

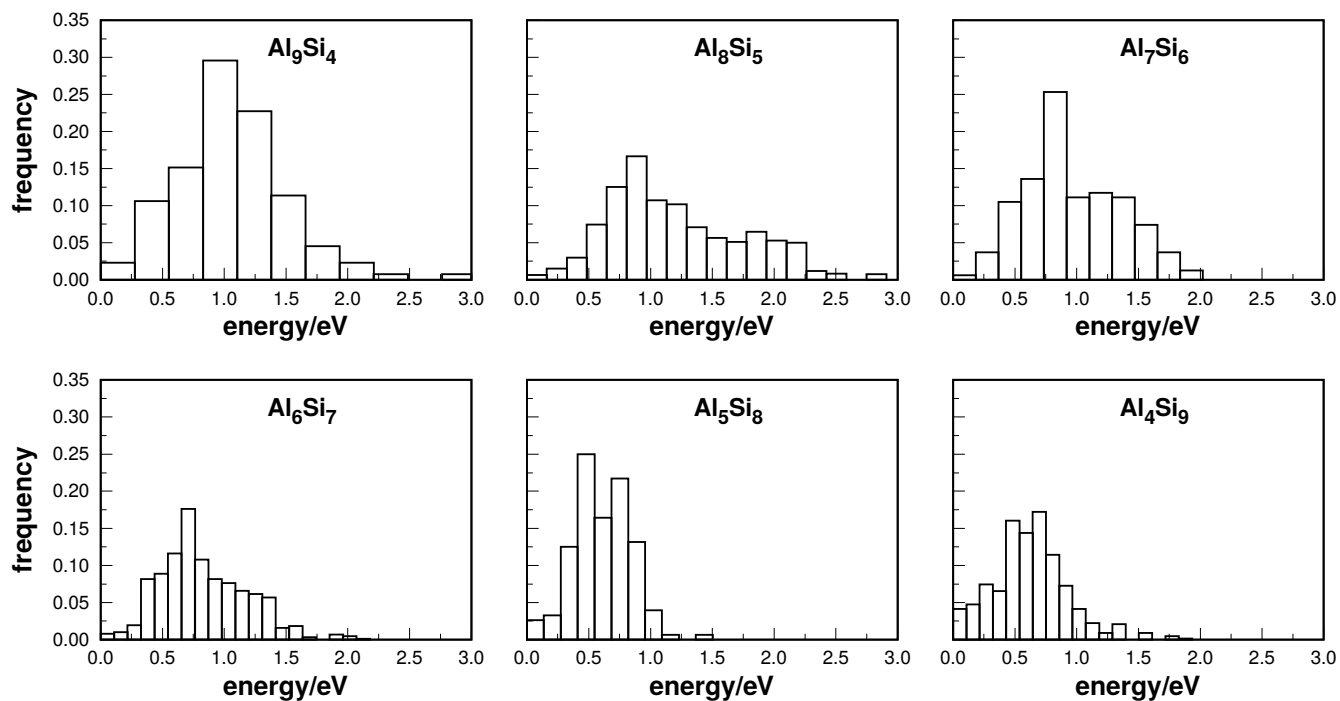
# Structural and homotop optimization of neutral Al-Si nanoclusters

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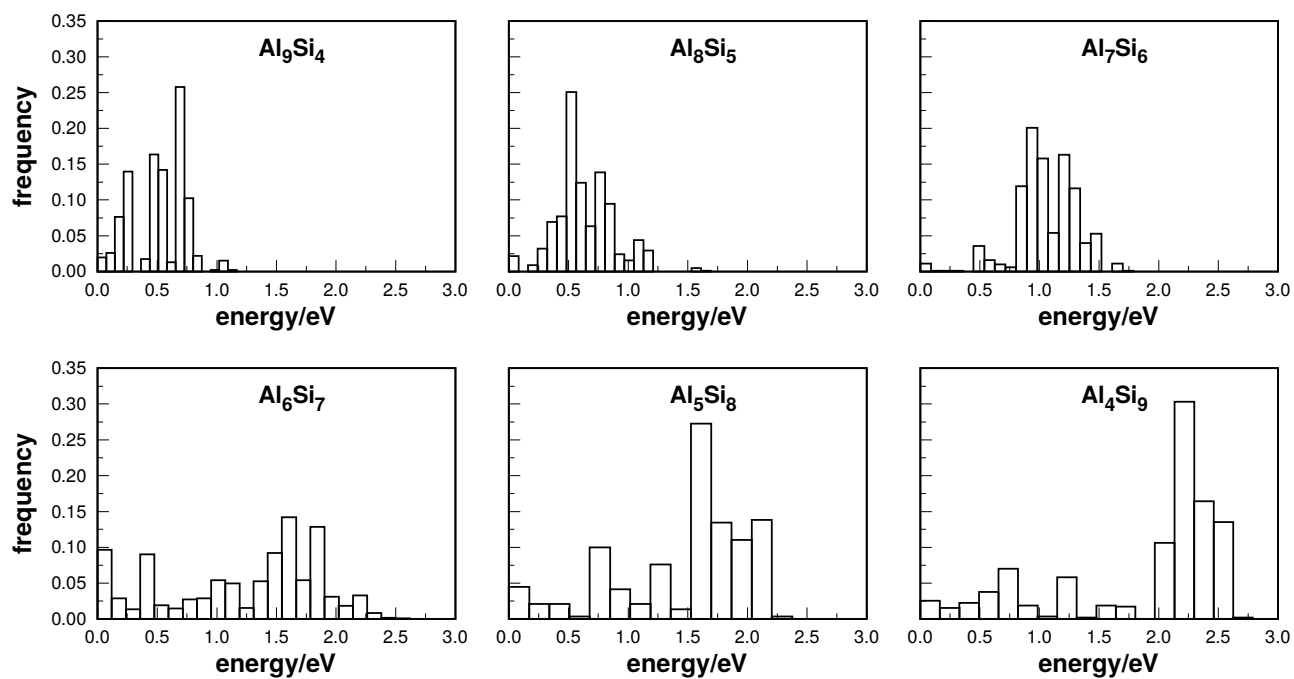
Supplementary Information

## **Part I**

Probability distribution of the energy for homotops of the 13 atoms structures.



**Figure 1:** Probability distribution of the energy of the homotops for the HCTP structure. The zero of energy in each case corresponds to that of the best homotop obtained.



**Figure 2:** Probability distribution of the energy of the homotops for the icosahedral structure. The zero of energy in each case corresponds to that of the best homotop obtained.

