NOTE: All coordinates are in Angstroms.

pH 7 Geometric Coordinates

H_2O	Atom	x-coord	y-coord	z-coord
	O	-0.675	0.557	0.017
	H	-0.956	1.217	0.675
	H	0.297	0.593	0.047

$NaOH•3H_2O$	Atom	x-coord	y-coord	z-coord
	Na	-0.179	-0.947	1.016
	O	-2.012	-0.353	-0.002
	H	-2.848	-0.507	0.477
	O	-1.972	2.233	-0.563
	H	-2.336	2.304	-1.465
	H	-2.007	1.227	-0.356
	O	1.651	-1.649	2.207
	H	2.105	-1.040	2.822
	H	1.618	-2.497	2.692
	O	-2.312	-1.510	-2.363
	H	-2.203	-1.085	-1.433
	H	-2.105	-2.453	-2.222

$Si(OH)_4$	Atom	x-coord	y-coord	z-coord
	Si	-1.462	0.579	1.253
	O	-0.546	-0.720	1.723
	O	-0.882	2.053	1.740
	O	-2.955	0.392	1.948
	O	-1.463	0.588	-0.405
	H	0.332	-0.793	1.303
	H	-3.387	-0.468	1.784
	H	-1.900	1.354	-0.825
	H	-0.898	2.221	2.701

$Si(OH)4•3H_2O$	Atom	x-coord	y-coord	z-coord
	Si	-1.506	0.474	1.315
	O	-0.596	-0.838	1.732
	O	-1.053	1.888	2.076
	O	-3.040	0.285	1.900
	O	-1.393	0.608	-0.336
	H	0.264	-1.004	1.238
	H	-3.523	-0.495	1.568
	H	-1.804	1.408	-0.717
	H	-0.184	2.244	1.808
	O	-1.389	2.629	4.884
	H	-1.318	2.374	3.935
	H	-2.241	3.103	4.935
	O	-1.422	-3.187	3.203
	H	-1.293	-2.976	4.148
	H	-1.145	-2.363	2.736
	O	1.761	-1.323	0.476
	H	2.368	-1.695	1.148
	H	1.638	-2.055	-0.162

$SiO(OH)_3^-•Na^+•3H_2O$	Atom	x-coord	y-coord	z-coord
	O	-1.206	0.301	-0.342
	H	-1.735	-0.519	-0.334
	Si	-1.355	1.184	-1.769

	O	-0.732	2.692	-1.369
	O	-0.297	0.594	-2.931
	O	-2.844	1.179	-2.372
	H	-1.192	3.127	-0.627
	H	0.624	0.502	-2.623
	O	-4.431	-0.700	-3.460
	H	-3.686	-0.141	-3.069
	H	-4.073	-1.052	-4.298
	O	-5.240	1.795	-1.324
	H	-5.504	1.182	-0.611
	H	-4.275	1.571	-1.521
	O	-3.993	2.525	-4.390
	H	-3.402	2.144	-3.664
	H	-4.003	3.489	-4.231
	Na	-5.771	1.236	-3.546

$SiO(OH)_3^-•Na^+•6H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-0.821	0.047	1.933
	O	-1.121	-0.524	3.487
	O	-0.309	1.556	1.822
	O	-2.301	-0.105	1.145
	O	0.243	-1.106	1.306
	H	-0.388	-0.395	4.118
	H	-2.627	-1.017	1.029
	H	0.642	-0.859	0.450
	O	-2.084	3.628	1.488
	H	-1.552	2.806	1.710
	H	-2.734	3.277	0.829
	O	-3.720	1.991	-0.227
	H	-4.637	1.990	0.112
	H	-3.298	1.214	0.218
	O	0.998	3.702	2.847
	H	0.694	3.956	3.739
	H	0.577	2.808	2.674
	O	-3.590	-0.832	4.929
	H	-3.943	0.064	5.091
	H	-2.761	-0.673	4.416
	O	0.640	2.839	-0.366
	H	0.357	2.210	0.368
	H	1.599	2.688	-0.474
	O	2.302	-2.476	2.791
	H	1.575	-2.026	2.299
	H	1.973	-3.387	2.912
	Na	-0.054	4.658	0.950

