

Supporting Information

Bimetallic Al-Sn Clusters: Mixing at the Nanoscale

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Additional figure showing the Density of electronic States (DOS) of neutral AlSn_{10} . The spin up and spin down DOS are almost identical except around the Fermi energy due to the odd number of electrons of the cluster. Observation of the electronic levels close to the Fermi energy reveals that an electronic configuration having even number of electrons contributes to the stability of the cluster, but this contribution is not crucial because no big gaps are associated to this electron pairing effect.

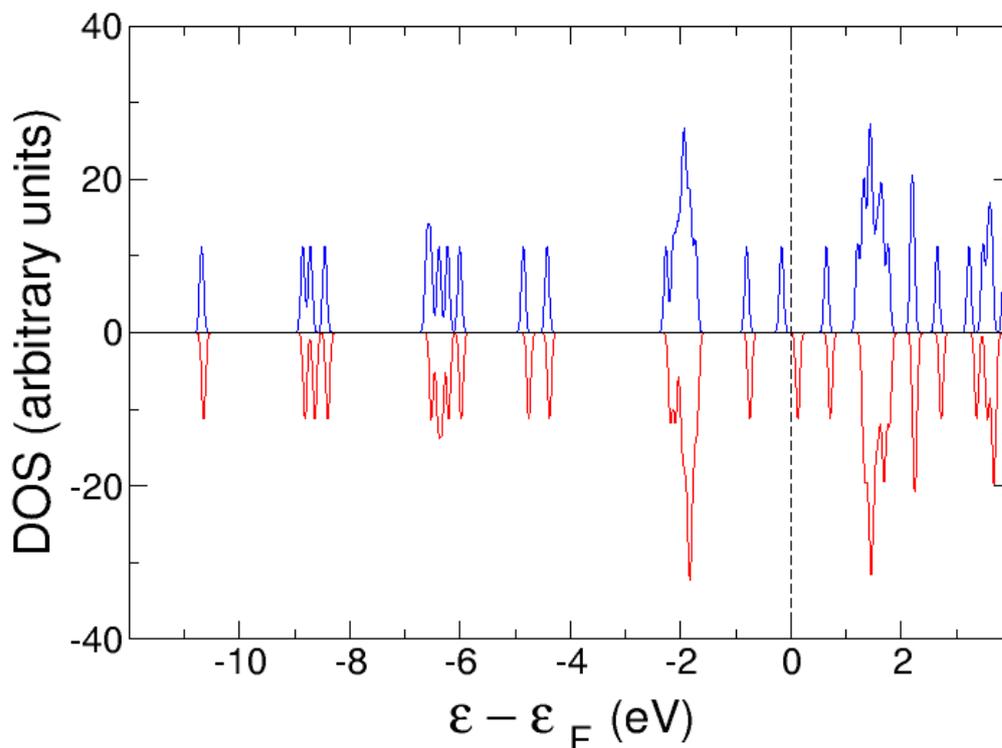


Figure S1. Density of electronic States (DOS) of the lowest energy structure of AlSn_{10} . The deeper levels (below -20 eV) originating from the 4d electrons of the Sn atoms are not shown in the figure. The DOS is separated into spin up (blue) and spin down (red) components. The Fermi level, at energy = 0, is indicated by a dashed vertical line.

Calculations using the PBE exchange-correlation functional have been performed for selected clusters to confirm the results obtained with the PW91 functional. The two functionals, PW91 and PBE, lead to the same structures and the energies are in excellent agreement (see Table 1). Therefore the calculations using the PBE functional fully support the conclusions obtained using the PW91 functional.

Table 1. Cohesive energy (eq. (2)) per atom and energy balance for the replacement reactions consisting in the elimination of a Sn atom from Al_mSn_n and the addition of an Al atom (eq. (7)) calculated using the PW91 and the PBE functionals.

| SYSTEM | PW91 | | PBE | |
|-------------|-------------------------------|---------------------------------|-------------------------------|---------------------------------|
| | $E_{\text{coh/atom}}$ (eV) | $E_{\text{Al repl Sn}}$ (eV) | $E_{\text{coh/atom}}$ (eV) | $E_{\text{Al repl Sn}}$ (eV) |
| Al_4Sn_2 | -2.33 | | -2.33 | |
| Al_3Sn_3 | -2.40 | 0.43 | -2.39 | 0.39 |
| Al_2Sn_4 | -2.53 | 0.80 | -2.52 | 0.77 |
| Sn_{10} | -2.89 | | -2.86 | |
| $AlSn_{10}$ | -2.87 | | -2.86 | |
| Sn_{11} | -2.84 | -0.39 | -2.81 | -0.51 |

In what follows we present a set of figures and tables showing the structures of the lowest energy configuration and several low-lying isomers of the investigated Al_mSn_n clusters at all compositions when the total number of atoms $N = m + n$ is equal to or smaller than $N = 6$, and for selected compositions for $N = 10$ and $N = 11$. The figures are ordered in families of increasing total number of atoms in the cluster. The members of a family with given cluster size are ordered by increasing content of Sn in the cluster. Finally for every cluster of fixed size and composition, the isomers are ordered by increasing energy. The reported Total Energy is the energy with respect to the lowest energy isomer of the cluster.

Each figure for a given Al_mSn_n cluster of fixed size and composition is followed by a table containing the energy (in eV), magnetic moment (in μ_B) and cartesian atomic coordinates (in Å) of the group of low-lying isomers, ordered by increasing energy. The isomers are numbered for easy identification. In the figures only a small number of low lying isomers have been plotted (between one to four for $N \leq 3$, and between four and six for $N > 3$). However, the table below each figure contains a more extensive account of all the isomers found in the calculations (about 10 isomers for $N > 3$, and in the case of $Al_{10}Sn$ we provide the coordinates of 43 isomers).

Al₂ isomers

Number of isomers: 1

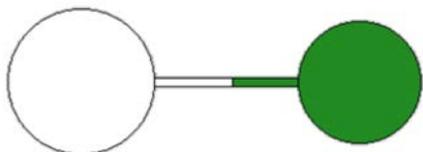


1

1
 Total energy 0
 Magnetic moment 2
 Geometry
 Al 1.369390 0.000003 -0.000002
 Al -1.369390 -0.000003 0.000002

AlSn isomers

Number of isomers: 1

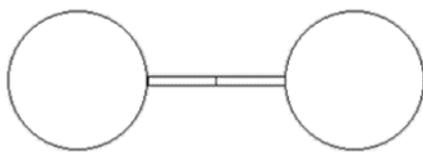


1

1
 Total energy 0
 Magnetic moment 1
 Geometry
 Al 1.334700 0.000000 0.000000
 Sn -1.337100 0.000000 0.000000

Sn2 isomers

Number of isomers: 1

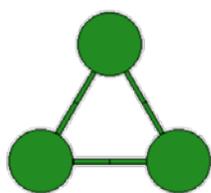


1

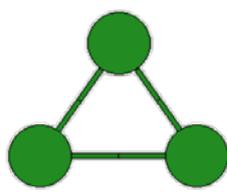
1
 Total energy 0
 Magnetic moment 2
 Geometry
 Sn 1.397236 0.000090 0.000107
 Sn -1.399713 0.000087 0.000075

Al3 isomers

Number of isomers: 3



1



2



3

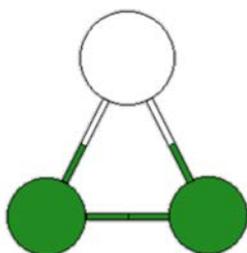
```
1
Total energy 0
Magnetic moment 1
Geometry
Al 1.254247 -0.088127 0.000000
Al -0.000367 2.085786 0.000000
Al -1.259409 -0.086547 0.000000
```

```
2
Total energy 0.19274
Magnetic moment 3
Geometry
Al 1.471982 -0.002467 0.000000
Al 0.000801 2.124050 -0.000001
Al -1.478779 0.001177 0.000003
```