## **Part II**

Cartesian coordinates for the putative global minimum  
for each composition at the MP2/cc-pVDZ level

2			
Al1Si1			
AL	0.0000000000	0.0000000000	1.0857393744
SI	0.0000000000	0.0000000000	-1.1758223744
2			
Al2Si0			
AL	0.0000000000	0.0000000000	1.2345674789
AL	0.0000000000	0.0000000000	-1.3246504789
2			
Al0Si2			
SI	0.0000000000	0.0000000000	0.9982457427
SI	0.0000000000	0.0000000000	-1.0883287427
3			
Al1Si2			
SI	0.1365187929	1.2374616024	-0.0000000000
AL	-1.3173726140	-0.6215928950	0.0000000000
SI	1.2758898212	-0.6710877075	0.0000000000
3			
Al2Si1			
AL	0.1160345010	1.3855063295	0.0000000000
AL	-1.1958428437	-0.7049222082	-0.0000000000
SI	1.1748443426	-0.7358031213	0.0000000000
3			
Al3Si0			
AL	0.0846842135	1.4386385714	0.0000000000
AL	-1.2566902196	-0.7009483587	-0.0000000000
AL	1.2670420061	-0.7929092128	0.0000000000
3			
Al0Si3			
SI	0.0810605633	1.1135504933	0.0000000000
SI	-1.3844660065	-0.5236884686	0.0000000000
SI	1.3984414432	-0.6450810247	0.0000000000
4			
Al1Si3			
SI	0.0000000000	1.2997543702	0.0306374449
SI	0.0000000000	-1.2997543738	0.0306374675
SI	-0.0000000000	-0.0000000055	1.9072426539
AL	-0.0000000000	0.0000000092	-2.1187735663
4			
Al2Si2			
SI	-0.0000000000	1.4504977557	-0.0375660065
SI	-0.0000000000	-1.4504977414	-0.0375659871
AL	0.0000000000	-0.0000000156	1.8963021479
AL	0.0000000000	0.0000000014	-1.9714261544
4			
Al3Si1			
AL	0.0000000000	1.4163280444	-0.0350332730
SI	0.0000000000	-1.3026696760	-0.0399002349
AL	-0.0000000000	-0.0605178388	2.0118584941
AL	-0.0000000000	-0.0531405296	-2.0871809862
4			
Al4Si0			
AL	0.0642521279	1.4211274490	-0.0872506691
AL	-0.0176771753	-1.3820469211	-0.1184455799
AL	-0.0022360693	-0.1436079956	2.0720314281
AL	0.0516011167	0.1825774677	-2.2777051791
4			
Al0Si4			
SI	-0.0000000000	1.2227510255	-0.0375623763
SI	-0.0000000000	-1.2227510171	-0.0375623580
SI	0.0000000000	-0.0000000102	1.9569638264
SI	0.0000000000	0.0000000017	-2.0320950920
5			
Al1Si4			
SI	-0.0121900931	1.5759255280	0.0369278814
SI	-0.0121141532	-1.5759274027	0.0369946279
SI	-1.5229649200	-0.0000545872	-0.8527134479
AL	1.5406982256	0.0000182683	-0.8616946119
SI	0.0065709405	0.0000381729	1.7901765606
5			
Al2Si3			
SI	-0.0000000550	1.6136356528	0.1758483352
SI	-0.0000000397	-1.6136031809	0.1762032014
AL	-1.5463744988	-0.0001128932	-0.9993323370

SI	0.0000000262	0.0001933317	1.7822921155
AL	1.5463745678	-0.0001129119	-0.9993323150

5  
Al3Si2

AL	1.5226325346	2.2406114769	-0.1579338291
SI	0.0030344091	-1.5291425687	0.1720009140
AL	-2.6808594279	-1.2438741441	0.1100714749
SI	1.8566995104	-0.2753170910	0.0842542694
AL	-0.7015070263	0.8077223070	-0.0587018192

5  
Al5Si0

AL	-0.4117418717	-0.8723218015	-1.6573187856
AL	1.5144443882	1.4530622878	0.0302408602
AL	-0.8561274386	1.3913271213	-0.7248226963
AL	-1.6401597513	-1.0016862270	0.7048993919
AL	-0.1393841867	0.8103838793	2.0205466498

5  
Al0Si5

SI	-0.0000000055	1.5072269452	-0.8430572305
SI	0.0000000195	-1.5072269420	-0.8430570591
SI	-1.5403469087	0.0000000841	0.0271330111
SI	0.0000000196	-0.0000001468	1.7675272531
SI	1.5403468751	0.0000000595	0.0271330254

6  
Al1Si5

SI	-0.0582995173	-0.1476465274	1.4127279076
SI	-2.0196175551	0.1003356244	-0.0000001109
SI	-0.1291375166	1.7703367953	0.0000001236
SI	-0.0582994916	-0.1476465130	-1.4127278406
AL	0.3976466346	-2.1295326470	0.0000000738
SI	1.9010444460	0.4007342677	-0.0000001533

6  
Al2Si4

SI	-0.0372228536	-0.3343034588	1.4963387752
AL	-1.8735191560	0.2968783399	-0.0000000763
SI	-0.1241790157	2.1069267473	0.0000001754
SI	-0.0372228443	-0.3343035744	-1.4963388407
AL	0.5518224899	-2.3741466610	0.0000000578
SI	1.5536583799	0.4855296070	-0.0000000910

6  
Al3Si3

SI	-0.0650526047	-0.0321823205	1.5540302052
AL	-2.0461888250	-0.2207106735	0.0000000473
AL	-0.0212347776	1.8930705002	-0.0000000855
SI	-0.0650526042	-0.0321823563	-1.5540302285
AL	0.3412968082	-1.9150196326	-0.0000000441
SI	1.8895690035	0.1536054827	0.0000001048

6  
Al4Si2

AL	0.0055655592	-0.0255732623	1.9417489930
SI	-1.6143041817	-0.1811466711	0.0000000123
AL	-0.1800952741	1.9072871645	-0.0000000213
AL	0.0055655529	-0.0255733075	-1.9417489424
AL	0.1911871532	-1.9584218353	-0.0000000666
SI	1.6254181904	0.1300089117	0.0000000249

6  
Al5Si1

AL	-0.0114983423	-0.0262700216	1.8329217676
AL	-1.9107692748	-0.2242084266	-0.0381435805
AL	-0.1937991622	1.8913638350	-0.0209392755
SI	0.0219437645	-0.0250836516	-1.7531390517
AL	0.2052380150	-1.9422095855	-0.0186183790
AL	1.9222219998	0.1729888503	-0.0020814810

6  
Al6Si0

AL	-0.6951053082	-0.8823121128	1.9534338397
AL	-2.0066400712	0.4303520992	0.1162910498
AL	0.0194633748	2.1306885914	-0.3153245625
AL	-0.2443434879	-0.3260635743	-1.5456416964
AL	0.8423130897	-1.9118019197	0.1109745302
AL	2.1176494028	0.4057179164	-0.3197331612

6  
Al0Si6

SI	-0.6925494483	-1.4174090033	1.1936323532
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SI	-1.4211409578	1.1890484388	0.5818120701
SI	0.7035844775	1.3662231350	-1.1936851180
SI	-0.7964604095	-0.4859097241	-1.0057642134
SI	1.4323366016	-1.2401130886	-0.5817818366
SI	0.8075667364	0.4347412422	1.0057867482

7  
Al1Si6

SI	0.0000000264	2.0554723139	0.6827284603
SI	0.0000000095	1.3100333620	-1.6775109452
SI	-0.0000000005	-1.3100333753	-1.6775109094
SI	0.0000000291	-2.0554723085	0.6827284782
SI	-1.3022977602	0.0000000264	-0.0199918709
AL	-0.0000000348	-0.0000000500	2.1849826967
SI	1.3022977304	0.0000000315	-0.0199919097

7  
Al2Si5

AL	0.0000000984	2.2922617530	0.9484739658
SI	0.0000000533	1.7255516860	-1.4619045812
SI	-0.0000000245	-1.7255516938	-1.4619045950
AL	0.0000001416	-2.2922617084	0.9484739392
SI	-1.2934149489	-0.0000000360	-0.2945381521
SI	-0.0000001228	0.0000000122	1.7713714522
SI	1.2934148009	-0.0000000130	-0.2945380288

7  
Al3Si4

AL	-0.0000009440	2.4733150642	0.8422893745
SI	0.0000001640	1.5289841607	-1.4728265135
SI	0.0000000740	-1.5315190692	-1.4698251530
AL	-0.0000007905	-2.4719172081	0.8481672988
SI	-1.3701768616	-0.0002391596	-0.2202599562
AL	0.0000005630	0.0016153934	1.8481492519
SI	1.3701777944	-0.0002391817	-0.2202603024