$SiO_2(OH)_2^{2-}•2Na^+•9H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	O	-3.224	1.026	-0.202
	Si	-1.779	1.495	0.384
	O	-0.504	1.166	-0.559
	O	-1.852	3.188	0.712
	O	-1.459	0.823	1.908
	H	-2.566	3.624	0.211
	H	-2.175	0.995	2.574
	Na	1.190	0.321	-3.016
	O	-0.822	-0.727	-2.446
	H	-0.820	-0.085	-1.661
	H	-1.718	-0.584	-2.827

	O	0.456	2.521	-2.631
	H	-0.249	2.872	-3.207
	H	-0.025	2.152	-1.813
	O	1.903	0.069	-0.775
	H	2.614	0.652	-0.448
	H	1.042	0.512	-0.478
	Na	-5.698	-0.304	-1.528
	O	-4.463	-1.308	0.201
	H	-3.894	-0.468	0.216
	H	-4.882	-1.350	1.082
	O	-5.739	1.832	-0.512
	H	-6.217	1.910	0.335
	H	-4.768	1.685	-0.256
	O	-3.664	0.166	-2.660
	H	-3.706	0.906	-3.296
	H	-3.366	0.587	-1.774
	O	0.568	2.166	3.458
	H	-0.026	1.621	2.882
	H	0.006	2.949	3.641
	O	-1.826	3.965	3.370
	H	-2.176	4.867	3.503
	H	-1.864	3.804	2.384
	O	-3.256	1.628	3.959
	H	-4.182	1.703	3.655
	H	-2.888	2.547	3.867

$(OH)_3SiOSi(OH)_3$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.237	0.330	1.098
	O	0.104	-0.424	1.707
	O	-1.277	1.971	1.338
	O	-2.544	-0.333	1.857
	O	-1.311	0.149	-0.542
	H	0.945	-0.225	1.252
	H	-2.532	-1.304	1.964
	H	-1.138	2.277	2.255
	Si	-1.306	1.105	-1.892
	O	-0.687	2.603	-1.539
	O	-0.400	0.441	-3.105
	O	-2.876	1.120	-2.410
	H	-0.842	2.884	-0.613
	H	-3.055	1.654	-3.207
	H	0.566	0.463	-2.966

$(OH)_3SiOSi(OH)_2O^-•Na^+•3H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.615	0.282	1.837
	O	-0.021	0.486	1.915
	O	-2.521	1.158	2.937
	O	-2.089	-1.315	2.035
	O	-2.256	0.826	0.385
	H	-1.395	-1.958	1.799
	H	-2.329	0.938	3.868
	Si	-1.776	1.317	-1.106
	O	-1.206	2.877	-0.883
	O	-0.662	0.335	-1.824
	O	-3.043	1.268	-2.173
	H	-0.919	3.317	-1.708
	H	0.179	0.189	-1.308

	H	-3.801	1.837	-1.943
	O	0.939	2.954	1.224
	H	0.474	2.135	1.576
	H	0.390	3.179	0.440
	O	2.475	0.555	3.015
	H	2.552	1.060	3.847
	H	1.492	0.459	2.859
	O	1.530	-0.030	-0.143
	H	0.899	0.005	0.663
	H	1.846	-0.954	-0.196
	Na	2.862	1.629	0.949