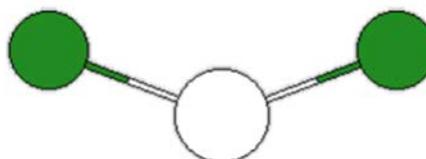
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3
Total energy 0.62348
Magnetic moment 3
Geometry
Al 2.614727 0.000000 0.000000
Al -0.000984 0.000000 0.000000
Al -2.615495 0.000000 0.000000
```

Al₂Sn isomers

Number of isomers: 4



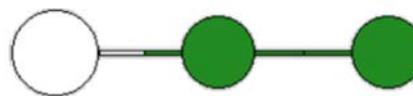
1



2



3



4

1

Total energy 0
Magnetic moment 0
Geometry
Al 0.087382 2.068273 0.000000
Al 1.292865 -0.037519 0.000000
Sn -1.395413 -0.173240 0.000000

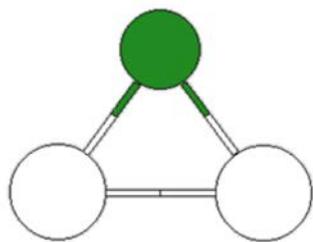
2
Total energy 0.45295
Magnetic moment 2
Geometry
Al -2.597734 0.998956 -0.000002
Al 2.597764 0.998966 0.000004
Sn 0.000009 0.001476 0.000000

3
Total energy 0.61775
Magnetic moment 0
Geometry
Al 2.795302 0.000002 -0.000004
Al -2.795302 -0.000002 0.000004
Sn 0.000000 0.000000 0.000000

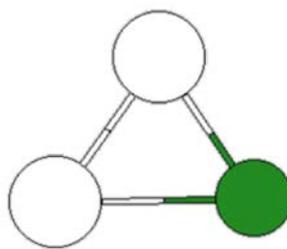
4
Total energy 0.66619
Magnetic moment 2
Geometry
Al 2.735049 -0.000015 0.000000
Al -0.041477 0.000010 0.000000
Sn -2.680579 -0.000001 0.000000

AlSn2 isomers

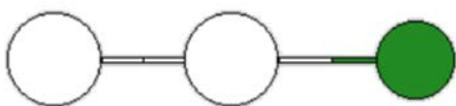
Number of isomers: 4



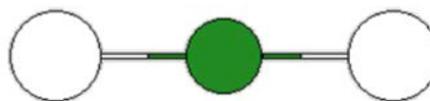
1



2



3



4

1
Total energy 0

Magnetic moment 1
 Geometry
 Al -0.001316 2.032896 0.000000
 Sn 1.505024 -0.068806 0.000000
 Sn -1.506921 -0.068200 0.000000

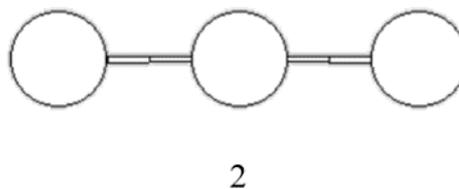
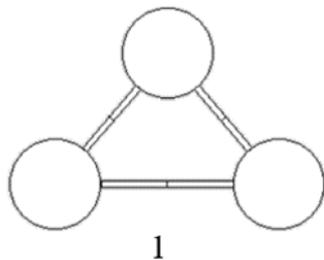
2
 Total energy 0.11412
 Magnetic moment 1
 Geometry
 Al 1.469146 -0.058665 0.000000
 Sn 0.014826 2.116175 -0.000002
 Sn -1.561901 -0.116580 -0.000007

3
 Total energy 0.55003
 Magnetic moment 1
 Geometry
 Al 2.743856 0.000000 -0.000002
 Sn -0.021536 0.000000 0.000000
 Sn -2.702084 0.000000 0.000000

4
 Total energy 0.99098
 Magnetic moment 1
 Geometry
 Al 0.016617 0.000000 -0.000005
 Sn 2.640529 0.000001 0.000062
 Sn -2.609932 0.000000 -0.000008

Sn3 isomers

Number of isomers: 2

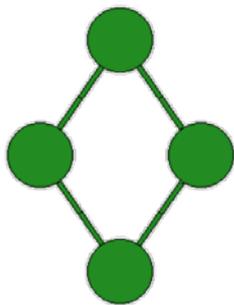


1
 Total energy 0
 Magnetic moment 0
 Geometry
 Sn 1.732984 0.088982 0.000000
 Sn -0.000985 2.154585 0.000000
 Sn -1.741692 0.095007 0.000000

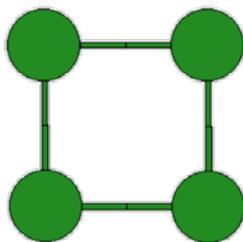
2
 Total energy 0.39121
 Magnetic moment 0
 Geometry
 Sn 2.656849 -0.001962 -0.001830
 Sn 0.000700 -0.000064 0.000018
 Sn -2.655466 -0.001651 -0.001515

Al4 isomers

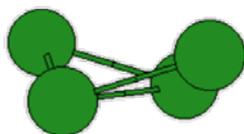
Number of isomers: 4



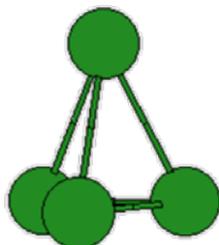
1



2



3



4

1

Total energy 0

Magnetic moment 2

Geometry

Al 0.000120 2.106835 0.000016

Al 1.439396 0.002268 0.000004

Al -0.000076 -2.100058 0.000025

Al -1.439592 0.002513 0.000006

2

Total energy 0.12097

Magnetic moment 2

Geometry

Al 0.000000 1.873977 0.000414

Al 1.872777 0.000000 0.000315

Al 0.000000 -1.873977 0.000414

Al -1.872777 0.000000 0.000315

3

Total energy 0.3024

Magnetic moment 4

Geometry

Al 0.000217 2.193410 0.863337

Al 0.000216 -2.193155 0.863173

Al 1.361808 0.000198 0.090303

Al -1.361172 0.000194 0.090547

4

Total energy 0.56843

Magnetic moment 0

Geometry

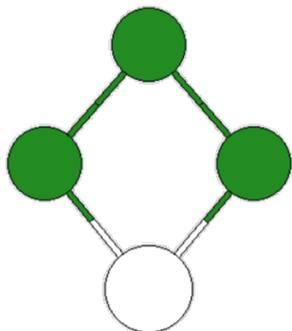
Al -0.041924 0.705807 2.598810

Al -0.015043 2.255816 -0.186767

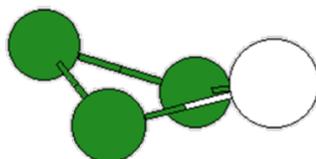
Al 1.241687 0.056907 -0.128510
Al -1.245205 0.056827 -0.102701

Al₃Sn isomers

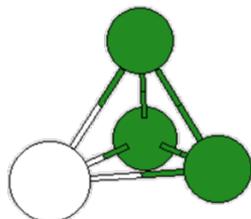
Number of isomers: 4



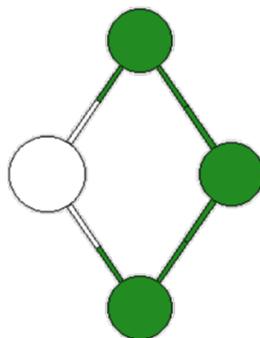
1



2



3



4

1
Total energy 0
Magnetic moment 1
Geometry
Al 0.000691 1.942754 -0.000002
Al 1.668102 0.021538 -0.000020
Al -1.671469 0.029262 -0.000021
Sn -0.006583 -2.000304 -0.000018

2
Total energy 0.39649
Magnetic moment 3
Geometry
Al -0.000163 2.152961 0.866864
Al 1.351693 0.045114 0.119054
Al -1.351996 0.045015 0.119204
Sn 0.000032 -2.159764 0.873150

3
Total energy 0.73984
Magnetic moment 3
Geometry
Al 0.118063 0.849461 2.213591
Al 0.112830 2.371889 0.053725
Al 1.451133 0.087420 0.057260

Sn -1.481181 -0.097590 -0.068727

4

Total energy 1.07907

Magnetic moment 1

Geometry

Al -0.000197 2.497353 -0.000003

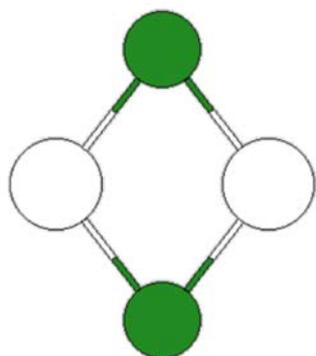
Al 1.698500 0.000000 -0.000001

Al -0.000196 -2.497354 0.000001

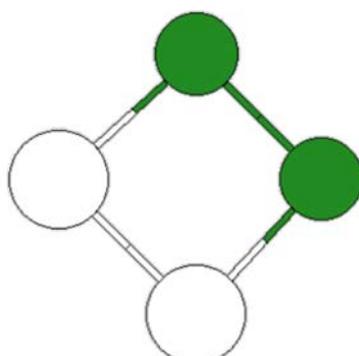
Sn -1.698020 -0.000001 -0.000001

Al₂Sn₂ isomers

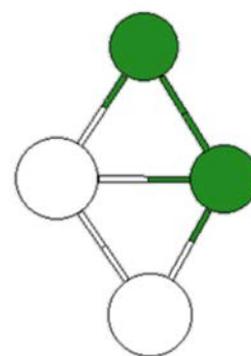
Number of isomers: 6



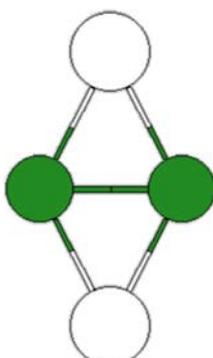
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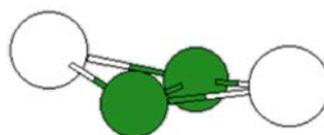
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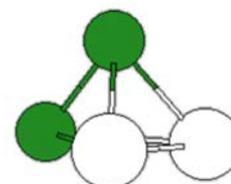
3



4



5



6

1

Total energy 0

Magnetic moment 0

Geometry

Al 0.000000 2.082283 -0.000001

Al 0.000000 -2.082281 0.000001

Sn 1.626248 0.000003 0.000001

Sn -1.626248 0.000003 -0.000001

2

Total energy 0.06937

Magnetic moment 0

Geometry

Al 1.782229 -0.003015 0.000000

Al -0.002431 1.782263 0.000000

Sn -0.005688 -1.945126 -0.000001

Sn -1.945614 -0.004481 0.000000

3

Total energy 0.72142

Magnetic moment 2

Geometry

Al 0.000621 2.332484 0.459441

Al 1.387562 0.045025 0.442896

Sn 0.102196 -2.268290 0.616171

Sn -1.484828 0.064315 0.317769

4

Total energy 0.76429

Magnetic moment 0

Geometry

Al 1.247564 -0.000087 0.000000

Al -1.247558 -0.000088 0.000000

Sn 0.000000 2.431217 0.000000

Sn 0.000000 -2.431398 0.000000

5

Total energy 0.77889

Magnetic moment 0

Geometry

Al 1.248599 0.000000 0.205035

Al -1.246955 -0.000006 0.203378

Sn 0.000455 2.384610 0.648678

Sn 0.000454 -2.384604 0.648703

6

Total energy 1.58265

Magnetic moment 0

Geometry

Al 0.000036 0.911693 2.023899

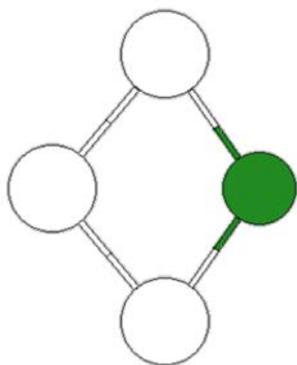
Al 0.006787 2.629083 0.213287

Sn 1.536124 -0.141701 -0.049552

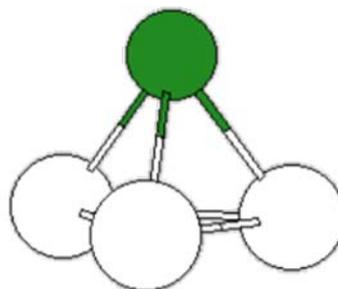
Sn -1.539547 -0.152206 -0.033393

AlSn3 isomers

Number of isomers: 2



1



2

1

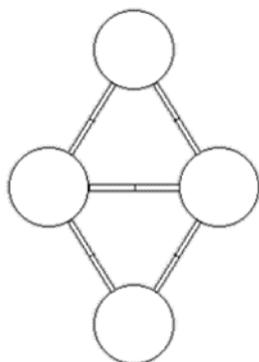
Total energy 0

Magnetic moment 1
 Geometry
 Al 1.573188 0.000235 0.000000
 Sn 0.059019 2.164261 0.000000
 Sn 0.058689 -2.163511 -0.000001
 Sn -1.752041 0.000479 0.000000

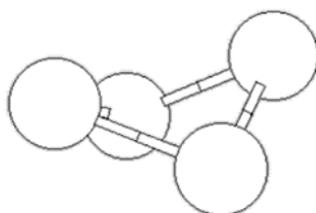
2
 Total energy 1.04974
 Magnetic moment 1
 Geometry
 Al 0.000769 0.769653 2.220899
 Sn -0.000533 2.462408 -0.011356
 Sn 1.464596 -0.073870 -0.010453
 Sn -1.464934 -0.073448 -0.011099

Sn4 isomers

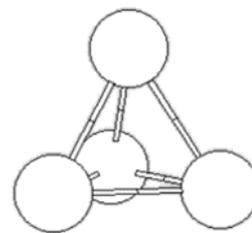
Number of isomers: 5



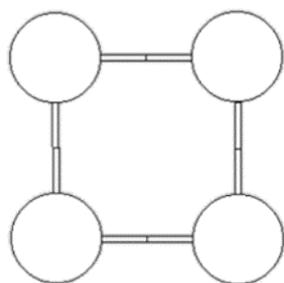
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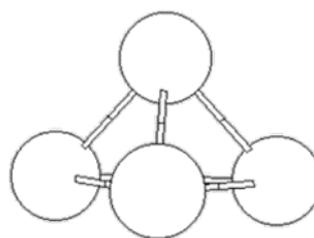
2



3



4



5

1
 Total energy 0
 Magnetic moment 0
 Geometry
 Sn 1.504995 0.000015 0.000035
 Sn 0.000006 2.429007 0.000221
 Sn 0.000026 -2.428994 0.000017
 Sn -1.504946 0.000002 0.000035

2
 Total energy 0.66967
 Magnetic moment 2

Geometry

Sn 1.758447 -1.037677 0.004881
Sn -0.141886 2.158865 -0.001984
Sn -0.076602 0.038593 1.843558
Sn -0.071385 0.033588 -1.841926

3

Total energy 1.18919

Magnetic moment 0

Geometry

Sn 0.000008 0.771162 2.407120
Sn 0.000002 2.526706 -0.075301
Sn 1.520314 -0.106380 -0.075189
Sn -1.520311 -0.106388 -0.075187

4

Total energy 1.28179

Magnetic moment 0

Geometry

Sn 2.010188 -0.000008 0.000000
Sn -0.000013 2.010373 0.000000
Sn 0.000013 -2.010373 0.000000
Sn -2.010188 0.000008 0.000000

5

Total energy 1.54847

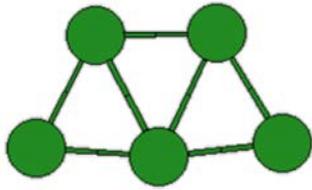
Magnetic moment 2

Geometry

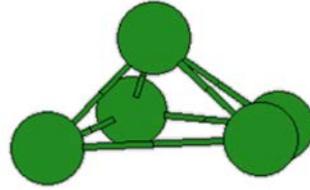
Sn -1.817061 -1.008215 0.084320
Sn 1.662011 -0.957728 0.089776
Sn -0.117636 2.033953 0.082809
Sn -0.090360 0.022483 -1.857832

A15 isomers

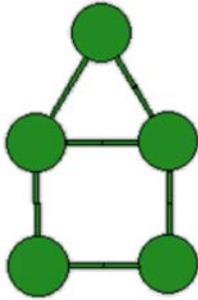
Number of isomers: 4



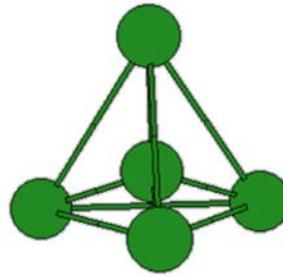
1



2



3



4

1

```
Total energy 0
Magnetic moment 1
Geometry
Al 2.665735 0.768596 0.000000
Al 0.738299 -0.841748 0.000000
Al -1.430949 -2.099234 0.000000
Al -1.732874 0.482078 0.000000
Al 0.306202 1.888216 0.000000
```

2

```
Total energy 0.04211
Magnetic moment 1
Geometry
Al 1.298194 -1.357246 0.020645
Al 0.110141 -0.390044 -2.064293
Al -1.536203 -0.405775 -0.178585
Al -0.999556 1.930091 0.408136
Al 0.220762 0.096959 1.876832
```

3

```
Total energy 0.14017
Magnetic moment 1
Geometry
Al -1.283124 -1.277279 0.000000
Al 1.282667 -1.277533 0.000000
Al -1.303461 1.206659 0.000000
Al 1.303536 1.206451 0.000000
Al 0.000111 3.462103 0.000000
```

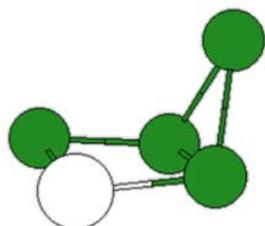
4

