	-3.202648	4.665574
O	5.797930	3.601571	-0.342952
O	5.392625	0.274207	3.418411
O	4.835238	-2.965549	-0.658096
O	5.157871	-1.053840	-2.920307
O	-3.422198	5.515166	-0.350954
O	0.429789	4.889861	2.933780
O	2.851284	4.979334	1.275463
O	0.537441	5.746777	-3.503417
O	-5.982614	-3.355862	0.544461
O	-5.124017	1.439935	2.739043
O	-4.893974	3.021658	0.312566
O	-5.437737	-0.603426	-3.418280
O	3.442223	-5.305694	0.459011
O	-0.511277	-5.453092	3.944354
O	-3.081148	-5.264830	-1.235256
O	-0.415900	-4.971402	-3.098411
O	-1.281633	2.879711	-4.868127
O	3.349568	0.602960	-5.931449
O	0.585777	-3.368644	-5.349026
O	-2.998216	0.456736	-4.837830
H	2.687380	-1.610612	5.047007
H	0.103045	4.276115	4.882588
H	-3.389321	0.057969	6.712603
H	0.626351	-4.136702	4.698606
H	6.668281	3.442260	0.065466
H	4.963707	-0.175294	4.178090
H	5.240164	-2.643320	-1.492522
H	5.730040	-0.734415	-3.641939
H	-4.235184	5.053513	-0.047068
H	1.302256	5.231395	2.633929
H	3.671018	5.448618	1.031978
H	0.200411	6.651653	-3.372470
H	-6.692694	-3.266105	-0.117319
H	-5.661344	1.269198	3.530122
H	-5.226011	2.707466	1.188221
H	-5.086847	-0.200841	-4.241071
H	4.188675	-4.897013	-0.029993
H	-0.143563	-6.349443	4.035977
H	-3.578741	-6.018163	-0.865523

H	-1.274159	-5.393027	-2.893289
H	-0.995991	3.674316	-5.356339
H	3.066036	0.172582	-6.758111
H	0.197973	-4.190538	-4.976437
H	-2.726745	1.350939	-5.143190
Al	-3.917257	0.318869	2.161391
Cu	-2.740331	-2.219587	2.331859
Al	-0.495645	-4.733074	2.327638
N	-3.994904	-4.564549	4.668926
N	-3.719722	-3.808865	3.893561

7. Zn^{2+}

O	1.408175	4.059323	7.883399
O	7.904084	4.211174	0.866949
O	8.168510	4.466945	8.190672
O	1.795201	5.015498	1.177354
O	8.008210	0.699006	4.722109
O	0.712748	8.084556	4.846880
O	8.048541	8.033433	4.382231
O	0.848132	0.740794	4.311559
O	3.812953	7.510310	1.141800
O	3.936459	1.358192	7.894837
O	4.843570	8.064814	8.148351
O	5.029840	1.914992	1.438638
O	5.908320	0.094631	3.200981
O	5.904398	8.671148	2.932662
O	2.904345	0.035739	5.868934
O	3.011211	8.304992	6.221313
O	3.390582	1.056778	3.399243
O	3.024565	8.021927	3.512303
O	5.521794	0.711553	5.814591
O	5.652626	8.168260	5.585409
O	3.345098	5.802772	-0.826603
O	3.510349	5.692983	8.332681
O	5.941212	3.256241	-0.698611
O	5.730228	3.301166	8.392337
O	3.301417	3.179250	-0.175467
O	3.319003	3.321754	9.584739
O	5.653146	5.651077	0.560173
O	6.121915	5.922538	9.050272
O	0.869646	3.181555	5.420896
O	8.126605	3.070749	5.909148
O	0.973899	5.795709	3.470671
O	7.961352	5.645518	3.148482
O	0.420383	2.883716	2.776049
O	7.986116	2.915143	3.192371
O	0.373949	5.768671	6.122913
O	8.128759	5.795682	5.867048
Si	2.408741	4.544589	-0.294683
Si	2.449882	4.603480	9.014694
Si	6.706390	4.615605	-0.170905