7  
Al4Si3

AL	-0.3549039539	1.5663123072	0.8626542388
AL	0.3125264573	1.5151506126	-2.0218308355
AL	0.0613568425	-1.3380055002	-1.6856084230
SI	-0.2798293864	-1.5192896584	0.8862788790
AL	-1.8718993273	-0.0780698893	-0.3511921714
SI	0.7554921781	-0.1632954776	2.4711823658
SI	1.3772571895	0.0171976059	-0.0060500538

7  
Al5Si2

AL	0.8359671098	2.3820631486	0.8938942553
AL	-0.3597905246	1.3025878213	-1.2792473712
SI	0.2766594839	-1.2072556382	-1.7472633489
AL	0.1977350400	-2.2012002496	0.8189587402
AL	-1.8476611947	-0.5135577365	-0.2953346934
AL	-0.4636092363	0.2861257576	1.7653488577
SI	1.3606993218	-0.0487631034	-0.0009224397

7  
Al6Si1

AL	1.2442851826	2.4927445761	0.7951883366
AL	-0.4119169403	1.2438628576	-1.0971267985
AL	0.1432501690	-1.2239193638	-1.6789621607
AL	-0.0491569397	-2.0497297173	0.8787571892
AL	-2.0939304161	-0.6687647055	-0.2833481730
SI	-0.4751780083	0.4007431711	1.3413218809
AL	1.7143569528	-0.1915368181	0.1109397254

7  
Al7Si0

AL	-0.8197566970	1.9271279076	0.9184022851
AL	0.3680000521	1.3230742007	-1.3519791202
AL	0.0520336754	-1.3907827041	-1.8967554032
AL	-0.3531197209	-1.7271057683	0.8388866339
AL	-1.8961419410	-0.0866325534	-0.3917139001
AL	0.7376694171	0.2715387756	2.1601474348
AL	1.9113152148	-0.3172198581	-0.1215539303

7  
Al0Si7

SI	0.0000000379	2.0379780620	0.6844459570
SI	-0.0000000841	1.2595404036	-1.7114178699
SI	0.0000000873	-1.2595403703	-1.7114178899
SI	-0.0000000762	-2.0379780735	0.6844459676



SI	-1.2773728980	-0.0000000335	0.0221612666
SI	0.0000000341	0.0000000323	2.165052683
SI	1.2773728991	-0.0000000205	0.0221613003

8

Al1Si7

SI	-0.1006291220	-2.4952095329	-0.0000007441
SI	-0.0112217747	-0.4635324029	1.3029209165
SI	1.3728439924	1.1914709559	0.0000011497
SI	2.0728490989	-1.0994727766	0.0000000051
SI	-0.0112218021	-0.4635310838	-1.3029203532
AL	-2.3989769406	-1.0649474285	-0.0000000797
SI	-1.1830889054	1.2565965802	0.0000012050
SI	0.1604934535	3.2392846885	-0.0000021006

8

Al2Si6

SI	-0.1310638786	-2.3766717578	0.0521837921
AL	-0.0123763691	0.0098847306	1.3244193529
SI	1.4485221807	1.1155580181	-0.5062186351
AL	2.2159992610	-1.2310037147	0.1120151399
SI	-0.0878279490	-0.4829625394	-1.3993795841
SI	-2.1377191544	-0.8709307164	0.1881156613
SI	-1.4619712071	1.3053211370	-0.5134497649
SI	0.0674851165	2.6314638427	0.7423140380

8

Al3Si5

AL	-0.0900426513	-2.5996405639	-0.1212712330
SI	-0.3249278094	-0.1484079685	1.3746960955
AL	2.6831432156	1.4068936793	-0.5154604214
SI	1.7159242670	-0.9821804239	0.3132936774
SI	-0.0177000061	0.0092578723	-1.1293095892
SI	-2.0499180743	-1.0416506887	-0.1103496273
AL	-2.1893897453	1.4581241227	-0.1233777963
SI	0.1739588039	1.9982629708	0.3117788934

8

Al4Si4

SI	-1.2689736256	-1.7217767926	0.0805081733
AL	-0.0288251659	-0.0095072866	1.5782878152
SI	2.0925358785	-0.2123195495	0.1045902528
AL	1.0675125489	-2.4219862853	-0.2425379992
SI	-0.0197574797	0.0145652107	-1.2013699540
AL	1.5346096094	2.1644070631	-0.2014090878
SI	-0.8956183969	1.9440065304	0.1134651106
AL	-2.6710303687	0.2758621098	-0.2315343109

8

Al5Si3

SI	-0.1138555453	-2.4573886935	-0.0000009107
SI	-0.0397123463	-0.4305028461	1.3419161457
AL	1.4703604920	1.1261808848	0.0000015710
AL	2.1633457181	-1.3560803276	-0.0000000850
SI	-0.0397121501	-0.4305010630	-1.3419155389
AL	-2.2145578658	-1.0849548632	-0.0000003508
AL	-1.4689906710	1.3068881330	0.0000018267
AL	0.1441703683	3.4270177757	-0.0000026593

8

Al6Si2

SI	-0.2438461887	-2.4408041838	-0.2729804024
AL	-0.2900087787	-0.0160635666	1.6560038219
AL	2.1960739883	1.3289573049	-0.6567735688
AL	1.7702478559	-1.0295375996	0.3583221282
AL	0.0849923160	-0.2429335157	-1.6567049467
SI	-2.1310906892	-1.2477159784	0.2609281776
AL	-1.7161826898	1.1798422561	-0.3576835239
AL	0.2308621860	2.5689142830	0.6688883070

8

Al7Si1

AL	-0.1541113026	-2.9697563223	0.1613641983
AL	-0.0635581409	-0.3744484573	1.6231585829
AL	1.7109914470	1.2785141672	0.5963207869
AL	1.7439209726	-1.2662450237	-0.3491923649
SI	0.0259646730	0.2284116018	-1.3964687747
AL	-1.8640952524	-1.0991981090	-0.4229658001
AL	-1.6337808212	1.4335620524	0.5275303086
AL	0.1357164244	2.8698190909	-0.7397469369

8

Al8Si0  
AL 0.0594778366 -2.6272044626 -0.5732118431  
AL 0.2786344299 0.2603359464 1.8324184982  
AL 1.6340856672 0.7895102376 -0.4352409460  
AL 1.9908813637 -1.6056912692 0.8197099101  
AL -0.3034283923 -0.2351164944 -1.8324253136  
AL -1.6587984547 -0.7644351283 0.4352600963  
AL -2.0156658366 1.6308511539 -0.8196060739  
AL -0.0841386139 2.6524090168 0.5730956677

8

Al0Si8  
SI -0.1252032804 -2.5516300812 -0.0003054216  
SI -0.0357058827 -0.5178583178 1.3817144630  
SI 1.2478777208 1.2285105439 0.0004546553  
SI 1.9715445148 -1.1695343236 -0.0000197234  
SI -0.0356810789 -0.5172944302 -1.3814746014  
SI -2.0924431756 -0.9906979843 -0.0000197700  
SI -1.1609484223 1.3345106008 0.0004547735  
SI 0.1316076044 3.2846529921 -0.0008043744

9

Al1Si8  
AL 1.5779843940 -1.2625177299 -0.0000003770  
SI -0.0393994894 -1.4357960157 1.8336418010  
SI -0.0394013577 -1.4357966353 -1.8336425269  
SI -1.4648862835 -1.9646302064 0.0000009104  
SI 1.7641893876 1.2829393223 0.0000008536  
SI 0.1445288383 1.0103005874 1.7718687679  
SI -0.5967278561 2.5093979803 -0.0000003258  
SI 0.1445304753 1.0103009433 -1.7718692567  
SI -1.6440771084 0.3340617540 0.0000001541