```
Total energy 1.19691
Magnetic moment 1
Geometry
```

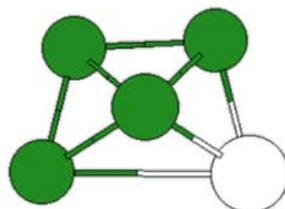
Al 0.155733 -0.001720 1.858368
 Al 2.633064 0.002552 0.978856
 Al -1.422631 2.070312 0.377275
 Al -1.412932 -2.064286 0.411650
 Al 0.013205 0.003356 -0.560571

Al4Sn isomers

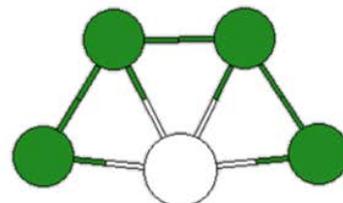
Number of isomers: 9



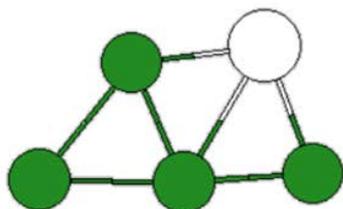
1



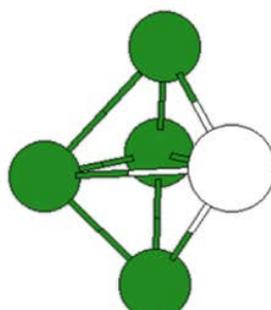
2



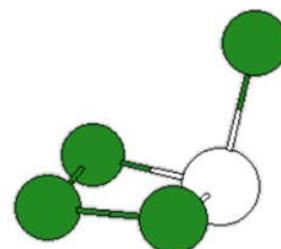
3



4



5



6

1

Total energy 0
 Magnetic moment 0
 Geometry

Al -0.236154 -0.458823 1.718103
 Al -2.133008 0.846830 0.677997
 Al 1.819331 0.197408 0.375861
 Al 0.708525 -2.342808 0.090533
 Sn -0.004710 1.861801 -0.516886

2

Total energy 0.0305
 Magnetic moment 0
 Geometry

Al -1.885133 0.040100 -0.022210
 Al -0.098885 1.956875 -0.004533
 Al -0.589382 -2.107112 0.379561
 Al 0.114479 -0.186724 1.848689
 Sn 2.136725 0.489003 0.371145

3

Total energy 0.04053
 Magnetic moment 0
 Geometry

Al -2.664552 0.035095 -0.000002
 Al 2.664552 0.035096 -0.000002
 Al -1.257754 2.284161 0.000000

Al 1.257753 2.284162 0.000000
Sn -0.000010 -0.244368 -0.000002

4

Total energy 0.10973
Magnetic moment 0
Geometry
Al -0.048658 -0.215487 0.000001
Al -2.809917 -0.216572 -0.000008
Al 2.457049 0.011036 -0.000003
Al -1.052693 2.099190 0.000000
Sn 1.521396 2.496022 -0.000004

5

Total energy 0.16842
Magnetic moment 2
Geometry
Al 1.231923 -1.219467 -0.198650
Al -0.184877 0.189636 1.964350
Al 0.005342 0.187703 -1.991537
Al -1.304086 -1.250761 0.152799
Sn -0.054530 1.999969 -0.021739

6

Total energy 0.17435
Magnetic moment 0
Geometry
Al -1.966400 -0.005172 -0.546321
Al 2.715168 -0.050127 0.394670
Al -0.696835 2.017966 0.416104
Al -0.694287 -2.028773 0.421705
Sn 0.378130 -0.000306 1.774404

7

Total energy 0.49893
Magnetic moment 0
Geometry
Al 1.434319 -0.905372 -0.077927
Al -0.086910 0.007949 -1.995144
Al -1.613770 -0.884768 -0.083861
Al -0.154984 1.802581 -0.081913
Sn -0.091784 0.029620 2.001749

8

Total energy 1.26397
Magnetic moment 0
Geometry
Al -0.000796 0.000000 2.712387
Al 2.546742 0.000000 -0.910441
Al -1.275817 2.214890 -0.896786
Al -1.275817 -2.214890 -0.896786
Sn -0.000126 0.000000 0.000117

9

Total energy 1.5452
Magnetic moment 0
Geometry
Al 0.178313 0.288615 0.159102

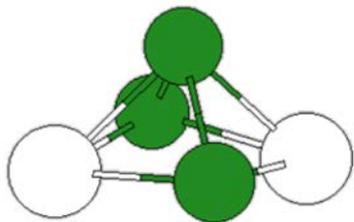
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Al -0.505949 -0.857187 2.435145
Al 2.231913 -0.677780 -1.176036
Al -1.680654 1.577378 -1.202477
Sn -1.029962 -1.782461 -0.816900

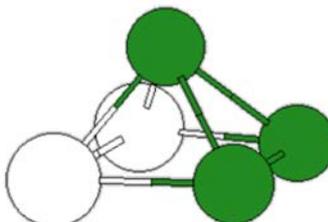
```

Al3Sn2 isomers

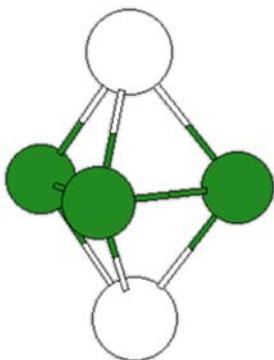
Number of isomers: 4



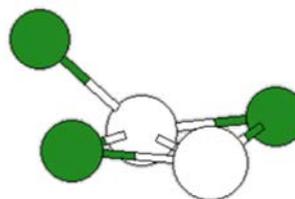
1



2



3



4

1

```

Total energy 0
Magnetic moment 1
Geometry
Al -2.041711 -0.000025 0.273162
Al -0.018644 -0.000037 1.880751
Al 2.052689 -0.000033 0.348589
Sn -0.004317 -1.964205 0.002041
Sn -0.004244 1.964078 0.002074

```

2

```

Total energy 0.08605
Magnetic moment 1
Geometry
Al -0.044198 0.041671 1.743295
Al 1.945037 -0.052287 -0.063818
Al 0.076170 -1.939114 -0.032535
Sn 0.212097 2.090559 0.075485
Sn -2.091797 -0.234293 0.061429

```

3

```

Total energy 0.38227
Magnetic moment 1
Geometry
Al -1.228973 -0.701208 0.000206
Al 1.303295 -1.225785 0.000286

```

Al -0.423336 1.754321 0.000912
Sn 0.146895 0.086636 2.260391
Sn 0.147313 0.086550 -2.260058

4

Total energy 0.45858

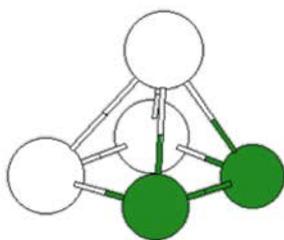
Magnetic moment 1

Geometry

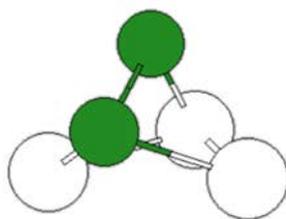
Al 1.870047 -0.003387 0.100711
Al 0.000099 1.979989 0.166408
Al -0.026743 -1.972927 0.091019
Sn 0.152036 -0.038973 2.274276
Sn -1.900262 0.020511 -0.075341

Al₂Sn₃ isomers

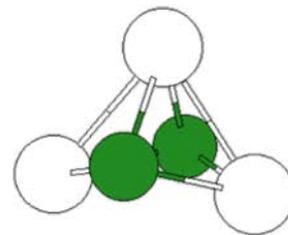
Number of isomers:6



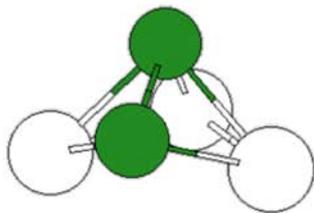
1



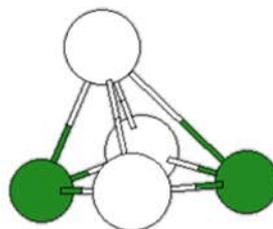
2



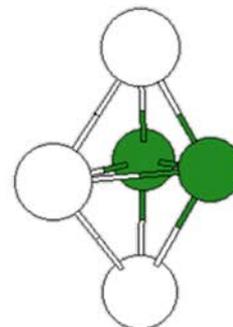
3



4



5



6

1

Total energy 0

Magnetic moment 2

Geometry

Al -0.023969 1.836649 -0.090317
Al -1.825901 0.007929 -0.151124
Sn -0.055210 0.095736 2.261467
Sn 1.944925 0.011799 -0.336845
Sn -0.012573 -1.962952 -0.211377

2

Total energy 0.03664

Magnetic moment 0

Geometry

Al -0.006192 0.000025 1.997745

Al -1.900935 -0.000053 0.432736
Sn 2.109097 0.008903 0.525301
Sn -0.068472 1.905909 -0.314996
Sn -0.059035 -1.892389 -0.327607

3

Total energy 0.0872

Magnetic moment 2

Geometry

Al 0.129204 0.091480 2.012400
Al 0.155298 0.099317 -2.002167
Sn -1.540886 -0.876691 -0.000904
Sn 1.503526 -1.266786 0.005482
Sn -0.350297 1.955332 0.003045

4

Total energy 0.17533

Magnetic moment 2

Geometry

Al 0.029210 0.020165 2.200986
Al -1.155527 -0.659082 0.066146
Sn 0.043939 0.028708 -2.276006
Sn 1.494751 -1.304395 0.031925
Sn -0.374675 1.953039 0.030597

5

Total energy 0.18583

Magnetic moment 0

Geometry

Al -0.001229 -1.958021 -0.373371
Al -0.001852 1.843416 0.054252
Sn -1.854578 0.010742 0.151403
Sn 0.004296 0.261792 2.562799
Sn 1.851708 0.015152 0.135899

6

Total energy 0.23781

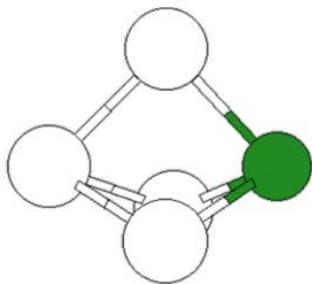
Magnetic moment 0

Geometry

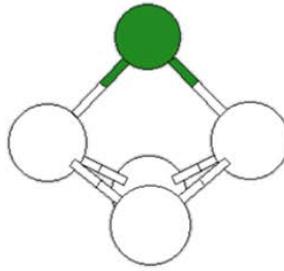
Al 1.304776 -0.960059 -0.330535
Al -1.130119 -0.865853 0.155902
Sn -0.255165 0.090013 2.445519
Sn 0.148376 -0.139727 -2.503396
Sn 0.040175 1.786296 0.074102

AlSn4 isomers

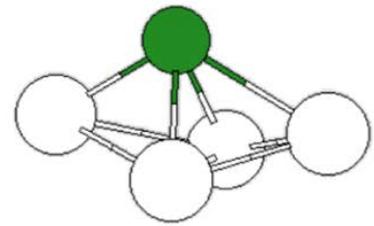
Number of isomers: 5



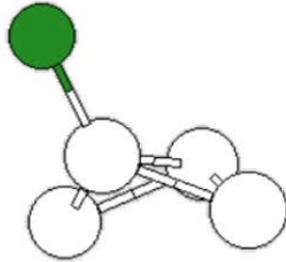
1



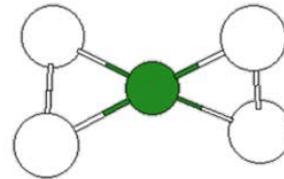
2



3



4



5

1

Total energy 0

Magnetic moment 1

Geometry

| | | | |
|----|-----------|-----------|-----------|
| Al | -0.060382 | 0.005043 | 1.868008 |
| Sn | -0.115944 | 0.039168 | -2.041046 |
| Sn | -1.780623 | -1.098728 | 0.012271 |
| Sn | 1.582535 | -0.907619 | 0.034136 |
| Sn | -0.040583 | 2.055971 | 0.005750 |

2

Total energy 0.05879

Magnetic moment 1

Geometry

| | | | |
|----|-----------|-----------|-----------|
| Al | 1.672106 | -0.962138 | 0.000327 |
| Sn | 0.002948 | -0.027084 | 1.827168 |
| Sn | 0.004281 | -0.030213 | -1.828809 |
| Sn | -1.984663 | -1.033912 | -0.000714 |
| Sn | -0.183133 | 2.191174 | -0.002825 |

3

Total energy 0.45836

Magnetic moment 1

Geometry

| | | | |
|----|-----------|-----------|-----------|
| Al | 0.000068 | 0.588492 | 1.711210 |
| Sn | 1.645093 | -0.012843 | -0.409696 |
| Sn | -0.000491 | 2.676370 | 0.137136 |
| Sn | -0.000201 | -2.237860 | 0.442759 |
| Sn | -1.645275 | -0.012378 | -0.409848 |

4

Total energy 0.9835

Magnetic moment 1

Geometry

| | | | |
|----|----------|-----------|----------|
| Al | 0.000511 | -0.113931 | 3.356275 |
|----|----------|-----------|----------|

Sn -0.014752 1.462244 -1.672019
 Sn 2.119781 -0.367400 -1.201124
 Sn -2.146696 -0.362498 -1.172355
 Sn -0.002522 -0.574976 0.680566

5

Total energy 1.323

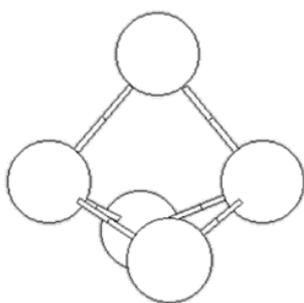
Magnetic moment 1

Geometry

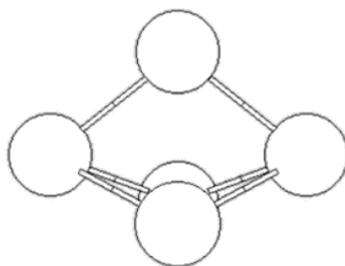
Al -0.000318 -0.007069 -0.006718
 Sn -0.214153 1.062796 2.461191
 Sn 0.220707 2.674309 0.201046
 Sn 1.402595 -1.777401 -1.485320
 Sn -1.380643 -2.007014 -1.179690

Sn5 isomers

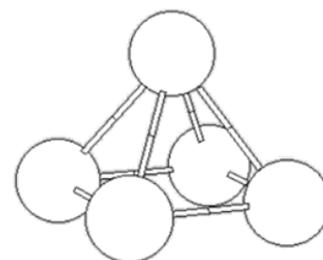
Number of isomers: 5



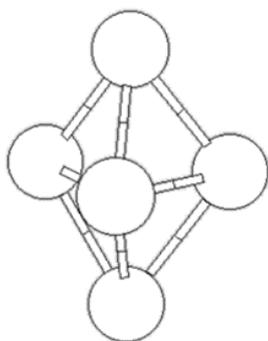
1



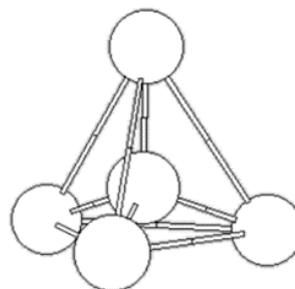
2



3



4



5

Sn

Total energy 0

Magnetic moment 0

Geometry

Sn -1.953710 -1.090931 -0.000269
 Sn 1.800421 -1.035660 0.005286
 Sn -0.119573 2.194940 -0.002079
 Sn -0.096008 0.027908 1.827619
 Sn -0.090373 0.022145 -1.826005

2

Total energy 0.5338

Magnetic moment 2

Geometry

Sn -2.188766 0.060947 -0.223952
Sn 2.189547 -0.059581 -0.223172
Sn 0.047978 1.724789 -1.213049
Sn -0.046702 -1.721743 -1.214638
Sn 0.000037 0.000021 1.541339

3

Total energy 0.74008

Magnetic moment 0

Geometry

Sn -2.010066 0.000001 -0.156452
Sn 2.010066 -0.000001 -0.156452
Sn 0.000000 2.009998 -0.156408
Sn 0.000000 -2.009998 -0.156408
Sn 0.000000 0.000000 2.175532