Si	6.758914	4.400129	9.037365
Si	0.142750	2.240397	4.248595
Si	8.591431	2.223733	4.569931
Si	0.109773	6.549328	4.695385
Si	8.576404	6.498211	4.434181
Si	4.596711	0.627521	2.360275
Si	4.550398	8.717647	6.672699
Si	4.707141	2.313081	-0.134963
Si	4.538484	2.341403	9.055591
Si	4.540656	6.690195	-0.098820
Si	4.651836	6.669654	8.990548
Si	2.366769	0.147057	4.323506
Si	2.235399	8.702413	4.819582
Si	6.518210	-0.000359	4.728083
Si	6.607854	8.850277	4.392536
Si	0.390712	4.190098	6.618819
Si	8.487217	4.275910	2.392699
O	1.112756	4.292058	-1.279152
O	1.582763	5.304304	10.226043
O	7.293026	5.449914	-1.482876
O	7.062722	3.870526	10.584410
O	-1.473308	2.096376	4.548675
O	10.254105	2.210248	4.533108
O	-1.478857	6.572451	4.293775
O	10.239125	6.428334	4.278106
O	4.083349	-0.549833	1.298268
O	3.548072	10.372153	2.140242
O	4.649669	-1.212570	7.529346
O	4.699530	10.376426	6.774466
O	4.586832	0.994457	-1.104644
O	5.135658	1.441250	10.295333
O	5.227892	7.760709	-1.135864
O	4.105120	7.017215	10.525809
O	2.401907	-1.352370	3.580807
O	2.288932	10.345595	4.661277
O	6.647610	-1.584437	5.213131
O	6.917531	10.430761	4.757813
O	-1.143155	3.677008	7.018944
O	10.347216	4.493808	6.566263
O	-1.161617	5.253254	1.800947
O	10.154244	4.230532	2.376873
H	1.252438	3.645532	-1.994499
H	2.116553	5.929964	10.757874
H	7.743498	4.921342	-2.166482
H	7.617522	4.445438	11.141508
H	-1.728136	2.414883	5.441592
H	10.596742	2.640254	3.716036
H	-1.637333	6.200439	3.384831
H	10.670156	6.093802	5.095823
H	3.464252	-1.184708	1.722221
H	4.112723	11.095037	1.816341
H	5.297772	-1.750113	7.029999

H	3.913347	10.842368	6.420192
H	4.326761	0.189908	-0.601323
H	5.775024	1.931405	10.850746
H	6.023787	7.406267	-1.584110
H	4.560472	7.737233	10.997967
H	1.913064	-2.065032	4.031115
H	2.590254	10.619233	3.750933
H	7.205314	-2.166204	4.665828
H	6.382728	10.754320	5.514527
H	-1.654278	4.260826	7.608470
H	10.726838	3.662486	6.206607
H	-1.835632	4.678582	1.398568
H	10.534423	5.046114	2.781656
Al	0.387207	4.543015	2.261124
Al	4.260782	8.776352	2.385180
Zn	2.293723	6.672628	2.238709
Si	8.682516	4.443563	6.636751
Si	4.269405	0.206329	6.786029
N	-0.085783	8.683080	0.751705
N	0.695012	8.041097	1.224974

8. Cu^{+}

O	0.916674	4.600492	8.301550
O	7.925793	4.364589	0.885832
O	7.927908	4.293341	8.220742
O	1.358498	4.947435	0.922345
O	8.135269	0.664501	4.612073
O	0.767617	8.313011	4.733991
O	7.791154	7.994275	4.480732
O	1.220593	0.852292	4.833586
O	3.691809	7.530548	1.238171
O	3.933452	1.017346	7.718473
O	5.163659	7.367215	7.417836
O	5.198243	1.769223	1.529330
O	6.037284	-0.163132	3.182609
O	5.389281	8.190105	3.245509
O	3.272558	-0.628766	5.735058
O	3.305782	8.295828	5.701912
O	3.575109	0.879785	3.498652
O	2.786242	9.018725	3.153707
O	5.752063	0.424518	5.837437
O	5.793504	9.313969	5.685197
O	3.275189	5.769740	-0.692519
O	3.408404	5.550554	8.311695
O	5.915020	3.299591	-0.552316
O	5.519699	3.105331	8.359925
O	3.362731	3.241715	0.280984
O	2.923551	3.004656	9.102396
O	5.625021	5.731473	0.667257
O	5.901272	5.639761	9.329320
O	1.067356	3.249870	5.997131