9

Al2Si7  
SI 1.3035900471 -1.3570934924 -0.0027035380  
AL -0.1240350429 -1.4577640300 2.0476686349  
SI -0.0940721490 -1.2696821252 -1.8951328624  
SI -1.2846920114 -2.2121968646 -0.0806489767  
SI 1.7087326664 1.1772563584 -0.0245066570  
SI 0.1860335855 1.2176924048 1.8056631039  
SI -0.6064637957 2.5760469910 -0.0417396138  
SI 0.1540986879 1.1869929684 -1.8394653930  
AL -1.3964509879 0.1870077895 0.0308653019

9

Al3Si6  
SI 2.2535763434 -0.8995993157 -0.8137547128  
AL 0.8849138026 -1.6364043156 1.4529349739  
SI 0.1056046891 -2.0311307385 -0.9983068557  
AL -1.6105945875 -0.5055323336 0.0905898865  
AL 1.0781651413 0.9307818358 0.3121039466  
SI -0.6973739620 0.2309709124 2.2605054854  
SI -0.8136857351 2.2645513819 0.9477778776  
SI 0.2389821447 0.1558445104 -2.0621321331  
SI -1.5928468365 1.5387780628 -1.1897184684

9

Al4Si5  
AL 2.1444041828 -1.6629361638 -0.2911275615  
SI 0.8747263303 -1.2974163604 1.8588805978  
SI 0.2775650903 -0.8288968949 -1.8212553932  
SI -0.8107377183 -1.6699115497 0.1852857338  
AL 0.6752153576 0.7189554519 0.3235859661  
AL -1.0647321333 0.1696846088 2.5328395941  
AL 0.7190876821 2.9852454904 -1.0975528821  
SI -0.9861977785 1.1716862630 -1.8582727690  
SI -1.9825900130 0.4618491549 0.1676167138

9

Al5Si4  
SI 1.0343525195 -1.0016992053 -0.0211869677  
SI -0.5525247304 -1.5332663467 1.8723913822  
SI -0.8621483553 -0.6181562454 -1.7353842619  
AL -1.2348309521 -2.5511719254 -0.2629536863  
AL 1.3492570469 1.7573456996 0.4932889992  
AL 1.2606363790 0.0999063020 2.4914474682  
AL -1.0415583525 2.4427808285 -1.5903927431  
SI 1.0383964199 0.8299260636 -1.7730628665  
AL -1.1448389750 0.6225948293 0.5258526759

9  
Al6Si3  
AL 1.1809107483 -0.9180809939 0.0000000259  
AL -0.4754300141 -1.5350588073 2.3463414840  
AL -0.4754303502 -1.5350585794 -2.3463414032  
SI -0.9270901832 -2.3135057323 0.0000000862  
AL 1.8787833723 1.6913402040 0.0000000921  
SI 0.3515943048 0.7572193513 1.7970541754  
AL -0.6253742181 2.9138444216 -0.0000000741  
SI 0.3515946003 0.7572193273 -1.7970542484  
AL -1.4128172599 0.2303408088 -0.0000001368

9  
Al7Si2  
AL 1.1859056746 -0.7227526518 0.0013106684  
AL -0.6464492862 -1.4047809319 2.2701246230  
AL -0.6122434631 -1.3964270667 -2.3443847738  
AL -0.9095222080 -2.6271471517 -0.0440494815  
AL 2.0644148277 1.7531434150 -0.1344524450  
AL 0.2951846181 1.0008140141 2.1143134839  
AL -0.4743366965 2.4678584479 0.0729961595  
SI 0.1626764613 0.9377321096 -1.9192092298  
SI -1.2188889279 0.0398198156 -0.0166490046

9  
Al8Si1  
AL 1.5697990954 -0.4267972809 -0.1255072544  
AL -1.6409581323 -1.5151769554 2.3056173982  
AL 0.2430782430 -2.2110866041 -2.2998967067  
SI -0.6537626929 -1.7404106530 0.0028713068  
AL 1.5076258190 2.1159140539 -1.0967358787  
AL 0.3160037903 0.1786555104 2.1091936760  
AL 0.1777431576 2.6046932958 1.0871946657  
AL -0.1629844864 0.3456439303 -2.1089009545  
AL -1.5098037937 0.6968247029 0.1261637444

9  
Al9Si0  
AL 2.0785385295 -0.8431167315 -0.0105392579  
AL 0.3166248868 -2.2777911647 1.2896470610  
AL 0.3201180121 -2.3812437339 -1.4866999507  
AL -1.7884601684 -1.3992584010 0.0050049954  
AL 1.7934202082 1.8933561335 0.1027722769  
AL -0.0615817276 0.3582506475 1.5274947348  
AL -0.4600233296 3.0795665705 -0.1528954489  
AL -0.0666062385 0.3118985219 -1.3934674595  
AL -2.2852891726 1.3065981579 0.1186830489

9  
Al0Si9  
SI 1.4528649277 -1.1366732358 -0.0000000599  
SI 0.2256574988 -1.6941143596 1.9416934728  
SI 0.2256574890 -1.6941144173 -1.9416935457  
SI -1.1085806644 -1.5023539393 -0.0000000107  
SI 1.7962877853 1.4236373236 0.0000001606  
SI -0.1084948700 0.6452166433 1.5229816938  
SI -0.3733450314 2.5018380415 -0.0000001223  
SI -0.1084948511 0.6452165681 -1.5229817089  
SI -2.1548112839 0.8596073753 0.0000001203

10  
Al1Si9  
SI 0.6953765661 -1.6854714598 1.3399532081  
SI 1.0868080161 0.9805991819 1.6933661096  
SI 0.6953766522 -1.6854714254 -1.3399532288  
AL -1.4957955817 -1.6015954415 -0.0000000580  
SI -1.0394643998 0.0181664225 -1.9707666311  
SI -1.0394643220 0.0181663540 1.9707666830  
SI 0.0039759331 2.2377193338 -0.0000000625  
SI 1.0868080459 0.9805990791 -1.6933661440  
SI -2.0048523097 1.0106005462 0.0000000642  
SI 2.1890213999 -0.3001325907 0.0000000592

10  
Al2Si8  
SI 0.0511401628 -1.7743579651 1.7235619244  
SI 1.6143861861 1.1150509337 0.8855106755  
SI 0.9490632272 -1.2160468519 -1.4976907056  
SI -1.1262637036 -1.7731245000 -0.3735109573  
AL -1.2829035677 -0.3007138147 -2.5487644402

SI	-0.4609000668	0.5580222237	2.0097773801
AL	-0.4038820139	2.7792480145	0.6000928153
SI	0.4547902201	1.1963551972	-1.2948042226
SI	-1.6840107756	0.6222127711	-0.1361182286
SI	2.0663703314	-1.2334660085	0.6319457593

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Al3Si7

AL	0.8301116791	2.7471037630	0.0907241787
SI	1.6279589979	0.2493681227	-0.5888068553
AL	0.6920444037	0.8395295113	1.8805984322
SI	-1.4451313440	1.1187551444	0.2548096289
SI	-1.4622382954	-0.4395226640	2.1775669823
SI	-0.1340118308	1.4234710914	-1.8209271437
SI	1.6048242860	-2.0115662344	-1.1422746201
SI	-0.3619850433	-0.9777601355	-1.9083243878
SI	-1.9160657614	-1.2768702207	-0.0023507882
AL	0.4605389083	-1.7861333782	1.0589845731