4

Total energy 0.80034

Magnetic moment 0

Geometry

Sn -1.327547 -0.760963 0.000436
Sn 1.581460 -1.106572 -0.000471
Sn -0.165310 1.928220 -0.000237
Sn -0.077725 -0.039680 2.425235
Sn -0.077132 -0.039632 -2.424796

5

Total energy 4.2563

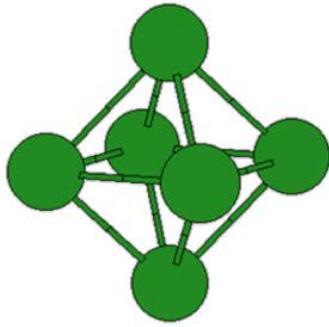
Magnetic moment 0

Geometry

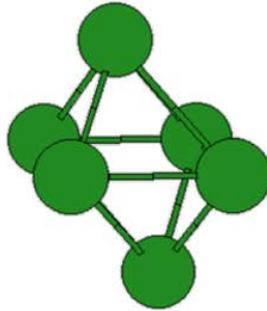
Sn -0.000227 0.002133 2.723974
Sn -0.000295 2.569509 -0.905851
Sn 2.231325 -1.278499 -0.906890
Sn -2.231425 -1.278329 -0.906814
Sn 0.000045 -0.000846 -0.000882

A16 isomers

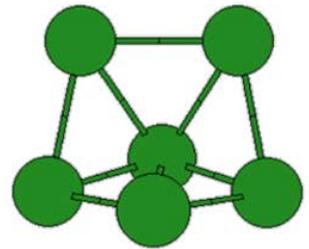
Number of isomers: 5



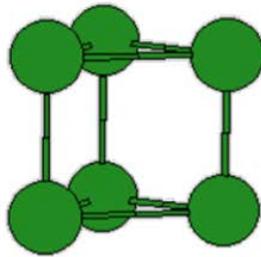
1



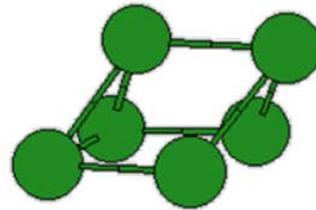
2



3



4



5

1

```
Total energy 0
Magnetic moment 2
Geometry
Al 1.332447 -0.914618 -1.041890
Al 0.102885 1.521687 -1.161907
Al -0.123612 -1.548703 1.160150
Al -1.336629 0.883002 1.045647
Al 1.387519 0.931677 0.964766
Al -1.391589 -0.947303 -0.972439
```

2

```
Total energy 0.01701
Magnetic moment 0
Geometry
Al -1.500001 -1.139634 0.176442
Al 1.025710 -1.516097 -0.122733
Al 0.172395 0.074448 -1.947298
Al 1.451201 1.401496 -0.165566
Al -0.196805 0.188072 1.948006
Al -1.069799 1.772893 0.118145
```

3

```
Total energy 0.18212
Magnetic moment 0
Geometry
Al -1.972134 0.758059 -0.113328
Al 1.329376 -1.488568 0.491829
Al -1.219337 -1.763592 -0.006455
Al -0.208381 -0.053086 1.872844
Al 0.252851 1.981770 0.466652
Al 1.581528 0.476867 -1.186014
```

4

```
Total energy 0.24475
```

Magnetic moment 0

Geometry

Al -1.490067 -0.696185 -0.028049
Al -0.002289 1.405765 2.561275
Al 1.502315 -0.669851 2.548092
Al -1.479362 -0.686799 2.553771
Al 0.000348 1.390161 -0.094430
Al 1.497112 -0.689565 -0.032868

5

Total energy 0.52912

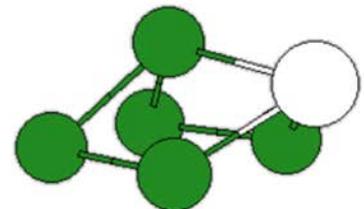
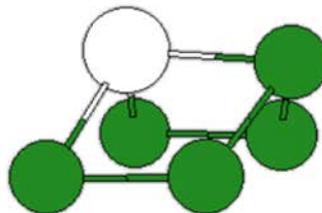
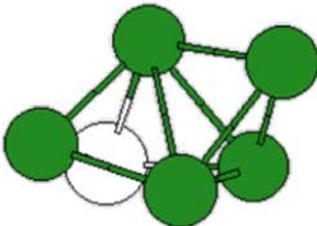
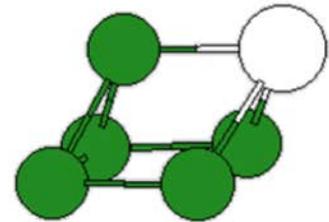
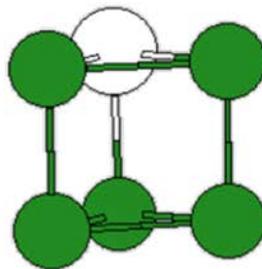
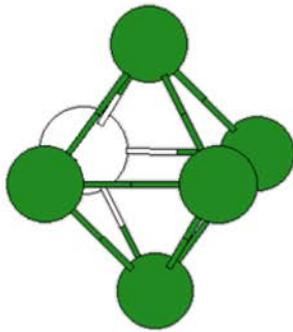
Magnetic moment 2

Geometry

Al -1.846830 -0.023678 -0.053785
Al 1.969909 -0.085665 -0.063498
Al -0.087121 1.969289 -0.062287
Al -0.024491 -1.844208 -0.056398
Al -0.069076 -0.068945 1.833304
Al 1.840595 1.840236 1.737156

Al5Sn isomers

Number of isomers: 6



1

Total energy 0

Magnetic moment 1

Geometry

Al 1.416987 -0.875304 -1.036979
Al 0.016900 1.511091 -1.228230
Al 0.030382 -1.478393 1.295054

Al -1.327537 0.911967 1.108907
Al 1.311008 0.825456 0.977828
Sn -1.399319 -0.906245 -1.061525

2

Total energy 0.25939

Magnetic moment 1

Geometry

Al 1.573666 1.572373 1.649505
Al -1.703499 0.255934 -0.005606
Al 2.023320 0.070041 -0.463911
Al 0.063644 2.030689 -0.457297
Al 0.257502 -1.702543 -0.003858
Sn -0.239430 -0.239915 2.299457

3

Total energy 0.89962

Magnetic moment 1

Geometry

Al -1.795495 0.033651 -0.007475
Al 2.149591 -0.285688 -0.085770
Al -0.252813 2.094279 -0.136369
Al 0.062501 -1.797869 -0.013006
Al -0.098433 -0.112776 1.909688
Sn 1.785204 1.783960 1.750187

4

Total energy 0.91912

Magnetic moment 1

Geometry

Al 1.841714 1.647432 1.753635
Al 1.914615 0.020351 -0.383531
Al -0.066407 1.987089 -0.047765
Al 0.195087 -1.818429 0.196523
Al -0.220630 0.060055 1.975845
Sn -1.909116 -0.001484 -0.187272

5

Total energy 1.1138

Magnetic moment 1

Geometry

Al 0.002476 2.197221 0.583633
Al 1.864877 0.794392 -0.480247
Al -1.864837 0.801909 -0.480329
Al 1.947928 -1.626274 0.547182
Al -1.972239 -1.609959 0.564234
Sn -0.000830 -0.272175 1.879315

6

Total energy 1.16288

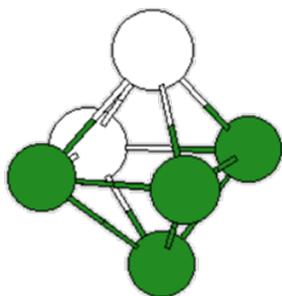
Magnetic moment 3

Geometry

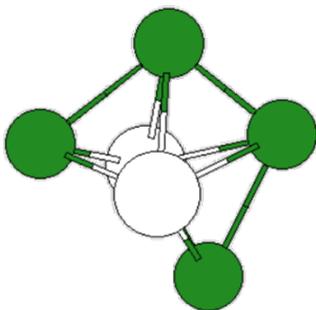
Al 1.612015 0.686548 -0.304102
Al -1.639276 0.683841 -0.273567
Al 1.392316 -1.873738 0.304244
Al -1.355658 -1.875709 0.293488
Al 0.008361 -0.174857 1.727344
Sn -0.003152 2.568454 0.744583

Al₄Sn₂ isomers

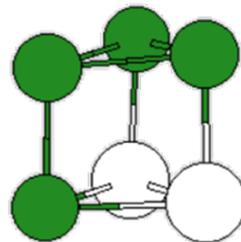
Number of isomers: 12



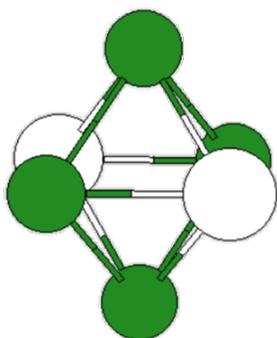
1



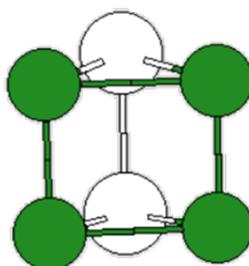
2



3



4



5

1

Total energy 0
Magnetic moment 0
Geometry

Al 0.939800 -1.348071 0.049492
Al -1.347833 -0.175794 0.069786
Al -0.759845 1.422188 2.384330
Al -0.763094 -1.150748 2.355445
Sn 1.787372 -0.087473 2.326107
Sn 0.770177 1.604658 0.125291

2

Total energy 0.28546
Magnetic moment 0
Geometry

Al -0.393293 0.486939 2.132328
Al -1.222790 1.709564 -0.192160
Al 1.146349 -1.604408 -0.474434
Al -0.183988 0.295049 -1.940796
Sn -1.386705 -1.210559 0.313549
Sn 1.576709 0.907676 0.366215

3

Total energy 0.35684
Magnetic moment 0
Geometry

Al -1.438065 -0.843962 -0.026389

Al 0.097792 1.543781 2.601797
Al 1.406692 -0.686276 2.605081
Al -1.318149 -0.766177 2.441202
Sn -0.097964 1.635064 -0.000193
Sn 1.369060 -0.923451 0.007312

4

Total energy 0.48816

Magnetic moment 0

Geometry

Al 1.417742 -0.933508 -1.093615
Al -0.004219 1.535524 -1.283110
Al -0.010075 -1.546834 1.303382
Al -1.417353 0.906829 1.095681
Sn 1.334546 0.828444 1.006649
Sn -1.320787 -0.858976 -1.015014

5

Total energy 0.60955

Magnetic moment 0

Geometry

Al -1.675100 0.279380 0.012242
Al 1.981648 0.002146 -0.556093
Al -0.001498 1.984283 -0.556995
Al 0.284210 -1.677076 0.014143
Sn -0.396587 -0.393954 2.390230
Sn 1.507695 1.509353 1.716585

6

Total energy 0.6313

Magnetic moment 0

Geometry

Al -1.203580 1.669353 -0.010299
Al -1.600621 -1.029867 -0.006189
Al 1.069147 -1.424219 0.005152
Al 1.494859 1.239500 0.009170
Sn -0.058121 0.126812 -2.096943
Sn -0.081485 0.129218 2.092788

7

Total energy 0.67496

Magnetic moment 2

Geometry

Al 0.172533 -0.422988 2.066803
Al 1.208547 1.980361 1.761462
Al -1.857995 0.423761 0.551600
Al 2.011651 -0.062308 0.197404
Sn 0.030557 1.784704 -0.768642
Sn -0.199512 -1.511469 -0.592358

8

Total energy 0.79376

Magnetic moment 2

Geometry

Al -0.352951 0.178069 2.150948
Al 2.034103 1.206063 1.877606
Al -1.792404 -0.120450 -0.452835
Al -0.229563 1.860750 0.158317

Sn 0.280851 -1.791057 0.319430
Sn 1.891371 0.282047 -0.733897

9

Total energy 0.89989

Magnetic moment 0

Geometry

Al -2.250330 0.481381 0.836975
Al 1.131592 -1.594926 -0.082903
Al -1.442607 -1.792347 0.195440
Al 0.095326 -0.045291 1.731139
Sn -0.117858 1.473562 -0.690991
Sn 2.451500 0.862604 0.732867

10

Total energy 1.03044

Magnetic moment 2

Geometry

Al -0.050670 -0.050030 1.957992
Al 1.766829 1.765749 1.910809
Al -1.828335 -0.021033 -0.001836
Al -0.022065 -1.825292 -0.002630
Sn 2.030805 -0.120990 -0.273379
Sn -0.122352 2.030253 -0.272585

11

Total energy 1.51659

Magnetic moment 2

Geometry

Al 1.655349 0.688205 -0.483863
Al -1.621402 0.681796 -0.497767
Al 1.894692 -1.709939 0.479100
Al -1.875640 -1.714719 0.474376
Sn 0.006461 -0.321746 1.883738
Sn 0.006406 2.494288 0.627804