$(OH)_2O^-SiOSi(OH)_2O^-•2Na^+•6H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.820	0.053	1.798
	O	-0.268	0.263	2.180
	O	-2.923	0.668	2.903
	O	-2.226	-1.573	1.634
	O	-2.273	0.856	0.413
	H	-1.464	-2.142	1.421
	H	-2.839	0.277	3.792
	Si	-1.673	1.354	-1.056
	O	-0.974	2.857	-0.678
	O	-0.472	0.323	-1.598
	O	-2.823	1.460	-2.173
	H	-0.565	3.294	-1.450
	H	0.306	0.219	-0.993
	O	-4.064	-0.395	-3.660
	H	-3.469	0.149	-3.051
	H	-3.456	-0.844	-4.278
	O	0.635	2.825	1.732
	H	0.183	1.968	1.996
	H	0.205	3.013	0.863
	O	-5.355	2.341	-2.132
	H	-5.921	1.820	-1.531
	H	-4.412	2.031	-1.941
	O	2.021	0.395	3.639
	H	1.937	0.864	4.491
	H	1.081	0.266	3.319
	O	-3.013	2.697	-4.545
	H	-2.772	2.340	-3.630
	H	-3.001	3.669	-4.450
	O	1.591	-0.031	0.343
	H	0.843	-0.073	1.042
	H	1.945	-0.940	0.277
	Na	-5.090	1.604	-4.352
	Na	2.644	1.603	1.708

pH 11 Geometric Coordinates

H_2O	**Atom**	**x-coord**	**y-coord**	**z-coord**
	O	-0.678	0.554	0.014
	H	-0.954	1.218	0.676
	H	0.297	0.596	0.049

$NaOH•3H_2O$	Atom	x-coord	y-coord	z-coord
	Na	-0.318	0.045	-1.907
	O	-2.315	-0.536	0.117
	H	-2.986	-0.730	0.797
	O	-1.475	1.761	-0.769
	H	-2.166	2.232	-1.273
	H	-1.961	0.972	-0.317
	O	0.213	-1.148	0.065
	H	-0.779	-0.979	0.289
	H	0.715	-0.657	0.744
	O	-2.247	-1.221	-2.389
	H	-2.442	-1.088	-1.385
	H	-2.123	-2.183	-2.501

$Si(OH)_4$	Atom	x-coord	y-coord	z-coord
	Si	-1.462	0.579	1.253
	O	-0.546	-0.720	1.723
	O	-0.882	2.053	1.740
	O	-2.955	0.392	1.948
	O	-1.463	0.588	-0.405
	H	0.332	-0.793	1.303
	H	-3.387	-0.468	1.784
	H	-1.900	1.354	-0.824
	H	-0.898	2.221	2.701

$Si(OH)4•3H_2O$	Atom	x-coord	y-coord	z-coord
	Si	-1.506	0.474	1.315
	O	-0.597	-0.838	1.732
	O	-1.053	1.888	2.077
	O	-3.040	0.285	1.900
	O	-1.393	0.608	-0.336
	H	0.263	-1.004	1.238
	H	-3.522	-0.495	1.568
	H	-1.803	1.407	-0.719
	H	-0.184	2.243	1.809
	O	-1.389	2.629	4.885
	H	-1.319	2.373	3.936
	H	-2.241	3.103	4.935
	O	-1.423	-3.187	3.203
	H	-1.293	-2.976	4.148
	H	-1.145	-2.363	2.736
	O	1.762	-1.323	0.476
	H	2.368	-1.696	1.148
	H	1.637	-2.054	-0.162

$SiO(OH)_3^-•Na^+•3H_2O$	Atom	x-coord	y-coord	z-coord
	O	-1.206	0.302	-0.341
	H	-1.737	-0.517	-0.332
	Si	-1.355	1.184	-1.769
	O	-0.732	2.692	-1.371
	O	-0.297	0.593	-2.930
	O	-2.845	1.178	-2.372
	H	-1.192	3.128	-0.629
	H	0.624	0.503	-2.621
	O	-4.432	-0.699	-3.461
	H	-3.688	-0.141	-3.068
	H	-4.071	-1.052	-4.297