10

Al4Si6

SI	0.3696200690	2.0921653438	0.1865342321
SI	2.3430911784	-0.0298345281	-0.3281049902
AL	2.0526761202	1.1535691209	1.8399649330
SI	-1.8808082208	1.0185467497	0.2122737304
AL	-2.1792487217	-0.8653873435	1.8883534474
SI	0.8903422635	1.0320061186	-1.8661948457
AL	0.9738468125	-2.0981417149	-0.9920137858
SI	-1.4224510602	-0.0714501271	-1.8396934572
SI	-1.4825115949	-1.8549943770	-0.2843365049
AL	0.2314891539	-0.4901042424	1.1832172408

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Al5Si5

AL	-0.2407304118	-1.5230112767	2.0486673666
SI	0.9477069921	0.8424173134	1.7889328454
SI	1.0297586499	-0.3994173648	-1.6675800143
SI	-0.4423778656	-2.0616529023	-0.4317458895
SI	-1.3510607457	-0.7376961239	-2.1450643952
SI	-1.3562666158	0.6470800447	2.5101340122
AL	1.2063201547	2.0795355454	-0.3990015568
AL	-0.4888479979	1.6253542565	-2.3663495824
AL	-1.1234872794	0.6072185200	0.0473730657
AL	1.9967751194	-1.1066480123	0.6146341485

10

Al6Si4

AL	0.9766294866	-2.9262745954	0.3138360052
AL	1.0901939730	1.1476913366	1.7693868543
SI	0.8554667545	-1.5073552626	-1.7900836094
AL	-0.5448518356	-0.8452842040	0.6145500485
AL	-1.1937576936	0.0053347776	-2.1005162738
AL	-1.5009234710	1.1559576021	2.1877452867
SI	-0.5744351574	2.0563286979	-0.1381306934
AL	1.3306566024	0.8642335143	-1.2053276546
SI	-2.5320291981	0.6888396026	-0.0797327878
SI	2.2708405392	-0.6662914689	0.4282728241

10

Al7Si3

AL	0.7419733398	-2.3796808247	1.2894291288
AL	1.8461607670	1.5455068569	1.6016076447
AL	0.6895741083	-1.6743853368	-1.4049542026
SI	-1.5970995656	-2.2384504632	0.3872023145
AL	-1.7045135723	-0.5055084027	-1.6772989379
AL	-0.5348842618	0.0288896346	0.9536984125
SI	-0.1340404513	2.6478253797	0.6638561350
AL	0.6300758588	0.9961879896	-1.1800147287
AL	-1.9266327576	1.9933713491	-0.9197112144
SI	2.1671765347	-0.4405761826	0.2861854482

10

Al8Si2

AL	1.4802287721	-2.1136649537	1.4970171373
AL	0.3577930849	0.4173212855	0.9670813779
AL	0.6254375103	-1.6545950609	-1.5474944178
AL	-0.9992561809	-2.0327936048	0.4323022955
AL	-1.2938635797	0.2824297449	-1.1330550990
SI	-2.4099429477	-0.1547709555	1.0890309557
SI	-0.1403347654	2.5125337343	-0.8670735830

AL	1.4177726656	0.8078553478	-1.6510155624
AL	-1.8181837016	2.2858521387	0.9903436079
AL	2.9581391425	-0.3769876762	0.2228632879

10

Al10Si0

AL	0.4798368078	-1.7535829593	1.1700920314
AL	0.7075950919	0.9523814171	1.0131581581
AL	0.9525541526	-1.6798343476	-1.4470192723
AL	-1.8655307820	-2.7271713851	-0.0167540570
AL	-0.8387277695	0.0819966757	-0.8895200284
AL	-1.7592851108	-0.5405855221	1.7503353161
AL	0.0596296395	2.9895177177	-0.7792285339
AL	1.6632966895	1.1161920339	-1.7791099335
AL	-1.9253467709	1.9995896771	0.8877523141
AL	2.7037680520	-0.4653233075	0.0902940054

10

Al0Si10

SI	0.0186330039	2.2318643395	0.0000000201
SI	2.1836116150	-0.1339076174	-0.0000000544
SI	0.9977361373	0.9667732654	1.7326952327
SI	-1.9957804964	1.0064542374	-0.0000000072
SI	-1.1118993829	-0.1021597963	1.8996333171
SI	0.9977361067	0.9667733235	-1.7326952451
SI	0.7077584986	-1.6566970226	-1.2733142816
SI	-1.1118993532	-0.1021598288	-1.8996333547
SI	-1.4976085415	-1.6338688327	0.0000000460
SI	0.7077584125	-1.6566970680	1.2733143270

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Al1Si10

SI	-1.5442219195	-1.4610148891	0.1142404521
SI	-1.2880164757	0.2909312517	1.7742853367
SI	1.0000013437	-1.2633519848	-1.3632236728
SI	0.7046739001	-1.0985813842	1.0929017129
SI	-1.1092795912	-0.1381134437	-1.9025901148
AL	1.1432494137	1.1642563636	2.1519083665
SI	0.6137273132	1.5363251187	-1.7928223888
SI	0.2748610333	-3.2103589636	0.0706500737
SI	2.1075507496	0.5553010609	-0.1972284545
SI	-2.0509919411	1.3296348028	-0.2455151283
SI	-0.0331348263	2.4513430678	0.2973938174

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Al2Si9

SI	-1.1145369806	-1.8061663650	0.2525607050
SI	-1.4464316480	0.4325331075	1.2976747795
AL	-0.1223288580	-1.8071350452	-2.0715223670
SI	0.4566701737	-1.5242458859	2.0000954879
SI	-1.3703970813	0.2892238700	-1.1671479810
SI	0.8713609182	0.8153239323	1.8255235416
SI	1.0935580998	0.3904944488	-1.7918083687
SI	1.5154784625	-1.6741878816	-0.1616270822
SI	2.4977458804	0.5129827737	0.1101377430
AL	-2.6739174153	2.5480368619	-0.1537442614
SI	0.1112174485	1.9795111835	-0.1401421965

11

Al3Si8

SI	-1.9261322502	-2.1155692686	0.2574974745
SI	-1.5978437571	-0.1159981235	1.4135858259
AL	1.1034591681	-1.0809283989	-2.3077964895
SI	1.3528397978	-1.0426849110	1.9191411469
SI	-1.3856863124	-0.4469891339	-1.2912055060
SI	0.3330075610	1.0853426162	1.8714314635
SI	0.3101674866	1.1958985141	-1.7250366606
SI	0.4499752823	-2.0043284086	-0.0504893610
SI	1.9704087910	0.0741714042	-0.0985997952
AL	-1.7507952138	1.8713639476	-0.1137551472
AL	0.9590184467	2.7360927623	0.1252270487

11

Al4Si7

SI	-1.6098385139	-1.1818279322	0.0000001947
AL	-1.1962618447	0.2938782919	2.0665156001
SI	-0.1256693189	1.5409297264	0.0000000850
SI	0.9730297460	-1.1793181722	-1.4658658732
SI	0.9730295341	-1.1793182032	1.4658658171
AL	-1.1962617618	0.2938778906	-2.0665156177

SI	1.1627048856	1.1837279891	2.0306975103
AL	-2.6534180655	1.1872009585	-0.0000001368
AL	2.4671550076	0.3888757615	-0.0000000231
SI	1.1627046187	1.1837281819	-2.0306974561
SI	0.0949527127	-2.7870644923	-0.0000001018