O	8.001630	3.020723	5.856488
O	1.126120	6.066564	3.291690
O	7.866666	5.645107	3.239328
O	1.165687	3.038808	3.276518
O	8.035415	2.919329	3.136816
O	0.872651	5.974380	6.000556
O	7.877751	5.743827	5.966645
Si	2.375227	4.428674	-0.260422
Si	2.354407	4.539760	9.102627
Si	6.655598	4.692035	-0.097801
Si	6.547649	4.138231	9.105637
Si	0.604683	2.376175	4.654600
Si	8.599044	2.228530	4.533609
Si	0.356749	6.707790	4.612786
Si	8.384589	6.471943	4.572845
Si	4.726578	0.459831	2.398146
Si	4.599745	8.690647	6.642681
Si	4.715293	2.327993	0.047444
Si	4.287058	2.109448	8.884878
Si	4.448501	6.688862	0.001927
Si	4.645168	6.537761	8.754674
Si	2.527190	-0.018529	4.399040
Si	2.232021	9.047708	4.716800
Si	6.728934	-0.194675	4.678802
Si	6.476772	8.933126	4.234097
Si	0.412145	4.564715	6.742324
Si	8.475940	4.343146	2.422035
O	1.578116	3.858446	-1.584970
O	2.170925	4.993416	10.678009
O	7.162000	5.496470	-1.462745
O	6.892555	3.481541	10.591977
O	-1.058531	2.279009	4.623602
O	10.260178	2.343669	4.598198
O	-1.283245	6.539701	4.480742
O	10.048453	6.522954	4.523412
O	4.121959	-0.647425	1.310419
O	4.603319	10.084520	1.450675
O	4.986083	-1.458385	7.652816
O	4.168708	9.783564	7.817819
O	4.493156	1.107965	-1.027228
O	4.735273	1.325394	10.259652
O	5.077673	7.772703	-1.058753
O	4.161795	7.583570	9.943261
O	2.118370	-1.291329	3.396649
O	2.121926	10.597868	5.295322
O	7.043592	-1.760098	5.127316
O	6.892835	10.328475	3.435239
O	-1.248452	4.428988	6.675500
O	10.132428	4.504858	6.645078
O	-1.172430	4.643157	2.517355
O	10.143285	4.386441	2.451388
H	0.801056	4.376313	-1.860629

H	2.162240	5.958003	10.826142
H	7.451197	4.928171	-2.200203
H	7.182277	4.111830	11.276359
H	-1.467789	2.724837	5.397893
H	10.622571	2.787883	3.798298
H	-1.486640	5.917758	3.714038
H	10.441805	6.081949	5.312605
H	3.385541	-1.176812	1.691121
H	5.428663	10.500673	1.776492
H	5.615899	-2.043261	7.187895
H	3.554127	10.479880	7.512013
H	4.228021	0.270673	-0.585742
H	5.411284	1.803190	10.782482
H	5.832544	7.408408	-1.566454
H	4.083848	8.511264	9.634948
H	1.549268	-1.980784	3.784021
H	1.459699	11.176125	4.875263
H	7.478543	-2.320400	4.459516
H	7.491438	10.942602	3.897716
H	-1.656736	5.186671	6.199635
H	10.553409	3.705488	6.254399
H	-1.609609	3.814536	2.800078
H	10.482493	5.215924	2.857138
Al	0.603312	4.494560	2.487740
Si	4.163818	8.741346	2.284511
Cu	1.442578	7.040838	1.516867
Si	8.468982	4.367826	6.684253
Si	4.496781	-0.171150	6.753130
N	0.246079	9.375865	0.123821
N	0.695882	8.480428	0.640902

9. Ag^+

Si	2.057421	0.169392	3.740492
Si	-0.259099	2.060349	4.480737
Si	-2.132741	-0.418326	4.673115
Si	0.193397	-2.192010	3.815364
Si	4.667549	2.159371	-0.539542
Si	4.464004	0.437537	2.036783
Si	3.785729	-2.044780	0.178335
Si	3.688241	-0.155485	-2.271052
Si	-2.178324	4.530773	-0.172032
Si	-0.112824	3.691976	1.988309
Si	2.133910	3.915878	-0.027960
Si	0.142299	4.722740	-2.174543
Si	-4.746610	-2.134750	0.371104
Si	-3.906724	0.156586	2.175007
Si	-3.782717	2.018266	-0.203449
Si	-4.549946	-0.300072	-2.166398
Si	2.087408	-4.492885	0.234872
Si	-0.431276	-4.692437	2.087837
Si	-2.215366	-3.886190	-0.181666