	O	-5.240	1.794	-1.324
	H	-5.502	1.181	-0.610
	H	-4.275	1.571	-1.522
	O	-3.994	2.525	-4.390
	H	-3.402	2.143	-3.665
	H	-4.001	3.488	-4.230
	Na	-5.772	1.237	-3.547

$SiO(OH)_3^-•Na^+•6H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.260	0.103	1.928
	O	-1.679	-0.346	3.474
	O	-0.471	1.494	1.775
	O	-2.687	0.139	1.053
	O	-0.351	-1.241	1.351
	H	-0.948	-0.678	4.065
	H	-3.013	-0.773	0.860
	H	0.146	-1.041	0.533
	O	-1.136	3.781	0.512
	H	-1.042	2.842	0.873
	H	-1.181	3.680	-0.460
	O	-2.784	-2.695	0.455
	H	-3.147	-3.272	1.157
	H	-1.852	-2.535	0.732
	O	0.270	3.380	3.553
	H	-0.485	3.765	4.042
	H	-0.110	2.590	3.054
	O	0.303	-1.407	5.136
	H	-0.164	-2.088	5.659
	H	0.812	-1.926	4.451
	O	1.908	2.318	0.819
	H	1.100	1.821	1.161
	H	2.660	1.967	1.334
	O	1.582	-2.568	2.958
	H	0.906	-2.191	2.335
	H	1.430	-3.533	2.927
	Na	0.921	4.349	1.503

$SiO_2(OH)_2^{2-}•2Na^+•6H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	O	-3.155	0.938	-0.592
	Si	-1.529	1.358	-0.301
	O	-0.706	-0.045	-0.311
	O	-1.035	2.362	-1.587
	O	-1.397	2.273	1.037
	H	-1.024	1.895	-2.443
	H	-3.750	1.709	-0.544
	Na	0.944	-2.633	-0.207
	O	-1.361	-2.550	0.266
	H	-1.310	-1.558	0.042
	H	-1.962	-2.931	-0.403
	O	0.842	-1.237	-2.104
	H	0.325	-1.556	-2.869
	H	0.194	-0.667	-1.564
	O	1.307	-0.811	1.238
	H	2.107	-0.273	1.089
	H	0.566	-0.337	0.725
	Na	-1.118	3.947	3.590
	O	-2.649	2.176	3.374

	H	-2.257	2.034	2.446
	H	-2.445	1.357	3.866
	O	0.687	2.806	2.581
	H	1.013	2.001	3.026
	H	0.001	2.473	1.903
	O	-1.851	4.837	1.539
	H	-1.240	5.421	1.051
	H	-1.699	3.908	1.151

$SiO_2(OH)_2^{2-}•2Na^+•9H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-0.578	-0.095	2.256
	O	0.607	0.706	3.138
	O	-1.230	0.823	1.085
	O	-1.614	-0.747	3.324
	O	0.321	-1.368	1.475
	H	1.312	1.136	2.590
	H	-0.146	-1.681	0.676
	O	-3.461	0.823	-0.367
	H	-2.675	0.633	0.247
	H	-3.517	0.049	-0.960
	O	-1.822	3.422	1.089
	H	-2.568	3.623	1.685
	H	-1.579	2.454	1.284
	O	2.760	1.760	1.589
	H	3.488	1.881	2.230
	H	2.938	0.867	1.179
	O	-0.281	1.568	-1.285
	H	-0.468	1.206	-0.352
	H	0.554	2.067	-1.204
	O	2.884	-0.797	0.489
	H	1.992	-1.056	0.851
	H	3.519	-1.346	0.989
	Na	-2.312	2.737	-1.107
	O	0.439	-3.934	2.890
	H	-0.466	-3.882	3.279
	H	0.506	-3.070	2.418
	O	-2.266	-3.238	3.787
	H	-1.975	-2.309	3.453
	H	-2.839	-3.600	3.083
	O	-1.403	-0.824	5.987
	H	-0.609	-1.309	6.285
	H	-1.290	-0.717	4.984
	O	-4.150	-0.411	4.043
	H	-3.216	-0.360	3.648
	H	-4.330	0.482	4.394
	Na	-3.354	-2.047	5.536