12

Total energy 1.52705

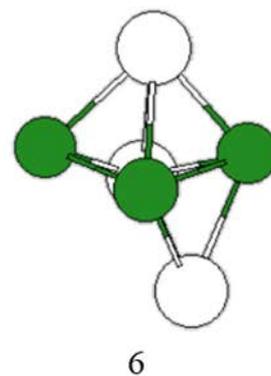
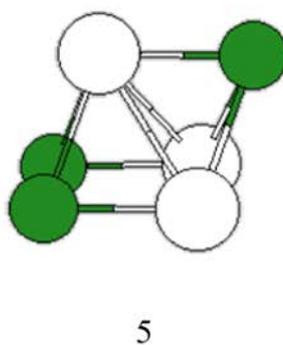
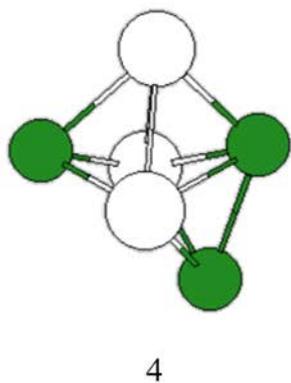
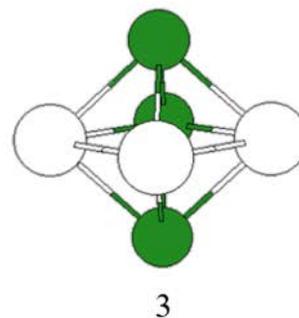
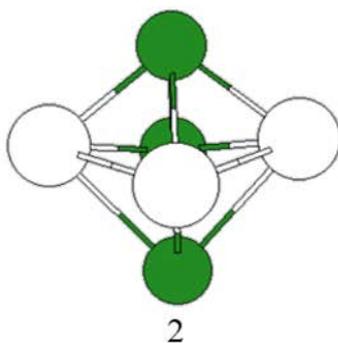
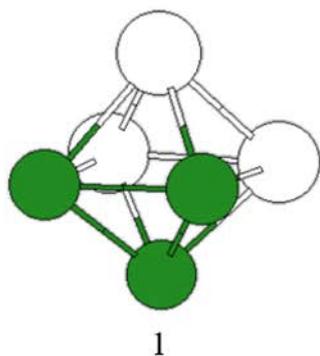
Magnetic moment 0

Geometry

Al -0.021876 -0.015576 1.717291
Al 1.947104 1.937601 1.930047
Al 1.926837 -0.018666 -0.115711
Al -0.022430 1.919712 -0.114838
Sn 0.069117 -2.046993 -0.049636
Sn -2.056000 0.065314 -0.058061

Al3Sn3 isomers

Number of isomers: 13



```

1
Total energy 0
Magnetic moment 1
Geometry
Al -1.459403 -1.029161 0.011490
Al 1.154990 -1.645766 0.067086
Al -0.064590 0.055619 1.815806
Sn -1.399676 1.864979 0.071661
Sn -0.048226 0.106408 -2.002578
Sn 1.609779 1.252120 0.060706

2
Total energy 0.06362
Magnetic moment 1
Geometry
Al -1.213554 1.700997 -0.011689
Al -1.407792 -1.106462 -0.007905
Al 1.124080 -1.490733 0.007064
Sn -0.345252 0.228936 2.133329
Sn -0.303252 0.223817 -2.135982
Sn 1.594331 1.169007 0.017431

3
Total energy 0.09516
Magnetic moment 1
Geometry
Al -1.290905 -0.849259 -0.983125
Al 1.363061 -0.920211 -1.064865
Al -1.391473 0.870418 1.061032
Sn -0.126944 1.554834 -1.435392
Sn -0.115534 -1.699583 1.309656
Sn 1.400273 0.869484 1.052507

```

4

Total energy 0.16945

Magnetic moment 1

Geometry

Al 1.986908 1.482376 1.684742
Al -0.193920 2.072477 0.180227
Al 0.285566 -1.895676 0.461572
Sn -1.535731 -0.001494 -0.690671
Sn 1.657908 0.093062 -0.704322
Sn -0.307664 0.049410 2.220136

5

Total energy 0.36187

Magnetic moment 1

Geometry

Al 1.785935 1.786149 1.888299
Al -0.001012 -1.809375 -0.080632
Al -1.811291 0.001723 -0.079573
Sn 1.971566 -0.086086 -0.347719
Sn -0.086664 1.972633 -0.347756
Sn -0.071341 -0.069727 2.222718

6

Total energy 0.39946

Magnetic moment 1

Geometry

Al -0.083408 1.980872 0.119683
Al 0.373617 -1.848853 0.509048
Al -0.370279 0.199335 1.976683
Sn -1.635201 -0.157859 -0.611652
Sn 1.795682 0.039302 -0.751309
Sn 2.107821 1.402836 1.887684

7

Total energy

0.42742

Magnetic moment

1

Geometry

Al 0.154731 1.600275 -0.205976
Al 1.499831 -0.633614 -0.219299
Al -1.149362 -0.696243 0.199622
Sn -0.041820 1.621979 2.440417
Sn 1.384204 -0.875261 2.419171
Sn -1.638978 -0.945588 2.745026

8

Total energy

0.48617

Magnetic moment

1

Geometry

Al 1.721276 1.721338 1.824785
Al 1.907833 0.092498 -0.394794
Al 0.093560 1.908703 -0.393096
Sn -1.875778 0.206652 -0.042775
Sn 0.203538 -1.876188 -0.043747

Sn -0.131829 -0.133737 2.326094

9

Total energy

0.70422

Magnetic moment

1

Geometry

Al -1.955893 0.705939 0.000341
Al -1.144616 -1.724573 -0.011891
Al -0.080260 -0.032045 1.745148
Sn -0.190380 2.581656 0.891459
Sn 1.601687 0.526252 -0.430805
Sn 1.380273 -2.203767 0.867825

10

Total energy

0.73805

Magnetic moment

1

Geometry

Al 0.053506 -0.083149 1.966316
Al -0.077703 1.958753 -0.158551
Al -1.758854 0.074533 -0.109039
Sn 1.950487 -0.073128 -0.357191
Sn -0.122122 -2.067398 0.107940
Sn 1.674525 2.006548 2.008910

11

Total energy

0.8247

Magnetic moment

3

Geometry

Al -0.297242 0.110246 2.036432
Al 1.912028 1.501962 1.768893
Al -0.272185 2.225339 0.403752
Sn -1.641892 -0.001498 -0.486279
Sn 1.594128 0.108312 -0.680622
Sn 0.232736 -2.128686 0.550469

12

Total energy

0.94455

Magnetic moment

1

Geometry

Al 0.006773 0.006081 1.991375
Al 1.864346 -0.015498 -0.275525
Al -0.016808 1.864140 -0.280591
Sn -1.972251 0.075290 -0.024878
Sn 0.074302 -1.970972 -0.029570
Sn 1.881818 1.882839 1.965301

13

Total energy

0.96531

Magnetic moment

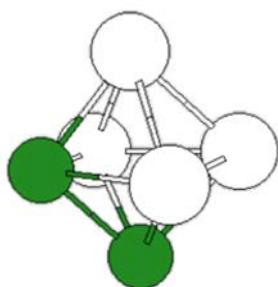
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1
Geometry
Al -0.233845 -0.079601 1.763895
Al 0.224561 1.653002 -0.109988
Al 1.131248 -1.207575 -0.123063
Sn -2.389042 0.816038 0.338758
Sn -1.434221 -2.148679 0.489549
Sn 2.647498 0.861619 0.743733

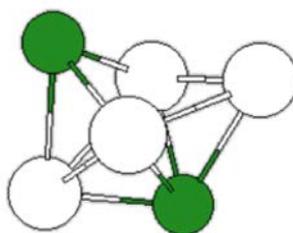
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Al₂Sn₄ isomers

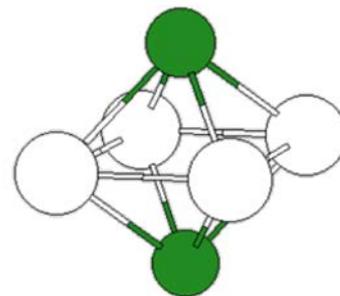
Number of isomers: 13



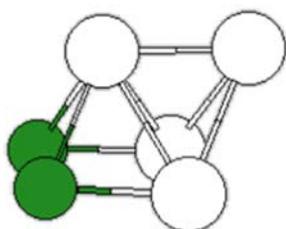
1



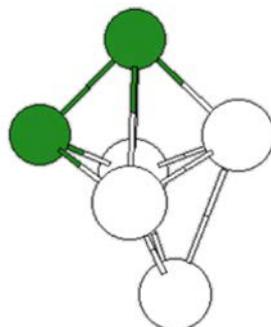
2



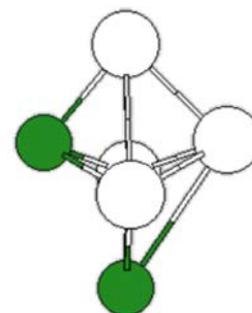
3



4



5



6

```

1
Total energy 0
Magnetic moment 0
Geometry
Al -0.100763 0.114859 1.795259
Al -1.471443 -0.954769 -0.005503
Sn -1.516507 1.923999 0.107068
Sn 1.230070 -1.829323 0.122590
Sn -0.049081 0.146288 -1.990589
Sn 1.582935 1.274103 0.064081

```

```

2
Total energy 0.26386
Magnetic moment 0
Geometry
Al 1.904056 1.220291 1.788856
Al -1.197100 0.080616 -0.483034
Sn -0.483475 0.075880 2.184623
Sn 1.566484 0.188673 -0.664275
Sn -0.356603 2.521918 0.193118

```

Sn 0.353721 -2.197214 0.525435

3

Total energy 0.35413

Magnetic moment 0

Geometry

Al 1.420627 0.872807 1.080831
Al -1.419315 -0.932938 -1.068385
Sn 1.267873 -0.837221 -0.990476
Sn 0.006055 1.805770 -1.509045
Sn 0.004576 -1.817978 1.527564
Sn -1.274036 0.813772 0.978976

4

Total energy 0.47231

Magnetic moment 0

Geometry

Al -0.063466 -1.854326 -0.098638
Al -1.855701 -0.062313 -0.097993
Sn -0.059439 -0.060023 2.165620
Sn 1.912736 1.913109 2.032302
Sn 1.936789 -0.097461 -0.354383
Sn -0.098135 1.936695 -0.353994

5

Total energy 0.48913

Magnetic moment 0

Geometry

Al -0.495737 0.738458 1.858594
Al -1.531417 2.145936 -0.119015
Sn -1.220435 -1.232613 0.167938
Sn 1.474974 -1.979602 -0.535313
Sn -0.335084 0.505797 -1.964429
Sn 1.593239 0.816087 0.164968

6

Total energy 0.51717

Magnetic moment 0

Geometry

Al 1.909315 -0.368980 0.102304
Al 0.843938 2.547917 1.830663
Sn 0.286740 -0.216758 2.206644
Sn -1.860782 0.276646 0.393614
Sn 0.365566 1.596770 -0.808279
Sn -0.179743 -1.796442 -0.808650

7

Total energy

0.72585

Magnetic moment

0

Geometry

Al -0.097400 1.413366 0.148628
Al 1.192254 -0.781152 0.158809
Sn -1.677839 -0.972121 -0.479684
Sn 0.200087 1.801464 2.736582
Sn 1.669075 -0.721056 2.747394
Sn -1.296189 -0.759606 2.298737

8

Total energy
0.7907
Magnetic moment
0

Geometry

Al -1.892289 0.514490 -0.080783
Al 0.058730 1.926386 -0.099585
Sn 2.374529 0.864264 0.762782
Sn 0.681751 -0.944093 -0.831655
Sn -1.527816 -1.991833 0.806063
Sn -0.012872 0.054805 2.280873

9

Total energy
0.97936
Magnetic moment
2

Geometry

Al -0.223097 1.841097 -0.266102
Al 1.824415 0.370041 -0.263278
Sn -2.510189 0.829717 0.849641
Sn 1.594955 -2.130432 0.826800
Sn -0.833911 -1.164250 -0.544759
Sn 0.009422 -0.005315 2.194674

10

Total energy
0.99128
Magnetic moment
2

Geometry

Al -1.348924 -0.909542 -0.001922
Al 1.292355 1.035604 0.010228
Sn -0.134860 0.191940 2.145072
Sn -1.443054 1.993835 -0.048490
Sn 1.331708 -1.793342 0.031246
Sn -0.072477 0.143451 -2.145300

11

Total energy
1.20409
Magnetic moment
0

Geometry

Al -0.001094 -0.184424 1.722895
Al 0.007753 1.510445 -0.410700
Sn 2.371967 1.105985 0.985304
Sn -2.355859 1.120373 0.978268
Sn 1.449917 -1.672489 0.026077
Sn -1.445563 -1.703860 0.052170

12

Total energy
1.42106
Magnetic moment
2

```

Geometry
Al 0.000127 1.584373 2.482516
Al -0.000168 1.590091 0.005290
Sn 1.502874 -0.785342 -0.159821
Sn -1.502981 -0.786222 -0.157402
Sn 1.504766 -0.788201 2.662861
Sn -1.504938 -0.787383 2.665295

```

```

13
Total energy
1.44913
Magnetic moment
0

```

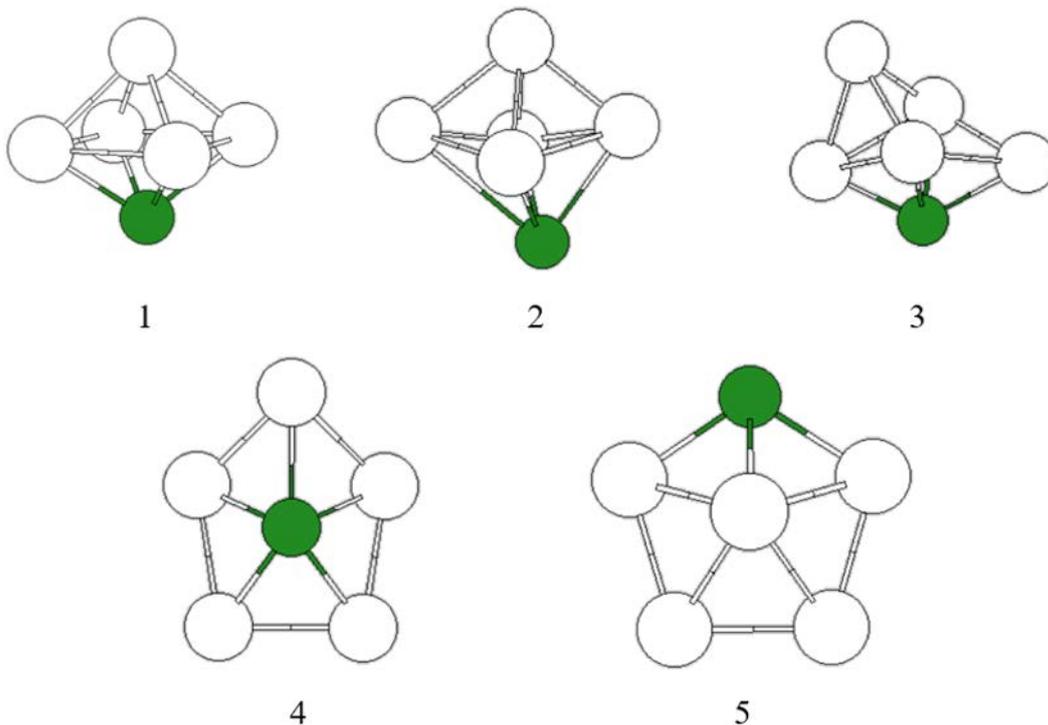
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Geometry
Al -0.172360 -0.173774 1.431204
Al 1.975914 1.964443 1.773115
Sn -2.366286 0.155978 -0.062018
Sn 2.142771 -0.191117 -0.032770
Sn -0.189244 2.151651 -0.014055
Sn 0.150611 -2.372217 -0.054577

```

AlSn5 isomers

Number of isomers: 5