Si	0.182728	-3.615014	-2.039739
Si	-0.437610	2.237720	-3.949060
Si	2.023811	0.668115	-4.579144
Si	-2.209614	-0.274491	-3.993073
O	1.236370	1.344305	4.537014
O	-1.400003	1.010334	5.034374
O	-1.029946	-1.645198	4.780182
O	0.993824	-0.935727	3.120076
O	4.998755	1.557334	0.959292
O	4.416301	-1.055185	1.314459
O	3.191787	-1.186927	-1.097912
O	4.766806	0.927718	-1.641443
O	-1.418204	4.400227	1.292986
O	0.936793	3.171576	0.814864
O	1.527492	4.816226	-1.270215
O	-1.137549	5.209137	-1.258462
O	-4.863656	-1.078876	1.638514
O	-3.201935	0.947163	0.922063
O	-4.381800	1.202828	-1.487103
O	-5.105407	-1.359297	-1.029384
O	0.957482	-5.061328	1.282495
O	-1.723373	-4.850129	1.075900
O	-0.908528	-3.176714	-0.868666
O	1.477379	-4.355630	-1.290857
O	0.950615	1.906590	-4.790478
O	1.449894	-0.745842	-5.112621
O	-1.413161	-1.477528	-4.725844
O	-1.143615	0.869187	-3.408112
O	2.936353	0.853609	2.525698
O	-0.627348	2.427946	2.905123
O	-2.749139	-0.454644	3.155238
O	-0.427834	-3.151543	2.649780
O	3.164067	2.800791	-0.641120
O	2.590806	-2.996494	0.769010
O	2.434967	0.631069	-2.964922
O	-2.584570	3.017620	-0.720738
O	-0.028918	3.177565	-2.669892
O	-3.226216	-2.745292	0.404719
O	-3.088590	-0.850716	-2.709467
O	0.741173	-2.346127	-2.884489
O	3.151791	-0.585004	4.745242
O	-0.290443	3.372713	5.466905
O	-3.387805	-0.643630	5.722649
O	1.327059	-2.959452	4.765704
O	5.751554	3.357890	-0.870519
O	5.540804	0.410884	3.276869
O	4.974520	-3.112168	-0.325236
O	4.465906	-1.108637	-3.422533
O	-3.484156	5.518099	-0.046341
O	0.657564	4.747580	3.021659
O	2.869213	4.930567	1.074609
O	0.244706	5.688989	-3.513638

O	-5.787971	-3.407154	0.547690
O	-4.873656	1.288823	2.924879
O	-4.940104	2.995006	0.499630
O	-5.679515	-0.238998	-3.359345
O	3.344464	-5.559772	0.229998
O	-0.557897	-5.683189	3.405541
O	-2.912189	-4.835039	-1.357312
O	-0.505648	-4.716933	-3.085856
O	-1.537261	2.968303	-4.962326
O	3.477130	1.005201	-5.345527
O	0.897270	-3.405402	-5.485135
O	-3.323084	0.491115	-4.983910
H	2.849190	-1.465844	5.058753
H	0.135118	4.148588	5.041221
H	-3.220545	-0.334205	6.631269
H	1.029861	-3.779128	5.203690
H	6.655708	3.194939	-0.546650
H	5.150764	-0.002792	4.077421
H	5.874448	-2.742362	-0.379553
H	4.637097	-0.578118	-4.235200
H	-4.278999	5.015558	0.239637
H	1.500004	5.101214	2.659073
H	3.563546	5.517397	0.722538
H	-0.021091	6.615627	-3.372186
H	-6.693337	-3.233794	0.231478
H	-5.368663	0.980603	3.706571
H	-5.240400	2.674062	1.378856
H	-5.276152	0.089952	-4.193451
H	4.206998	-5.107637	0.121295
H	-0.346387	-6.620069	3.241866
H	-3.799689	-5.188276	-1.161690
H	-1.405584	-5.010324	-2.825088
H	-1.281865	3.847564	-5.299153
H	3.428917	0.957793	-6.318328
H	0.451703	-4.229541	-5.200265
H	-3.029272	1.373878	-5.294611
Al	0.267721	-1.973306	-4.596350
Ag	2.876799	-3.068887	-4.102987
N	4.909477	-5.494315	-2.673115
N	4.350307	-4.705932	-3.235134

10. Au^{+}

O	1.413040	3.880736	7.938285
O	7.561245	3.920990	1.465191
O	8.116987	4.509268	8.452195
O	0.763418	4.640885	0.604674
O	8.039219	0.972215	4.691893
O	1.012641	7.976115	4.652067
O	8.049615	8.083216	4.499752
O	0.775906	0.605667	4.243155
O	4.365462	8.029567	0.839427