$SiO_3(OH)^{3-}•3Na^+•12H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	O	-3.184	0.966	-0.265
	Si	-1.778	1.444	0.454
	O	-0.501	1.233	-0.561
	O	-1.928	3.157	0.753
	O	-1.525	0.766	1.921
	H	-2.663	3.584	0.240
	Na	1.353	0.671	-2.896
	O	-0.662	-0.489	-2.581
	H	-0.720	0.085	-1.740

	H	-1.526	-0.302	-3.011
	O	0.455	2.809	-2.372
	H	-0.237	3.119	-2.988
	H	-0.047	2.273	-1.633
	O	1.954	0.293	-0.639
	H	2.600	0.910	-0.245
	H	1.037	0.670	-0.394
	Na	-5.595	0.064	-1.883
	O	-4.536	-1.314	-0.306
	H	-3.915	-0.530	-0.116
	H	-4.984	-1.498	0.542
	O	-5.488	2.049	-0.548
	H	-6.016	2.043	0.274
	H	-4.547	1.674	-0.286
	O	-3.476	0.522	-2.840
	H	-3.426	1.353	-3.352
	H	-3.214	0.777	-1.878
	Na	-0.992	0.207	4.854
	O	-1.677	-1.465	3.325
	H	-1.642	-0.736	2.613
	H	-0.999	-2.114	3.056
	O	0.619	1.136	3.408
	H	1.336	0.543	3.111
	H	-0.115	1.043	2.697
	O	-2.705	1.636	4.142
	H	-2.554	2.613	4.103
	H	-2.383	1.352	3.217
	O	-2.205	4.336	3.275
	H	-2.066	3.912	2.381
	H	-1.313	4.621	3.551
	O	0.231	4.797	-0.217
	H	0.465	4.268	-1.015
	H	-0.496	4.251	0.180
	O	-4.103	4.496	-0.537
	H	-4.708	3.711	-0.630
	H	-3.871	4.735	-1.456

$(OH)_3SiOSi(OH)_3$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.238	0.330	1.098
	O	0.104	-0.424	1.707
	O	-1.276	1.971	1.339
	O	-2.544	-0.333	1.857
	O	-1.311	0.150	-0.541
	H	0.945	-0.226	1.252
	H	-2.533	-1.303	1.963
	H	-1.137	2.277	2.256
	Si	-1.306	1.105	-1.892
	O	-0.687	2.603	-1.540
	O	-0.400	0.441	-3.104
	O	-2.876	1.119	-2.411
	H	-0.843	2.884	-0.614
	H	-3.055	1.653	-3.208
	H	0.566	0.464	-2.966

$(OH)_3SiOSi(OH)_2O^-•Na^+•3H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.616	0.260	1.835
	O	-0.023	0.466	1.929

	O	-2.533	1.131	2.930
	O	-2.094	-1.337	2.029
	O	-2.242	0.806	0.378
	H	-1.414	-1.984	1.766
	H	-2.351	0.907	3.861
	Si	-1.758	1.309	-1.107
	O	-1.199	2.873	-0.873
	O	-0.634	0.338	-1.824
	O	-3.019	1.258	-2.182
	H	-0.922	3.321	-1.696
	H	0.201	0.187	-1.299
	H	-3.781	1.822	-1.952
	O	0.923	2.945	1.248
	H	0.463	2.123	1.597
	H	0.374	3.169	0.464
	O	2.468	0.554	3.042
	H	2.539	1.065	3.871
	H	1.487	0.453	2.882
	O	1.541	-0.036	-0.122
	H	0.905	-0.003	0.681
	H	1.858	-0.959	-0.175
	Na	2.855	1.633	0.976