11

Al5Si6

SI	-1.8228561775	-1.6365533070	-0.1877435200
AL	-1.6756436981	-0.4118456888	1.9759722812
SI	1.6875955564	-0.9382346604	-1.4861791753
AL	0.9948775299	-1.3221107080	2.0110927233
SI	-1.9168052388	0.2987321611	-1.5248490018
SI	0.3320816050	1.0822699418	1.5114601025
SI	0.2527749709	0.7244996731	-2.3335145717
SI	0.4045955536	-2.3975440170	-0.1569601665
AL	2.5336706432	0.4280206624	0.4170305201
AL	-1.7862619546	1.9080703210	0.3722740427
AL	0.8143902103	2.4210666218	-0.5985832345

11

Al6Si5

SI	-1.1511277273	-1.0969783409	-0.0801122610
AL	-1.7222107035	0.4810518781	2.0578763764
SI	-0.0909866363	2.2200181470	0.9361597519
AL	0.6355039814	-1.4138357243	-2.0570353584
SI	0.2911939633	-0.9888140230	2.1580897611
AL	-1.5694612996	-0.1223647560	-2.4747574330
SI	1.7191068092	0.7945763318	1.4621625964
AL	-2.0839097250	1.3938427083	-0.4397366419
SI	2.3630752455	-0.3118764950	-0.5241805551
AL	0.5122552945	1.2692963971	-1.3897730287
AL	1.1486877979	-2.4802261232	0.3513067923

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Al7Si4

SI	-0.4222232644	-0.4200481982	0.0002397547
AL	-1.3947717312	0.6774050998	2.2148610592
AL	0.5428835767	-1.3559706615	-2.2599455655
AL	0.5478666328	-1.3581075285	2.2574104323
AL	-1.3996601889	0.6794989789	-2.2111936289
SI	1.0919458000	1.1389760276	1.5367484612
SI	1.0885605438	1.1404242232	-1.5381237691
AL	0.7786268738	-2.7415511394	-0.0021777813
AL	2.2806588631	-0.5376088132	-0.0027880237
SI	-2.6384426120	0.5634075054	0.0031500093
AL	-0.6570254937	2.3699455060	0.0018190482

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Al8Si3

AL	-2.3809776696	-1.1704220321	-0.1186482314
AL	-1.0530871275	-0.9455456378	2.2483915723
AL	0.0237413774	2.6623043207	-0.2652714519
AL	-0.2027077992	-1.5542525757	-2.0637372062
AL	1.7693102540	-1.2208647238	1.4483064916
AL	-0.0945242286	0.0292591183	0.0511722288
AL	0.4841680649	1.4454182419	2.1437875327
AL	-1.6802138247	1.0788339571	-1.7106070779
SI	2.2089230791	1.0590792703	0.0544458191
SI	1.0250378706	0.8594500222	-2.0522948756
SI	-0.0475429965	-2.4985699610	0.2644551982

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Al9Si2

SI	-1.2488884812	-1.4789222755	0.0019362060
AL	-1.5697631037	-0.0152878103	2.0436267790
SI	1.1506417606	2.5327929845	-0.0023657211
AL	0.7038135383	-1.5112978165	-2.2676775134
AL	0.7083037545	-1.5090950809	2.2677309973
AL	-1.5737910859	-0.0172509745	-2.0405240493
AL	0.5947163134	1.4266720078	2.2485896851
AL	-1.3828213150	1.7127771264	0.0005333077
AL	0.8373948968	-0.0226865803	-0.0008219910
AL	0.5902922625	1.4244878486	-2.2511469604
AL	1.2422284597	-2.7974994293	0.0001192354

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Al10Si1

SI	-0.0092712289	-0.0174807358	0.0319120995
AL	-1.2270724519	1.1014751794	2.1770873612

AL	0.2705344408	2.5791433366	0.3140393014
AL	1.2098114469	-1.1371341327	-2.1145762311
AL	-0.1735343419	-1.5038579920	2.1914827333
AL	-1.4175875030	-0.8561776693	-2.1252306082
AL	1.4004835461	0.8215299726	2.1899540703
AL	-2.6169657792	0.2593957798	0.0211177192
AL	2.5970246611	-0.2943523529	0.0425265617
AL	0.1602928545	1.4683172849	-2.1275411901
AL	-0.2837756444	-2.6145686704	-0.2501918170

11

Al11Si0

AL	-0.6542443174	-0.6733274890	-0.0000008795
AL	-1.4690326979	0.5819140578	2.2997722806
AL	-0.1093327995	2.0034424532	0.0000015382
AL	0.5901282487	-1.5049331503	-2.2996934739
AL	0.5901255380	-1.5049358666	2.2996922631
AL	-1.4690299162	0.5819158432	-2.2997739434
AL	1.1174040844	1.0746579509	2.2479376329
AL	-2.8236373025	1.1432885280	-0.0000017110
AL	2.0294795802	-0.1647777661	0.0000018378
AL	1.1174069697	1.0746604165	-2.2479341419
AL	1.1328596125	-2.8672149776	-0.0000014256

11

Al0Si11

SI	-1.4708862423	-1.8598811333	0.0479107930
SI	-1.3952096898	0.2019841272	1.3253203132
SI	0.7647203460	-1.1895380213	-1.2453649339
SI	0.8034836672	-1.1607435279	1.2552067491
SI	-1.4362239239	0.1713422089	-1.2783945715
SI	0.8086910177	1.1443377131	2.0650209051
SI	0.7428810395	1.0963556524	-2.1086979184
SI	0.5639640557	-3.2674155145	0.0320257074
SI	2.0002229742	0.5883213495	-0.0349338518
SI	-2.2817721130	1.9452780829	0.0164883883
SI	0.1523088688	2.3475290629	-0.0263415806

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Al1Si11

SI	3.5332793404	-0.0613334469	-0.0709297547
SI	1.8512715081	0.1166140527	1.6561261676
SI	1.6933856496	-1.6473386069	-0.3712751809
SI	0.0102371429	-0.9084463810	-2.0712083524
SI	-0.0053205075	1.5829332977	1.0989593279
SI	0.0369672993	-1.4642617136	1.4271977676
SI	-1.8160385511	0.0679080959	1.6764044963
SI	-1.4573487145	0.7233052489	-0.9404855262
SI	-1.6337898965	-1.6915232326	-0.3528755901
SI	-3.5117197789	-0.1548892803	-0.0319798117
SI	1.4463939691	0.7618668620	-0.9565421282
AL	-0.0330254610	2.7365751043	-1.1416284149

12

Al2Si10

SI	0.3360462488	0.0256584415	3.3484565421
SI	-0.0795458444	1.7060903052	1.6275086766
SI	0.8824180236	-1.4957493478	1.5089208894
SI	-1.4262788130	-0.4141993110	1.8479454057
AL	-1.1454135466	-2.0905800448	0.0002330324
SI	1.5996575109	1.7322207598	-0.0003083995
AL	-2.0271270178	1.1436447223	0.0001474617
SI	-0.0798734602	1.7056289419	-1.6274443184
SI	0.8819635636	-1.4961196743	-1.5089120640
SI	-1.4269346883	-0.4143889258	-1.8477742270
SI	0.3354042847	0.0252449910	-3.3483938925
SI	2.3444477388	-0.5040498582	-0.0003791048

12

Al4Si8

AL	-0.2042088875	-0.5578066621	3.6727318096
SI	0.0586011972	1.4871465487	2.0504705845
SI	0.8574697661	-0.9749416377	1.3082265085
AL	-1.7280773339	-0.3050280223	1.3453906559
SI	-0.7615716762	-2.2814766945	-0.0000000292
SI	1.3491736981	1.4296146307	0.0000000562
SI	-1.1216998928	1.9240911842	0.0000000446
SI	0.0586012397	1.4871465619	-2.0504705597
SI	0.8574696860	-0.9749415145	-1.3082265971