```

1
Total energy 0
Magnetic moment 1
Geometry
Al -1.207079 -0.777705 -0.922979
Sn 1.443663 -1.005254 -1.187439
Sn -0.031991 1.750016 -1.519870
Sn -0.039578 -1.812115 1.466063
Sn -1.538734 0.926203 1.111664

```

Sn 1.376982 0.864679 1.048182

2

Total energy 0.12814

Magnetic moment 1

Geometry

Al 1.171769 2.111443 1.727488
Sn -2.166633 0.444791 0.757358
Sn 2.507018 -0.263917 0.105845
Sn 0.143544 1.470679 -0.706146
Sn -0.082367 -1.488818 -0.594782
Sn 0.255239 -0.412148 2.151315

3

Total energy 0.34356

Magnetic moment 1

Geometry

Al 0.664433 1.316584 0.280768
Sn 1.356180 -1.224389 -0.696573
Sn -1.425308 -0.520777 0.233369
Sn -0.794367 1.718163 2.438192
Sn 1.265408 -0.646340 2.212052
Sn -1.441282 -1.241267 3.008561

4

Total energy 0.83325

Magnetic moment 1

Geometry

Al 0.000014 -0.052614 1.448195
Sn 0.000598 2.712373 0.762901
Sn 1.956908 0.775161 -0.260237
Sn -1.956780 0.776435 -0.259798
Sn 1.490860 -2.151095 0.431882
Sn -1.486477 -2.150932 0.426918

5

Total energy 1.70013

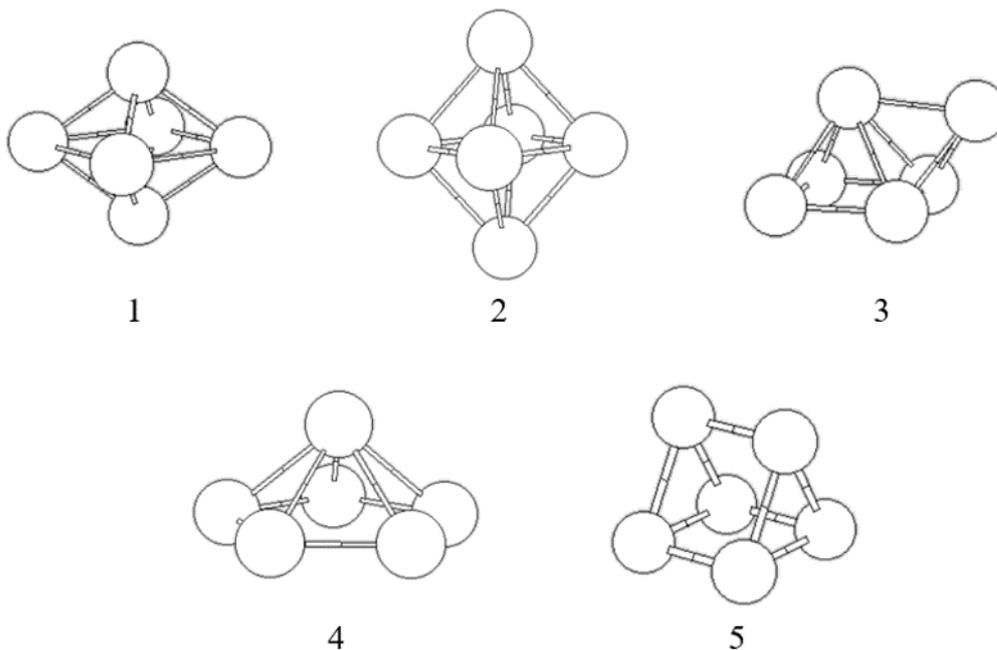
Magnetic moment 1

Geometry

Al 0.000000 2.377312 0.169119
Sn 2.286428 0.838250 0.153702
Sn -2.286430 0.838252 0.153731
Sn 1.458365 -2.011063 0.142724
Sn -1.458349 -2.011055 0.142727
Sn 0.000012 -0.033181 1.981050

Sn6 isomers

Number of isomers: 5



1

Total energy 0

Magnetic moment 0

Geometry

Sn 0.009835 1.926805 -0.129469
 Sn 1.690769 -0.974838 -0.100926
 Sn -1.197801 -0.703822 0.259811
 Sn -0.009056 -1.926513 2.630989
 Sn 1.197881 0.703470 2.241396
 Sn -1.690756 0.975560 2.600653

2

Total energy 0.6143

Magnetic moment 0

Geometry

Sn -1.457329 -0.944738 -1.117591
 Sn 1.447436 -0.952298 -1.123699
 Sn 0.001813 1.765473 -1.472860
 Sn -0.001983 -1.775414 1.490566
 Sn -1.455135 0.927092 1.120325
 Sn 1.466085 0.918508 1.114580

3

Total energy 0.77739

Magnetic moment 0

Geometry

Sn -2.119728 0.085438 -0.155007
 Sn 2.034084 -0.113879 -0.185173
 Sn -0.114427 2.033163 -0.185549
 Sn 0.084456 -2.116755 -0.158064
 Sn -0.086577 -0.086829 2.124699
 Sn 2.002938 2.002680 1.879838

4

Total energy 1.64692

Magnetic moment 0

Geometry

```

Sn 0.000002 2.422652 0.113666
Sn 2.305170 0.748871 0.111635
Sn -2.305173 0.748875 0.111656
Sn 1.425306 -1.962116 0.105759
Sn -1.425298 -1.962112 0.105770
Sn 0.000025 -0.012767 2.211837

```

5

Total energy 2.1954

Magnetic moment 2

Geometry

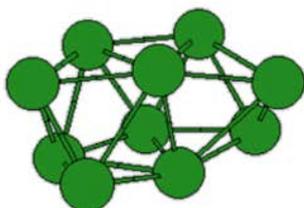
```

Sn 0.000311 1.736269 -0.183699
Sn 1.502587 -0.867518 -0.179697
Sn -1.501361 -0.866891 -0.175743
Sn 0.000055 1.732898 2.676594
Sn 1.502002 -0.867976 2.679818
Sn -1.503651 -0.869198 2.684444

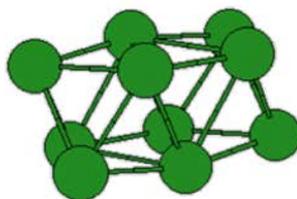
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All10 isomers

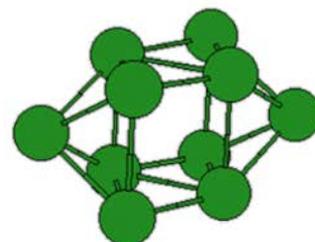
Number of isomers: 11



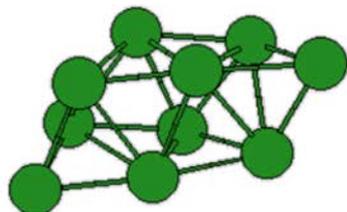
1



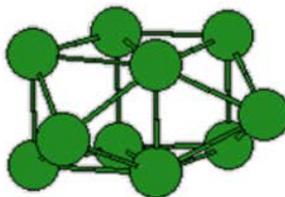
2



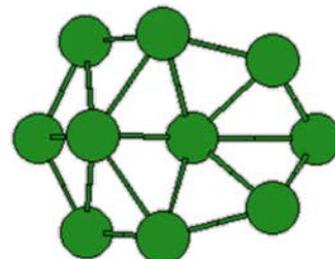
3



4



5



6

1

Total energy 0

Magnetic moment 0

Geometry

```

Al 2.248611 -0.766113 1.911314
Al 0.466485 1.415453 0.691073
Al -1.886596 0.099755 1.072120
Al -0.277999 -2.071505 1.236595
Al 0.958868 2.182203 -1.895048
Al -1.689528 1.243886 -1.253307
Al -1.226702 -1.415962 -1.104578
Al 1.325709 -0.598031 -0.660394
Al -0.066930 -0.085461 2.955715
Al -0.083055 0.024631 -2.975523

```

2

Total energy 0.09215

Magnetic moment 0

Geometry

Al 2.066157 -0.007166 0.694901
Al -2.344556 1.337340 1.219072
Al -2.320211 -1.335128 1.244235
Al -2.249322 0.018412 -1.055886
Al -0.092232 1.669294 -0.189838
Al 2.150149 1.335889 -1.609023
Al 2.170835 -1.333948 -1.573730
Al -0.087054 -1.670490 -0.182613
Al -0.228090 -0.012189 2.146285
Al 0.056594 0.011899 -2.517297

3

Total energy 0.11312

Magnetic moment 0

Geometry

Al 1.454487 0.000217 -2.557473
Al -0.763422 1.399534 -2.283343
Al -0.763137 -1.399411 -2.283162
Al 1.322902 1.335271 -0.274734
Al -1.323326 1.334712 0.274548
Al -1.322884 -1.335294 0.274744
Al 1.323308 -1.334731 -0.274557
Al -1.454487 -0.000216 2.557473
Al 0.763421 -1.399538 2.283344
Al 0.763138 1.399407 2.283161

4

Total energy 0.28048

Magnetic moment 2

Geometry

Al -1.505070 1.109125 1.460183
Al -2.143498 -1.626046 1.033702
Al 0.529881 -0.765971 1.068254
Al -2.060870 0.146341 -1.020246
Al 0.261917 1.402996 -0.549651
Al 1.909421 1.415239 -2.633089
Al 1.789035 -0.830149 -1.227444
Al -0.580557 -2.105289 -1.034996
Al -1.142632 -0.653720 3.270437
Al -0.188525 -0.242701 -2.918655

5

Total energy 0.3287

Magnetic moment 0

Geometry

Al 0.015102 0.148179 1.414963
Al -0.015072 0.148164 -1.414990
Al 2.380332 1.210561 1.356279
Al -2.379185 1.133500 1.335395
Al 2.379164 1.133565 -1.335379
Al -2.380284 1.210566 -1.356255
Al -0.000454 2.821389 1.267665
Al 0.000486 2.821395 -1.267660

Al 2.370070 3.411862 -0.032389
Al -2.370009 3.411792 0.032484

6

Total energy 0.90966

Magnetic moment 0

Geometry

Al 2.723815 1.125496 0.341611
Al 1.805366 2.674796 -1.426925
Al -0.014411 2.957396 0.294460
Al 0.276013 0.390531 -0.530710
Al -1.802080 1.329937 1.021555
Al -2.935675 -0.410199 -0.299321
Al -1.784222 -2.628995 -0.850505
Al 0.729307 -2.844906 -0.407011
Al 1.971819 -1.213017 0.941012
Al -0.789269 -1.228423 1.165713

7

Total energy

1.1394

Magnetic moment

2

Geometry

Al 1.914675 -0.000011 1.333833
Al 0.000040 1.913818 1.332560
Al -1.914674 0.000011 1.333832
Al -0.000037 -1.913818 1.332560
Al 1.914601 -0.000020 -1.333985
Al 0.000036 1.913805 -1.332546
Al -1.914599 0.000020 -1.333985
Al -0.000032 -1.913805 -1.332546
Al -0.000003 0.000000 3.270921
Al -0.000002 0.000000 -3.270995

8

Total energy

1.24159

Magnetic moment

0

Geometry

Al 2.903470 -0.007369 0.000000
Al 1.392506 1.939668 0.000000
Al 0.011825 4.141043 -0.000005
Al -1.387439 1.959521 0.000000
Al -2.885426 0.003340 0.000000
Al -1.392612 -1.958227 0.000000
Al -0.000669 -4.146453 0.000004
Al 1.386179 -1.951494 0.000000
Al -0.007128 -0.000269 1.388866
Al -0.007128 -0.000270 -1.388866

9

Total energy

1.26725

Magnetic moment

2

Geometry

Al 2.272461 -0.002339 -1.155256
Al 0.702732 2.159952 -1.168138
Al -1.836668 1.331849 -1.163245
Al -1.840607 -1.337614 -1.151365
Al 0.699017 -2.159734 -1.147815
Al -2.272461 0.002339 1.155256
Al -0.699017 2.159734 1.147815
Al 1.840607 1.337614 1.151365
Al 1.836668 -1.331849 1.163245
Al -0.702732 -2.159952 1.168138

10

Total energy

1.31319

Magnetic moment

2

Geometry

Al 2.571977 -0.000016 1.113648
Al -2.075437 1.325785 1.164871
Al -2.075438 -1.325785 1.164871
Al -2.536643 -0.000001 -1.077392
Al -0.773531 2.075154 -1.136820
Al 2.070837 1.402161 -1.217877
Al 2.070837 -1.402163 -1.217879
Al -0.773520 -2.075155 -1.136802
Al -0.102199 -0.000002 2.523713
Al 0.109487 0.000008 0.001488