$(OH)_2O^-SiOSi(OH)_2O^-•2Na^+•6H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.816	0.044	1.792
	O	-0.264	0.257	2.172
	O	-2.919	0.640	2.905
	O	-2.214	-1.582	1.609
	O	-2.274	0.863	0.417
	H	-1.448	-2.147	1.396
	H	-2.844	0.227	3.785
	Si	-1.677	1.364	-1.051
	O	-0.975	2.865	-0.672
	O	-0.479	0.334	-1.600
	O	-2.829	1.474	-2.165
	H	-0.566	3.302	-1.443
	H	0.303	0.229	-0.999
	O	-4.053	-0.392	-3.652
	H	-3.464	0.158	-3.042
	H	-3.439	-0.837	-4.268
	O	0.633	2.824	1.740
	H	0.182	1.965	1.998
	H	0.203	3.017	0.872
	O	-5.367	2.339	-2.129
	H	-5.932	1.818	-1.528
	H	-4.423	2.036	-1.934
	O	2.022	0.385	3.635
	H	1.936	0.846	4.491
	H	1.083	0.256	3.313
	O	-3.020	2.710	-4.537
	H	-2.779	2.355	-3.621
	H	-3.013	3.682	-4.443
	O	1.596	-0.024	0.334
	H	0.848	-0.070	1.033
	H	1.952	-0.931	0.265
	Na	-5.089	1.600	-4.347
	Na	2.644	1.605	1.710

$(OH)_3SiOSi(OH)O_2^{2-}•2Na^+•6H_2O$	Atom	x-coord	y-coord	z-coord
	Si	-3.519	-0.197	-0.623
	O	-3.179	0.720	0.775
	Si	-1.908	0.752	1.807
	O	-0.697	-0.253	1.265
	O	-2.293	0.316	3.367
	O	-1.448	2.347	1.904
	O	-1.969	-0.609	-1.238
	O	-4.315	0.752	-1.670
	O	-4.252	-1.576	-0.207
	H	-0.860	-0.487	0.314
	H	-2.419	-0.641	3.506
	H	-1.622	0.061	-1.857
	H	-0.732	2.530	2.542
	Na	-6.430	-3.781	0.066
	Na	-6.137	2.156	-3.771
	O	-4.105	-4.203	0.215
	H	-3.737	-4.425	1.092
	H	-3.937	-3.212	0.104
	O	-6.801	0.273	-2.471
	H	-7.444	0.490	-1.768
	H	-5.882	0.365	-2.033
	O	-6.065	-2.587	-1.922
	H	-6.590	-1.812	-2.224
	H	-5.317	-2.145	-1.401
	O	-4.155	1.029	-4.325
	H	-3.387	1.570	-4.590
	H	-4.026	0.852	-3.336
	O	-6.256	-1.932	1.509
	H	-5.484	-1.617	0.928
	H	-6.939	-1.240	1.426
	O	-5.267	3.232	-1.860
	H	-4.778	2.375	-1.631
	H	-4.566	3.900	-1.984

$(OH)_2O^-SiOSi(OH)O_2^{2-}•3Na^+•9H_2O$	Atom	x-coord	y-coord	z-coord
	Si	-3.844	-1.268	-1.352
	O	-2.303	-0.941	-0.736
	Si	-1.441	-1.652	0.503
	O	-0.145	-2.477	0.021
	O	-2.536	-2.599	1.359
	O	-0.884	-0.420	1.513
	O	-3.665	-2.518	-2.488
	O	-4.396	0.087	-2.068
	O	-4.797	-1.881	-0.173
	H	-3.443	-2.463	0.971
	H	-3.078	-2.282	-3.229
	H	-1.598	0.122	1.897
	Na	-7.683	-2.195	1.312
	Na	-5.752	2.469	-3.493
	Na	2.381	-4.051	-0.890
	O	-6.291	-3.974	0.632
	H	-5.825	-4.509	1.302
	H	-5.596	-3.339	0.269
	O	-6.681	1.290	-1.638
	H	-6.672	1.798	-0.804