O	4.021121	1.225215	7.911705
O	5.360894	7.321147	7.501391
O	4.527358	0.979365	0.745575
O	5.941809	0.934542	3.011578
O	5.704562	8.314359	3.170099
O	2.965496	0.225592	5.730866
O	3.586406	7.951904	5.569870
O	3.221885	0.779105	3.083252
O	2.983484	8.592622	2.996848
O	5.553816	1.021906	5.700025
O	5.947063	9.233089	5.715981
O	2.940827	5.993472	0.044416
O	3.612739	5.419069	8.208984
O	5.764250	3.106526	-0.300471
O	5.842728	3.076822	8.613557
O	3.211016	3.334757	0.468096
O	3.342130	3.153275	9.629042
O	5.516060	5.576602	0.838929
O	5.958581	5.659094	9.524645
O	0.977635	2.963878	5.485602
O	8.180614	3.294545	6.061782
O	0.940544	5.733667	3.187876
O	7.926057	5.589872	3.542720
O	0.247247	2.830535	2.872733
O	9.078867	3.143519	3.500207
O	1.071395	5.645530	5.937273
O	8.165700	6.009719	6.217350
Si	2.194924	4.482720	-0.125186
Si	2.521789	4.441176	9.001120
Si	6.553971	4.417569	0.277817
Si	6.756853	4.223469	9.338895
Si	0.108815	2.126351	4.329110
Si	8.894136	2.344325	4.924659
Si	0.447348	6.402162	4.608075
Si	8.590771	6.547458	4.711061
Si	4.582283	0.361565	2.253379
Si	4.742122	8.536457	6.601489
Si	4.320779	2.296491	-0.200286
Si	4.560372	2.147227	9.145290
Si	4.494440	6.593127	0.036179
Si	4.739302	6.472662	8.777953
Si	2.303179	0.040444	4.241896
Si	2.486660	8.674855	4.593584
Si	6.500057	0.432320	4.488861
Si	6.715565	8.999340	4.276947
Si	0.614188	4.165481	6.543518
Si	8.640161	4.440936	2.582242
O	2.054491	4.114118	-1.748884
O	1.763707	5.278101	10.201452
O	7.348083	5.187116	-0.970697
O	7.158858	3.640014	10.837504
O	-1.467096	1.971374	4.811586

O	10.396424	1.995035	5.550121
O	-1.205906	6.388104	4.718559
O	10.243915	6.528117	4.529329
O	4.739270	-1.298326	2.224544
O	4.575439	10.482743	1.966651
O	4.838153	-1.201616	7.094643
O	4.087956	9.625626	7.670651
O	3.856596	1.778570	-1.688019
O	5.028867	1.179256	10.390406
O	4.977836	6.851435	-1.512817
O	4.058410	7.484365	9.904835
O	2.324047	-1.569204	3.783477
O	2.434526	10.250427	5.125146
O	6.499000	-1.230232	4.572243
O	7.118738	10.472406	3.624051
O	-1.035869	4.160471	6.797657
O	10.351001	4.700206	6.893929
O	-1.602578	5.095854	2.338293
O	9.953954	5.043314	1.786439
H	1.269656	4.472953	-2.200270
H	2.252840	6.070972	10.501034
H	8.037517	4.673738	-1.429903
H	7.459082	4.303578	11.484685
H	-1.656711	2.493368	5.621517
H	10.962983	1.413320	5.011533
H	-1.592376	5.994076	3.876816
H	10.690497	6.108271	5.299260
H	3.903869	-1.750348	2.486479
H	5.445015	10.861948	2.214760
H	5.433544	-1.628841	6.441967
H	3.476232	10.263707	7.248560
H	3.233523	2.402318	-2.119624
H	5.638700	1.613483	11.018045
H	5.884531	6.518596	-1.695117
H	3.873812	8.383112	9.558767
H	1.876514	-2.188099	4.388798
H	1.995781	10.900020	4.546572
H	6.108759	-1.630992	3.760507
H	7.709588	11.039273	4.152350
H	-1.466131	4.944950	6.389922
H	10.785358	3.826256	6.787453
H	-2.324673	4.452287	2.226402
H	10.539485	5.563097	2.375068
Al	0.062428	4.446856	2.240943
Si	4.456284	8.863403	2.243292
Au	1.231645	7.386921	1.377764
Si	8.685926	4.606218	6.926969
Si	4.360140	0.300730	6.609600
N	-1.229802	9.603981	0.019691
N	-0.388425	8.975857	0.404762