11

Total energy

2.34658

Magnetic moment

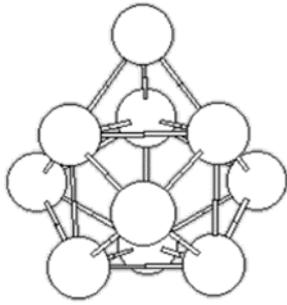
2

Geometry

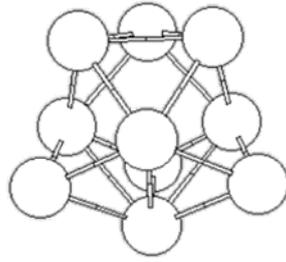
Al 2.245103 -0.004942 -1.313483
Al 0.687936 2.131746 -1.314759
Al -1.823348 1.324058 -1.313837
Al -1.819717 -1.317619 -1.315397
Al 0.686633 -2.140778 -1.313777
Al 2.245129 -0.004931 1.313471
Al 0.687926 2.131804 1.314821
Al -1.823360 1.324047 1.313840
Al -1.819756 -1.317620 1.315376
Al 0.686635 -2.140781 1.313685

Sn10 isomers

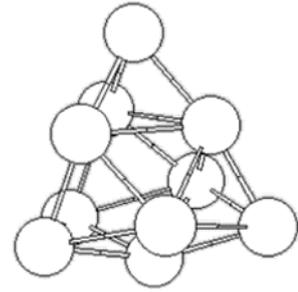
Number of isomers: 11



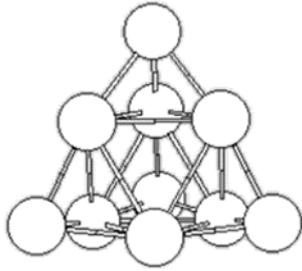
1



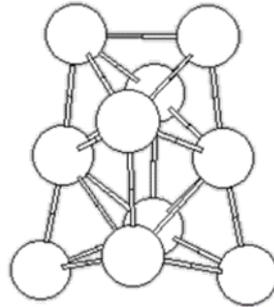
2



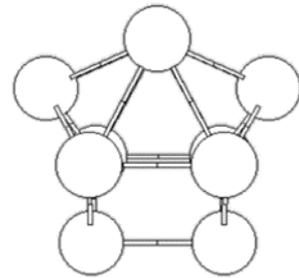
3



4



5



6

1

Total energy 0
Magnetic moment 0
Geometry

Sn 1.800286 0.000000 -1.546901
Sn -0.880601 1.551752 -1.547029
Sn -0.880601 -1.551752 -1.547029
Sn 1.944330 0.000000 1.518746
Sn -0.941189 1.672714 1.508610
Sn -0.941189 -1.672714 1.508610
Sn 1.524166 2.597911 0.043819
Sn 1.524166 -2.597910 0.043819
Sn -2.983868 0.000000 0.053223
Sn 0.005748 0.000000 3.685111

2

Total energy 0.08401
Magnetic moment 0
Geometry

Sn 2.886072 -0.000024 -1.527859
Sn -1.442058 2.503706 -1.499691
Sn -1.442110 -2.503714 -1.499763
Sn 1.784770 -0.000006 1.867507
Sn -0.901246 1.551251 1.856458
Sn -0.901269 -1.551244 1.856570
Sn 1.141100 1.959083 -0.343558
Sn 1.140973 -1.959085 -0.343514
Sn -2.288393 -0.000015 -0.345762
Sn -0.011371 0.000005 -2.659873

3

Total energy 0.7598
Magnetic moment 0
Geometry

Sn 0.067446 1.581583 -2.263154
Sn 0.067442 -1.581587 -2.263153
Sn 1.888570 -0.000003 -0.594969
Sn 1.071692 2.543700 0.749787
Sn -1.721855 1.631403 0.051823
Sn -1.721855 -1.631404 0.051825
Sn 1.071692 -2.543701 0.749792
Sn -3.003070 0.000000 2.056356
Sn -0.142714 0.000000 2.387436
Sn 2.676187 0.000002 2.184740

4

Total energy 0.96254

Magnetic moment 0

Geometry

Sn 2.090598 0.001270 1.533778
Sn -0.798823 1.642453 1.111692
Sn -0.799312 -1.639176 1.109338
Sn -1.316517 0.003834 -1.700625
Sn -1.008439 2.859153 -1.490995
Sn 1.562119 1.655588 -1.257408
Sn 1.561165 -1.650939 -1.262708
Sn -1.010734 -2.852156 -1.494445
Sn -0.088159 0.000087 3.369708
Sn 3.844711 0.000800 -0.739307

5

Total energy 1.01279

Magnetic moment 0

Geometry

Sn -0.411947 2.018494 -2.628193
Sn 0.165112 -0.519649 -1.543733
Sn 2.459164 -0.768757 0.577075
Sn 1.186337 2.108109 -0.056560
Sn -2.030335 1.317767 -0.166073
Sn -1.868578 -1.831001 0.424389
Sn 0.808952 -3.164847 -0.658755
Sn 0.539039 -2.623573 2.313359
Sn -0.107877 0.156657 2.087248
Sn -0.788123 2.892961 2.101604

6

Total energy 1.03236

Magnetic moment 0

Geometry

Sn -0.036087 1.434783 -2.344624
Sn -0.036087 -1.434787 -2.344630
Sn 2.445007 0.000000 -1.073952
Sn 1.049350 2.460289 0.187633
Sn -2.296042 1.471518 -0.537130
Sn -2.296039 -1.471514 -0.537130
Sn 1.049345 -2.460285 0.187632
Sn -0.983859 -1.435068 2.044724
Sn 1.798730 0.000000 1.921758
Sn -0.983858 1.435066 2.04471

7

Total energy

1.22959
Magnetic moment
0

Geometry
Sn 3.060703 -0.267903 -1.406630
Sn 0.952674 1.898359 -1.263988
Sn -1.855280 1.044246 -1.258052
Sn -2.373310 -1.930001 -1.404135
Sn 0.391569 -1.259652 -1.611558
Sn -3.060582 0.267666 1.406461
Sn -0.391229 1.259554 1.610940
Sn 2.373381 1.929946 1.404027
Sn 1.855321 -1.044176 1.257843
Sn -0.952537 -1.898481 1.263848

8
Total energy
1.30677
Magnetic moment
0

Geometry
Sn -2.070917 1.487564 1.281214
Sn -2.095053 -1.523823 1.311888
Sn 0.777165 -2.423904 1.272673
Sn -2.668204 -0.036589 -1.347578
Sn -0.776732 2.422037 -1.281141
Sn 1.744145 1.257433 -0.452499
Sn 2.059077 -1.500095 -1.295019
Sn -0.866355 -2.527529 -1.351807
Sn 0.451038 0.329271 2.124814
Sn 0.011402 0.011819 -2.903546

9
Total energy
2.09454
Magnetic moment
0

Geometry
Sn 2.804787 0.016713 -0.005862
Sn 0.538606 1.971840 -0.786352
Sn -0.012152 4.444126 0.518423
Sn -1.748461 2.366644 1.462071
Sn -2.207130 0.575627 -0.871151
Sn -1.527715 -2.171361 0.195390
Sn -0.183964 -4.690983 0.264443
Sn 1.672120 -2.595429 0.313444
Sn 0.132487 0.023196 1.613353
Sn 0.415693 -0.921463 -1.957980

10
Total energy
2.14922
Magnetic moment
0

Geometry
Sn 2.536901 0.000000 1.350271
Sn -1.961882 1.680225 1.360169
Sn -1.961883 -1.680226 1.360168

```

Sn -2.509800 -0.000001 -1.495393
Sn -0.890006 2.605245 -1.363704
Sn 2.029771 1.562395 -1.308629
Sn 2.029771 -1.562396 -1.308628
Sn -0.890007 -2.605246 -1.363705
Sn -0.042552 -0.000002 3.069844
Sn -0.013568 -0.000001 0.000227

```

11

Total energy

2.73998

Magnetic moment

2

Geometry

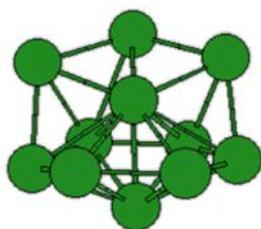
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Sn 2.136516 0.000007 1.481132
Sn 0.000003 2.136472 1.481163
Sn -2.136514 0.000007 1.481136
Sn 0.000003 -2.136469 1.481168
Sn 2.136515 0.000012 -1.481137
Sn 0.000007 2.136470 -1.481171
Sn -2.136515 0.000012 -1.481131
Sn 0.000007 -2.136471 -1.481160
Sn 0.000008 0.000013 3.664660
Sn -0.000008 -0.000012 -3.664660

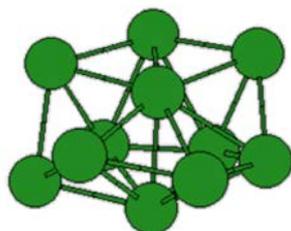
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All 11 isomers

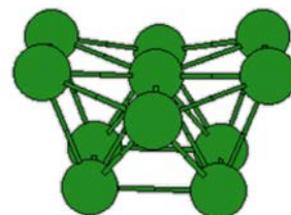
Number of isomers: 15



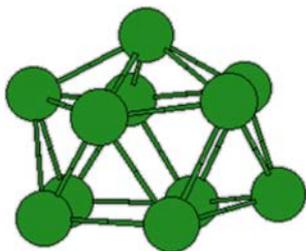
1



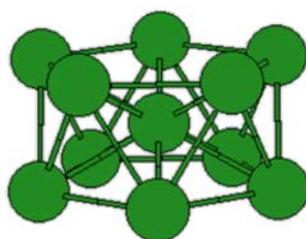
2



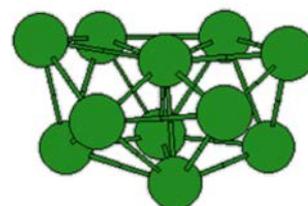
3



4



5



6

1

Total energy 0

Magnetic moment 1

Geometry

```

Al -0.017331 -0.001482 -1.468297
Al 2.617381 0.040658 -0.365892

```

Al 1.321777 2.247196 -0.461744
Al -1.236197 2.159055 -0.371435
Al -2.579753 -0.024659 -0.151645
Al -1.294819 -2.170500 -0.029551
Al 1.256533 -2.148507 -0.468365
Al 0.188313 0.130604 1.147620
Al -2.048990 1.438856 2.070275
Al 0.427502 -2.447735 2.056479
Al -1.773130 -1.105376 2.686491

2

Total energy 0.00969

Magnetic moment 1

Geometry

Al 2.060655 0.076893 1.358849
Al 1.824203 1.507321 -1.048631
Al 0.388565 1.978231 1.570449
Al -0.561028 2.632462 -0.865941
Al -2.120697 1.473469 0.986609
Al -2.859096 -0.981890 0.510803
Al -0.980028 -2.700540 -0.001695
Al 1.262911 -2.411017 1.296219
Al 1.991978 -1.236103 -1.006147
Al -0.568077 -0.597819 1.962455
Al -0.390637 -0.077879 -0.621960

3

Total energy 0.15392

Magnetic moment 1

Geometry

Al -0.320684 1.257533 -2.159115
Al -0.298715 -1.421557 -2.096451
Al 2.034932 -0.035812 -1.831453
Al 1.426930 2.363657 -0.430768
Al -1.976711 1.342084 -0.101650
Al -1.980649 -1.423474 -0.059165
Al 1.520484 -2.419373 -0.370188
Al -0.160651 -2.315840 1.705062
Al -1.519108 -0.021508 2.224862
Al -0.189117 2.264240 1.692082
Al 0.389206 -0.031511 0.292645

4

Total energy 0.20868

Magnetic moment 1

Geometry

Al 2.636402 -0.181800 0.995361
Al 0.094648 0.656378 0.459018
Al -2.459091 1.533213 0.985968
Al -1.898713 -1.045232 1.426778
Al 0.633379 -1.683184 1.752056
Al -2.372311 -0.206895 -1.127978
Al -1.408716 2.341799 -1.240778
Al 2.268225 1.379555 -1.077235
Al 1.975288 -1.340929 -1.344091
Al -0.414800 -1.849118 -0.788139
Al 0.109024 0.538361 -2.248353

5

Total energy 0.2839

Magnetic moment 1

Geometry

Al 2.376121 0.000056 -1.202919
Al 0.717744 2.276401 -1.169822
Al -1.963467 1.406780 -1.124788
Al -1.964353 -1.406994 -1.124573
Al 0.717792 -2.276391 -1.169723
Al -2.376127 0.000045 1.202919
Al -0.717747 2.276406 1.169841
Al 1.963650 1.406914 1.124826
Al 1.964626 -1.407132 1.124507
Al -0.717783 -2.276392 1.169744
Al -0.000006 0.000035 -0.000002

6

Total energy 0.47939

Magnetic moment 3

Geometry

Al -0.422318 0.910569 -2.081327
Al -0.027261 -1.715435 -2.188369
Al 2.095781 0.040738 -1.622392
Al 1.040636 2.431748 -0.513204
Al -1.790525 1.802443 0.046964
Al -1.819370 -0.824040 -0.466346
Al 1.611885 -2.336852 -0.228737
Al -0.525412 -2.353481 1.431731
Al -1.596067 -0.045967 2.233652
Al -0.073027 2.241307 1.973333
Al 0.550168 0.004785 0.51243

7

Total energy

0.48926

Magnetic moment

3

Geometry

Al 0.003052 -1.332903 2.659808
Al 0.000573 -1.354058 -2.633980
Al 2.312042 -0.437945 1.392106
Al -2.319994 -0.475123 1.396761
Al 2.320318 -0.463553 -1.354700
Al -2.329992 -0.490382 -1.350583
Al -0.005706 1.234520 2.261482
Al -0.008105 1.222064 -2.260753
Al 1.354820 1.664548 -0.003127
Al -1.379473 1.630477 0.000101
Al 0.000007 -0.759464 0.008875