AL	-1.7280774162	-0.3050279674	-1.3453906785
AL	-0.2042089743	-0.5578066913	-3.6727317270
SI	2.7612925938	-0.4475687358	-0.0000000847

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Al5Si7

SI	3.2350712545	-0.3705161441	-0.0776434277
AL	1.7901236632	1.1935871944	1.3486473599
AL	1.3683869322	-2.0887474069	-0.4412691092
SI	-0.0830175350	-1.0895268640	-2.3843697611
SI	-0.7976527061	1.0736347648	1.0684613326
SI	0.5072292653	-1.0377862613	1.7885151073
AL	-2.0377437229	-0.8876963660	2.1130010033
AL	-1.2587541243	1.0907269693	-1.6985236676
SI	-1.1010851815	-1.2873206629	-0.2191080445
AL	-3.2240067385	0.4047840165	0.0230381080
SI	1.3287530366	0.4916385861	-1.2095611840
SI	0.3869878567	2.5686321742	-0.3894247172

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Al6Si6

SI	2.3344089817	-0.0922857023	-0.9310863284
SI	2.2918412669	-0.0995918671	1.4328638275
AL	1.2988952660	-2.1671981319	0.2311422432
AL	0.2357563520	-1.1660612928	-2.0223225098
SI	0.6135234456	1.4760752673	1.9834877558
AL	0.0198275787	-0.9729344694	2.3003056537
AL	-1.7379655370	0.7905062565	1.3160827342
SI	-1.2108979784	0.6683338527	-1.1172422464
SI	-1.2369708170	-1.4923452506	0.1484706000
AL	-3.4420974451	-0.9455762573	-1.3007701813
AL	0.9857498572	1.5882075108	-2.0842849952
SI	-0.0377789704	2.4742800839	-0.0348835533

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Al8Si4

AL	2.6519388231	0.0670288507	-0.2427950443
AL	1.3034590373	1.2268611776	1.8890817540
AL	1.1222009819	-2.1178757854	-1.0140214378
AL	-1.2923864465	-1.2265187920	-1.8902178345
AL	-1.1111305790	2.1182069616	1.0128798455
SI	1.1700381753	-1.2325124742	1.3469293063
AL	-0.9362020991	-0.1890861258	2.4020990713
SI	-2.1558491479	-0.0047408976	0.1400172449
AL	-1.0500728243	-2.2902704528	0.5783752030
AL	-1.3447287441	1.5424058551	-1.6931243517
SI	0.8298611449	0.1862342425	-2.0829148161
SI	0.9271636786	1.9816774402	-0.5245459404

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Al10Si2

AL	-1.0633037550	0.1832820450	2.3891468613
AL	0.6033191627	1.9882770109	1.4059218383
AL	1.5738327634	-0.4828842957	1.9926965226
AL	-2.3461455746	-0.8014854434	0.2944987709
AL	-0.2502456344	-2.2080882958	1.3054014320
AL	2.3854039086	0.7746988922	-0.2772141071
SI	-1.6294406624	1.6468244419	0.2174441469
AL	0.3197325316	2.2790366124	-1.3266070649
SI	0.8978179980	-0.0743409010	-2.1694944025
AL	-0.5641346114	-2.0151321394	-1.3886390463
AL	-1.6105494922	0.4533352096	-2.0538383742
AL	1.8784773655	-1.8201221369	-0.3893165768

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Al11Si1

AL	2.4996374697	-0.1111586078	0.9299961933
AL	0.4311564302	0.5460399850	2.6801592030
AL	1.5872372694	-1.9297398858	-0.9325354727
AL	-0.6055659305	-0.6873749851	-2.4598616647
AL	0.9281766465	2.3683111887	0.6638165584
SI	0.6471895474	-1.9656085247	1.6056717771
AL	-0.3408901478	-0.1262742684	0.2936742362
AL	-1.7572496082	1.8242465407	1.1768196830
AL	-1.0972685295	-2.5013684372	-0.4345096855
AL	-2.6932153014	-0.0405363294	-0.7312072340
AL	1.4424344444	0.7538716531	-1.4409932493
AL	-0.9273502903	1.9310016711	-1.4292673448

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## Al12Si0

AL	-0.1722458601	-0.3373694964	3.9440260163
AL	1.3953571567	1.3320367416	2.2913855903
AL	0.9305238549	-2.2681337400	2.5899957442
AL	-1.1221673443	0.6357198091	1.6989707139
AL	-0.3877992844	-1.5621693275	0.3659872155
AL	0.4202394171	1.5493896693	-0.3660470117
AL	-2.1750779412	0.6689146941	-0.8586740750
AL	-0.8981887620	2.2553418396	-2.5900093501
AL	1.1546640200	-0.6485283391	-1.6989426754
AL	-1.3629022310	-1.3447275895	-2.2914630966
AL	0.2048242971	0.3246454656	-3.9439752313
AL	2.2075366776	-0.6817187306	0.8587461616

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## Al0Si12

SI	3.6883158288	-0.1305918184	-0.0653918053
SI	1.8120971137	0.2322619695	1.3926328846
SI	1.6587906320	-1.6148101918	-0.3466662640
SI	0.0075416301	-0.6897687406	-1.9208558019
SI	-0.0037363806	1.7038163256	1.5196381837
SI	0.0368050267	-1.3763441156	1.4900164381
SI	-1.7818351729	0.1847102279	1.4136998803
SI	-1.8047305041	0.7143464325	-1.2174899369
SI	-1.5999963109	-1.6579941531	-0.3274189443
SI	-3.6656012881	-0.2275246475	-0.0218506135
SI	1.7898792078	0.7619521065	-1.2389736794
SI	-0.0232377823	2.1613566048	-0.7555773414

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## Al1Si12

SI	1.1384714031	1.1929554732	-1.4857889230
SI	-0.0814399890	1.8021430561	0.7272530864
SI	0.0641821286	-0.0552303245	2.3575424231
SI	-2.3561765257	2.5570802056	0.0939818936
SI	-1.2229376918	1.1853497833	-1.5150697473
SI	-1.1723187312	-1.1642702199	-1.4754462023
SI	1.2347947648	-1.2353510660	-1.5444577906
SI	2.2847477093	2.2778493058	0.2636607859
SI	2.4027115096	-2.3651535962	0.1678487374
SI	1.9386494517	-0.0621849316	0.7617766874
SI	0.1009350957	-1.9018458537	0.7016708388
SI	-2.1900942793	-2.3572227011	0.2616979912
AL	-2.1415248458	0.1258808683	0.8225692196

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## Al2Si11

SI	1.2016480667	1.1880678359	-1.5214722485
SI	-0.0000000542	1.8007585250	0.6993519403
SI	0.0000001061	-0.0000000795	2.4099313210
SI	-2.2596786003	2.4099642596	0.1831550914
SI	-1.2016480092	1.1880679634	-1.5214723912
SI	-1.2016480488	-1.1880679082	-1.5214722792
SI	1.2016480635	-1.1880679945	-1.5214724166
SI	2.2596785161	2.4099643092	0.1831551986
SI	2.2596785895	-2.4099642192	0.1831551560
AL	2.1306233331	0.0000000499	0.8409362544
SI	-0.0000000424	-1.8007585311	0.6993519110
SI	-2.2596786451	-2.4099642520	0.1831551512
AL	-2.1306232748	0.0000000417	0.8409363118