	H	-5.791	0.773	-1.656
	O	2.217	-1.705	-0.957
	H	2.738	-1.188	-0.313
	H	1.297	-1.795	-0.544
	O	-7.464	-1.437	-0.893
	H	-7.492	-0.479	-1.128
	H	-6.480	-1.597	-0.784
	O	-5.354	0.407	-4.537
	H	-4.651	0.367	-5.213
	H	-4.911	0.111	-3.673
	O	0.304	-4.196	-1.975
	H	-0.217	-5.017	-1.889
	H	-0.073	-3.569	-1.275
	O	-5.898	-0.869	2.060
	H	-5.371	-1.091	1.225
	H	-5.995	0.102	2.056
	O	-3.649	2.608	-2.434
	H	-3.727	1.617	-2.231
	H	-2.857	2.692	-3.000
	O	1.514	-4.136	1.299
	H	0.772	-3.525	0.977
	H	1.064	-4.953	1.586

$(OH)O_2^{2-}SiOSi(OH)O_2^{2-}•4Na^+•12H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Na	-0.869	-3.011	0.288
	O	-2.919	-1.864	0.000
	H	-2.310	-1.040	-0.094
	H	-3.390	-1.930	-0.865
	O	0.306	-1.776	-1.345
	H	0.025	-1.860	-2.276
	H	-0.183	-0.954	-0.991
	O	-0.306	-1.472	1.973
	H	0.639	-1.328	2.170
	H	-0.553	-0.739	1.309
	Na	0.472	4.045	3.472
	O	-1.819	3.984	2.967
	H	-1.571	3.354	2.205
	H	-2.430	3.474	3.532
	O	0.891	1.757	3.111
	H	0.443	1.111	3.691
	H	0.276	1.853	2.300
	O	0.932	4.589	1.232
	H	1.824	4.382	0.892
	H	0.360	3.780	0.989
	O	-2.890	2.093	-0.400
	Si	-4.439	1.524	-0.127
	O	-4.961	0.710	-1.462
	O	-4.413	0.450	1.185
	O	-5.431	2.756	0.247
	H	-4.002	-0.408	0.932
	Si	-1.288	1.660	-0.146
	O	-1.125	0.035	-0.050
	O	-0.464	2.243	-1.520
	O	-0.670	2.487	1.114
	H	-0.720	1.771	-2.334
	Na	-6.417	-0.728	-3.616
	O	-5.904	1.609	-3.716

	H	-5.417	1.399	-2.834
	H	-5.206	1.889	-4.341
	O	-4.350	-1.509	-2.610
	H	-3.592	-1.407	-3.218
	H	-4.436	-0.603	-2.114
	O	-7.399	-0.285	-1.503
	H	-7.499	-1.052	-0.905
	H	-6.462	0.091	-1.312
	Na	-8.126	4.245	-0.485
	O	-6.335	4.030	-1.975
	H	-5.872	3.542	-1.215
	H	-6.360	3.355	-2.692
	O	-8.034	2.033	0.286
	H	-8.095	1.278	-0.344
	H	-7.031	2.192	0.343
	O	-6.596	4.967	1.174
	H	-6.861	4.889	2.110
	H	-6.020	4.157	0.996

$Al(OH)_4^-•Na^+$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	O	-1.698	-0.204	0.471
	H	-1.454	0.183	1.330
	Al	-1.274	0.789	-0.938
	O	-1.441	2.500	-0.493
	O	0.299	0.382	-1.720
	O	-2.234	0.256	-2.365
	H	-1.083	3.134	-1.141
	H	1.109	0.433	-1.187
	H	-3.195	0.393	-2.353
	Na	-0.522	-0.407	-3.663