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## Al4Si9

AL	-1.0010516975	2.9059314842	-1.5515156188
AL	1.5552524463	1.9340950276	-0.4317681369
AL	-2.4188948596	0.5280879614	2.3922939275
AL	0.5160674063	0.1920055380	2.4581453812
SI	-0.2257086391	0.4912645281	-2.2500917488
SI	1.9557433925	-0.3720382646	-1.8574870913
SI	-0.9115185901	-1.6884022241	-1.3457298329
SI	1.3416779958	-2.5338245944	-1.0452021299
SI	-0.4804910621	0.4828805030	0.1182785758
SI	-2.0492958876	2.1840460803	0.5799667844
SI	2.3013374876	-0.3649343204	0.6075599377
SI	0.8300085036	-2.2592335082	1.2728746933
SI	-1.4131264858	-1.4998782002	1.0526752489

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## Al5Si8

AL	0.0912878505	-2.2847535717	-1.7005013016
AL	-1.6187710827	1.6531924080	-1.6737669054
AL	2.7333734845	1.1974582075	-0.9007830789
AL	1.5547531245	-0.9827598668	0.1978812545
AL	0.3409918947	1.8123034324	0.2167809659
SI	0.5044103575	0.2364676310	-1.9166007730
SI	-1.5559405538	-0.6670679139	-0.6245459925
SI	1.1870675735	-3.4737191211	0.2165527546
SI	-1.7303042038	3.2432997015	0.2622586940
SI	-0.7477187465	-2.3451595399	0.9573802004
SI	-2.2230905730	1.0506416004	0.9804758047
SI	-0.3646465849	-0.1679742121	2.1139746909
SI	1.8285204395	0.7859357846	1.8708936865

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Al7Si6

AL	-0.3283673834	-1.0353349823	3.0346216412
AL	-2.2315881551	0.9786266967	3.3123325706
SI	-3.4617786596	1.3602686135	0.8886352505
SI	0.6605746428	2.3080129830	0.2685036263
SI	0.3661623298	1.5571858017	2.9476281279
SI	-0.4581190011	-1.7362303710	0.5418742284
AL	-2.9604583347	-1.2912476158	1.0084372837
AL	-1.6701285175	2.0488715516	-1.0012690985
SI	2.5029851419	1.8284161028	1.7506562780
SI	1.6692757927	-0.3851619867	1.2290215321
AL	-1.4201465323	3.0876562037	1.6596075668
AL	-1.0495082957	0.5584434889	1.0310162713
AL	0.2721969622	0.0702935141	-1.2009652782

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Al8Si5

AL	1.2827611177	1.2874070422	-1.6291937014
AL	-0.3595617997	1.9577569161	0.4280325344
AL	0.1551698353	0.1584379266	2.4170837920
AL	-2.9794509582	2.0813824386	-0.3445491610
SI	-1.2957074942	1.3813263369	-1.9903638475
AL	-1.0797823319	-1.0871778226	-1.9415933718
SI	1.3898047552	-1.2909483448	-1.9875655322
AL	2.0682608894	2.0798758858	1.3000042015
AL	2.0964212949	-2.9695132518	-0.3392534893
AL	1.9590931805	-0.3494385438	0.4304573614
SI	0.5495767107	-2.2447583924	1.5248326750
SI	-1.5375595648	-1.5444025810	0.7474533661
SI	-2.2490256349	0.5400523902	1.5218941728

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Al10Si3

AL	0.1407439935	0.8723497882	-2.5604124211
AL	-1.0879737125	-1.5448839987	-1.7209211311
AL	2.4612165128	1.1820085612	-1.1290307775
AL	0.2751307052	2.4941766798	-0.4041490246
AL	0.5266682090	-2.6820180863	0.2098882326
AL	-1.6214049971	-1.2722180111	0.9088347949
AL	-0.7415547064	1.1250799024	1.6332033995
AL	1.8669211914	1.4099320402	1.4891917927
AL	-3.4466321702	1.9956858685	1.2376102954
AL	0.6368824752	-1.0007266943	2.3350477142
SI	1.4080852427	-1.1749326335	-1.7737723137
SI	-1.5431473967	0.7120625254	-0.6854165180
SI	2.4072984232	-0.8911045717	0.4883298866

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Al11Si2

AL	-0.1629678689	-0.1706597380	3.6521087302
AL	-2.7237190263	-0.0980019406	2.5332107055
AL	-2.8427634900	2.0682310526	0.8184605265
AL	-0.3560638861	3.3445209006	0.8699374787
SI	1.2254261676	1.9079185131	2.5636220736
AL	-0.8476011751	-1.8708418687	1.5412413050
AL	-2.6849057896	-0.6057659447	-0.3410777081
AL	-1.0399233455	1.6344088100	-1.2330292199
AL	1.5255255613	1.5666351752	-0.1246931534
AL	1.6448025101	-0.6059839425	1.5947003941
AL	-1.3998324382	2.2707316541	3.2040839530
SI	-0.6401393343	0.7086920133	1.1778474061
AL	0.1932621047	-0.8000846844	-0.7863124912

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## Al12Si1

AL	-0.1917913211	-0.1995001629	3.6516406819
AL	-2.7605688539	-0.1155635723	2.5416293522
AL	-2.8816208774	2.0771239851	0.8053797565
AL	-0.3875974541	3.3486212335	0.8422349474
AL	1.2746386420	1.9415289737	2.6012234457
AL	-0.8599746028	-1.9102227917	1.5380191031
AL	-2.5223784904	-0.5029951025	-0.2211447699
AL	-1.0559232018	1.6381270650	-1.2716780937
AL	1.5132243497	1.5542154337	-0.1615944693
AL	1.6341862957	-0.6387490334	1.5748730036
AL	-1.4411142585	2.2641785039	3.1982067015
SI	-0.6236209845	0.7190832459	1.1897686600
AL	0.1936407473	-0.8260477782	-0.8184583189

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## Al13Si0

AL	-0.1737194232	-0.1806073834	3.7225049449
AL	-2.8129034245	-0.1702207026	2.5473724004
AL	-2.9180276985	2.1420050630	0.8187388876
AL	-0.4134033709	3.3366889631	0.7303348425
AL	1.3435358475	1.8495884175	2.5895791411
AL	-0.8341196301	-1.8982598510	1.6496809852
AL	-2.5910601719	-0.4111582803	-0.2095648089
AL	-1.0738037367	1.6190400782	-1.3424897817
AL	1.5653801119	1.6086523822	-0.1673560439
AL	1.6705057867	-0.7035735522	1.5612776319
AL	-1.5271380951	2.1909733435	3.2209346813
AL	-0.6237613660	0.7192152798	1.1900074500
AL	0.2796151607	-0.7525437575	-0.8409203301

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## Al0Si13

SI	1.1986071683	1.1985982613	-2.1040994026
SI	0.0000001232	2.2380918819	1.4818078379
SI	-0.0000000596	0.0000000635	2.3740814560
SI	-1.9099184872	1.9099616066	0.0631060799
SI	-1.1986070822	1.1985983240	-2.1040991749
SI	-1.1986071765	-1.1985981042	-2.1040990691
SI	1.1986070589	-1.1985981770	-2.1040992396
SI	1.9099185366	1.9099619431	0.0631056858
SI	1.9099184920	-1.9099620450	0.0631057066
SI	2.2380692492	-0.0000000254	1.4817572226
SI	0.0000001282	-2.2380918155	1.4818079747
SI	-1.9099184225	-1.9099618016	0.0631060665
SI	-2.2380695249	-0.0000001115	1.4817578561