$(OH)_3SiOAl(OH)_3^-•Na^+$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.182	-0.550	1.898
	O	0.445	-0.646	1.530
	O	-1.466	0.303	3.304
	O	-1.720	-2.096	2.237
	O	-1.991	0.202	0.708
	H	-1.429	-2.769	1.592
	H	-1.120	-0.118	4.113
	H	0.647	-0.087	0.731
	Al	-1.453	0.928	-0.822
	O	-2.188	2.522	-0.955
	O	0.369	0.904	-0.826
	O	-1.614	-0.150	-2.240
	H	-2.129	2.947	-1.829
	H	0.817	1.751	-0.654
	H	-2.492	-0.476	-2.497
	Na	0.575	-0.341	-2.757

$(OH)_2O^-SiOAl(OH)_3^-•2Na^+•3H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Si	-1.216	-0.458	1.931
	O	0.086	0.406	2.367
	O	-2.515	-0.325	3.002
	O	-0.858	-2.116	1.918
	O	-1.860	-0.020	0.491
	H	0.099	-2.289	1.856
	H	-2.300	-0.641	3.899

	Al	-1.359	0.818	-0.978
	O	-1.493	2.577	-0.666
	O	0.271	0.354	-1.571
	O	-2.217	0.250	-2.444
	H	-1.167	3.140	-1.391
	H	1.010	0.449	-0.932
	H	-3.176	0.382	-2.518
	O	-0.176	3.080	1.742
	H	-0.234	2.124	2.041
	H	-0.615	3.039	0.845
	O	1.897	1.567	3.976
	H	1.504	2.009	4.753
	H	1.144	1.034	3.571
	O	2.104	0.784	0.708
	H	1.337	0.487	1.321
	H	2.808	0.118	0.828
	Na	2.132	2.797	1.963
	Na	-0.393	-0.549	-3.521

$(OH)O_2^{2-}SiOAl(OH)_3^-•3Na^+•6H_2O$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	Na	-0.031	-2.517	1.979
	O	-2.118	-2.216	0.879
	H	-1.712	-1.296	0.628
	H	-2.164	-2.713	0.039
	O	1.257	-1.569	0.238
	H	1.247	-2.026	-0.625
	H	0.527	-0.863	0.172
	O	-0.239	-0.439	3.051
	H	0.598	0.000	3.298
	H	-0.463	-0.078	2.120
	Na	0.821	5.219	1.311
	O	-1.526	5.154	1.133
	H	-1.398	4.172	0.877
	H	-2.038	5.137	1.964
	O	1.053	3.129	2.375
	H	0.640	3.043	3.256
	H	0.343	2.806	1.712
	O	0.998	4.301	-0.846
	H	1.825	3.831	-1.066
	H	0.363	3.578	-0.504
	O	-3.118	1.521	0.419
	Al	-4.571	0.695	-0.157
	O	-4.515	0.640	-1.966
	O	-4.834	-0.883	0.608
	O	-6.075	1.672	-0.029
	H	-4.006	-1.379	0.785
	Si	-1.529	1.414	-0.018
	O	-0.840	0.022	0.519
	O	-1.608	1.354	-1.739
	O	-0.699	2.745	0.448
	H	-0.769	1.074	-2.147
	H	-6.570	1.657	0.807
	H	-3.605	0.843	-2.267
	Na	-6.366	1.929	-2.258

$(OH)_3^-AlOAl(OH)_3^-•2Na^+$	**Atom**	**x-coord**	**y-coord**	**z-coord**
	O	-1.185	-0.545	0.618

Al	-0.883	0.616	-0.637
O	-0.942	2.283	0.003
O	0.644	0.272	-1.556
O	-1.925	0.434	-2.113
H	-0.754	2.969	-0.663
H	1.415	-0.018	-1.042
H	-2.825	0.798	-2.075
Al	-1.897	-0.839	2.175
O	-3.667	-0.489	2.349
O	-1.673	-2.522	2.732
O	-1.379	0.356	3.444
H	-4.290	-1.169	2.043
H	-0.859	-2.941	2.401
H	-0.642	0.933	3.177
Na	-0.294	-0.089	-3.565
Na	-3.472	1.098	3.922