8

Total energy

0.56169

Magnetic moment

1

Geometry

Al 0.000320 0.000016 -1.634336
Al 2.577251 -0.050985 -0.423110

Al 1.228299 2.127702 -0.103101
Al -1.340013 2.276710 -0.226973
Al -2.576673 0.050750 -0.422512
Al -1.228091 -2.128002 -0.104185
Al 1.339756 -2.276799 -0.226322
Al -0.000291 -0.000034 0.986442
Al -2.153126 0.833933 2.182866
Al 2.152932 -0.835290 2.182197
Al -0.000137 -0.000641 3.665496

9

Total energy

0.65857

Magnetic moment

1

Geometry

Al 2.429155 -0.010445 1.177449
Al -1.854454 1.449978 1.208481
Al -1.934847 -1.436885 1.264111
Al -2.908369 0.002167 -0.745305
Al -0.901750 1.599096 -1.503431
Al 1.956426 1.436708 -1.141721
Al 2.009808 -1.459138 -1.190335
Al -0.985251 -1.580944 -1.627826
Al 0.015006 -0.002281 2.672293
Al 0.670766 -0.000776 -2.958551
Al 0.095699 -0.104212 0.114041

10

Total energy

0.66716

Magnetic moment

1

Geometry

Al -0.050582 1.424881 -1.867414
Al -0.046985 -1.464541 -1.850270
Al 2.235705 -0.010515 -1.874353
Al 1.977367 1.753361 0.007316
Al -2.355979 1.406240 -0.765824
Al -2.359739 -1.402820 -0.761114
Al 1.984127 -1.759357 0.025373
Al -2.457874 0.001885 1.445825
Al -0.292031 0.044902 3.023711
Al 2.144039 0.007545 1.970607
Al -0.072440 -0.004688 0.367281

11

Total energy

0.86343

Magnetic moment

1

Geometry

Al 0.000041 -0.015374 -1.303493
Al 2.609667 0.002231 -0.377439
Al 1.257053 2.243184 -0.127512
Al -1.257172 2.243085 -0.127016
Al -2.609670 0.001791 -0.376019
Al -1.353164 -2.167701 -0.199846

Al 1.353669 -2.167840 -0.199661
Al 0.000216 0.047310 1.347640
Al -2.514568 1.119853 2.014109
Al 2.516142 1.120128 2.011944
Al -0.000045 -2.571471 2.011047

12

Total energy

1.43309

Magnetic moment

1

Geometry

Al 2.377577 -0.000002 1.331408
Al -1.886044 1.384478 1.167922
Al -1.886043 -1.384478 1.167924
Al -2.347537 -0.000001 -1.167553
Al -0.704652 2.164891 -1.141455
Al 1.873601 1.519487 -1.276614
Al 1.873602 -1.519487 -1.276610
Al -0.704648 -2.164891 -1.141455
Al -0.000115 0.000000 2.536786
Al 3.942775 0.000001 -0.767357
Al 0.117227 0.000001 -0.026966

13

Total energy

1.77305

Magnetic moment

1

Geometry

Al 1.944045 0.000034 1.767405
Al -0.000001 1.944042 1.767185
Al -1.944001 0.000034 1.767316
Al -0.000001 -1.943963 1.767071
Al 1.943928 0.000039 -1.767089
Al 0.000012 1.944027 -1.766769
Al -1.943922 0.000038 -1.767127
Al 0.000012 -1.943958 -1.766667
Al 0.000002 -0.000004 3.744159
Al -0.000003 -0.000003 -3.744116
Al 0.000003 0.000014 0.000008

14

Total energy

1.96079

Magnetic moment

1

Geometry

Al 1.992744 0.000000 1.680757
Al 0.000000 1.991807 1.681627
Al -1.992744 0.000000 1.680757
Al 0.000000 -1.991807 1.681627
Al 1.411656 1.411650 -1.694487
Al -1.411656 1.411650 -1.694487
Al -1.411656 -1.411650 -1.694487
Al 1.411656 -1.411650 -1.694487
Al 0.000000 0.000000 3.447785
Al 0.000000 0.000000 -3.460187

Al 0.000000 0.000000 -0.007771

15

Total energy

4.50577

Magnetic moment

1

Geometry

Al 3.130068 0.000000 -0.000111

Al 2.214405 2.214464 0.000061

Al 0.000000 3.130408 -0.000109

Al -2.214405 2.214464 0.000061

Al -3.130068 0.000000 -0.000111

Al -2.214405 -2.214464 0.000061

Al 0.000000 -3.130408 -0.000109

Al 2.214405 -2.214464 0.000061

Al 0.000000 0.000000 2.636522

Al 0.000000 0.000000 -2.636535

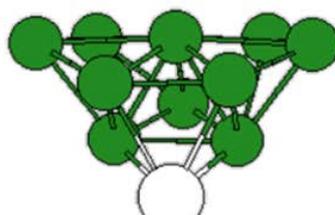
Al 0.000000 0.000000 -0.000004

Al₁₀Sn isomers

Number of isomers: 43



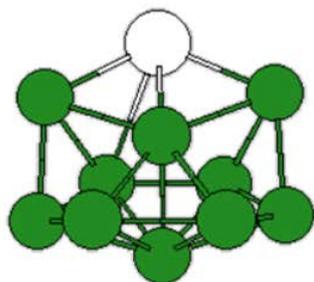
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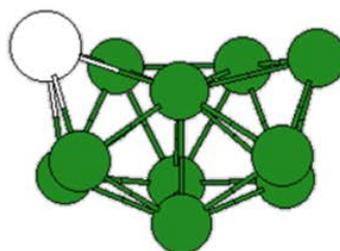
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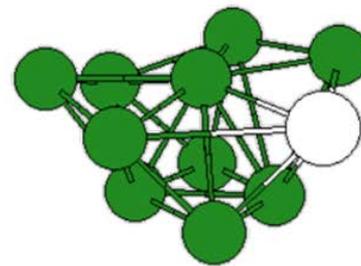
3



4



5



6

1

Total energy 0

Magnetic moment 0

Geometry

Al -0.073579 -0.092170 -1.379570

Al 2.517733 -0.277899 -0.269245

Al -1.217181 2.170799 -0.307249

Al -2.732065 0.121618 -0.602598

Al -1.228219 -1.751606 0.366539

Al 1.177029 -2.458909 -0.548865

Al 0.282663 0.407561 1.222599

Al -2.255148 0.846506 1.915306

Al 1.124487 -2.054903 2.052838

Al -1.024849 -1.063042 3.218084

Sn 1.514525 2.256567 -0.822324

2

Total energy 0.0328

Magnetic moment 0

Geometry

Al -0.076098 -0.051746 -1.433841

Al 2.534339 -0.009097 -0.402688

Al 1.423040 2.273828 -0.766877

Al -1.049265 2.167881 0.007631

Al -1.332265 -1.751807 0.316449

Al 1.305497 -2.247244 -0.399202

Al 0.342176 0.190260 1.224975

Al -2.253920 0.602373 1.777256

Al 0.746972 -2.383732 2.090920

Al -1.392909 -1.422686 3.138072

Sn -2.841697 0.204744 -0.981167

3

Total energy 0.05287

Magnetic moment 0

Geometry

Al -0.105297 -0.061310 -1.329350

Al 1.306016 2.197122 -0.309593

Al -2.164084 -0.376377 0.420771

Al -1.117050 -2.446160 -0.762158

Al 1.351121 -2.053088 -0.066461

Al 0.359316 0.117237 1.315100

Al -1.778851 1.694700 2.280595

Al -0.572193 -2.355689 1.790614

Al -1.828533 -0.671496 3.294119

Al 2.716412 0.070561 -0.636091

Sn -1.458427 2.312755 -0.396519

4

Total energy 0.13259

Magnetic moment 0

Geometry

Al -0.100461 -0.057566 -1.253398

Al 2.617032 -0.000922 -0.178924

Al 1.322424 2.272576 -0.190512

Al -1.269550 2.172898 -0.402293

Al -2.611568 -0.050757 -0.026200

Al -1.296917 -2.204632 0.003912

Al 1.282185 -2.219038 -0.511108

Al 0.186140 0.089918 1.281564

Al -1.969931 1.541402 2.065468

Al 0.521043 -2.535517 1.990361

Sn -1.645202 -1.080250 3.043493

5

Total energy 0.1534

Magnetic moment 0

Geometry

Al 0.172765 0.580300 0.375374

Al -2.362932 1.516257 1.063858

Al -1.714210 -1.066205 1.424769

Al 0.749850 -1.938209 1.354739

Al -2.320498 -0.078215 -1.119650
Al -1.319851 2.431803 -1.156486
Al 2.367239 1.120769 -1.326490
Al 1.914020 -1.484249 -1.125303
Al -0.562420 -1.841052 -1.048421
Al 0.078638 0.568303 -2.304729
Sn 2.824620 0.016249 1.18886

6

Total energy 0.20929

Magnetic moment 0

Geometry

Al -0.388970 -0.728499 2.936238
Al -0.122830 -1.062820 -2.839865
Al -2.282573 -0.850754 1.168795
Al 2.141475 -0.377262 -1.835775
Al -2.115431 -0.269044 -1.397288
Al 0.170389 1.776545 1.362981
Al -0.053817 1.417709 -1.337030
Al 2.371402 1.629141 -0.178589
Al -2.171725 1.683467 0.415998
Al 0.169613 -0.763783 0.133302
Sn 2.191537 -0.085653 2.060183

7

Total energy

0.22209

Magnetic moment

0

Geometry

Al -0.079532 -0.018361 -1.388833
Al 2.592679 0.020244 -0.286208
Al 1.357241 2.252000 -0.414364
Al -1.217537 2.131792 -0.362563
Al -2.640141 -0.038264 -0.185370
Al -1.297061 -2.118070 -0.002695
Al 1.240874 -2.176501 -0.577804
Al 0.135864 0.118164 1.206324
Al -2.106904 1.431145 1.997515
Al -1.791171 -0.980993 2.889654
Sn 0.444739 -2.517952 2.17847

8

Total energy

0.32011

Magnetic moment

0

Geometry

Al -0.000008 -1.343564 -2.734348
Al 2.236636 -0.174112 1.494232
Al -2.236631 -0.174127 1.494226
Al 2.178682 -0.301122 -1.502650
Al -2.178693 -0.301116 -1.502637
Al 0.000000 1.312707 2.244931
Al -0.000002 1.262132 -2.164132
Al 1.361095 1.750641 0.002983
Al -1.361086 1.750647 0.002987
Al 0.000000 -0.710054 0.013468

Sn 0.000000 -1.474793 2.729303

9

Total energy

0.32603

Magnetic moment

0

Geometry

Al 2.494286 -0.012160 -1.127386
Al 1.489776 1.250796 1.428906
Al 1.230549 2.396491 -1.027137
Al -0.679577 2.493248 0.951357
Al -2.896259 1.263295 0.363382
Al -2.886746 -1.327312 0.425743
Al -0.653531 -2.524155 1.017773
Al 1.289283 -2.441259 -0.944395
Al 1.495774 -1.236733 1.476888
Al -0.926896 -0.001721 1.959483
Sn -0.415204 -0.038263 -0.839792

10

Total energy

0.34104

Magnetic moment

0

Geometry

Al 1.490613 -0.193880 -2.345420
Al -0.364368 1.624389 -2.071073
Al -1.345515 -0.966613 -2.185184
Al 1.707870 1.723031 -0.294163
Al -2.438431 -1.502625 0.237937
Al 2.394573 -1.276461 -0.097878
Al -1.359509 -0.286325 2.378736
Al 1.160388 -1.222966 2.269402
Al 0.671205 1.454089 2.072795
Al -0.031814 -0.296956 0.002874
Sn -1.733902 1.824763 0.351785

11

Total energy

0.35834

Magnetic moment

0

Geometry

Al 2.646819 0.003752 0.085994
Al 1.333851 2.313902 0.045329
Al -1.261928 2.172394 -0.390290
Al -2.625207 -0.059842 -0.051272
Al -1.323729 -2.249117 0.033317
Al 1.271986 -2.191710 -0.423192
Al 0.057084 0.035710 0.925369
Al -1.970680 1.533809 2.061769
Al 0.512967 -2.448551 2.073249
Al -0.996623 -0.621999 3.262181
Sn -0.158137 -0.101969 -1.818047

12

Total energy

0.38373
Magnetic moment
0

Geometry

Al -0.295764 1.393374 -1.722198
Al -0.308370 -1.331170 -1.655403
Al 2.060718 -0.003471 -1.520472
Al 1.698094 2.342387 -0.345298
Al -2.343223 1.315736 -0.121595
Al -2.437281 -1.258953 -0.085430
Al 1.783108 -2.347972 -0.370191
Al -0.386580 -2.544057 1.106273
Al -0.292093 2.473399 1.400432
Al 0.298504 0.009300 0.551330
Sn -1.592242 -0.004587 2.489966

13

Total energy
0.39128
Magnetic moment
0

Geometry

Al -0.328636 1.252421 -2.331816
Al -0.386313 -1.323336 -2.303257
Al 1.129779 2.447757 -0.373992
Al -1.776602 1.321505 -0.121467
Al -1.858175 -1.397759 -0.141286
Al 1.199188 -2.546272 -0.389604
Al -0.358826 -2.421111 1.743027
Al -1.433883 -0.052792 2.229608
Al -0.280864 2.276917 1.838689
Al 0.460267 -0.071511 0.285461
Sn 2.287739 -0.063894 -1.722791

14

Total energy
0.42396
Magnetic moment
0

Geometry

Al -0.186731 1.668950 -1.758837
Al -0.397966 -0.949723 -2.076874
Al 2.067458 -0.124011 -1.781231
Al -2.159052 0.836303 -0.237856
Al -1.726368 -1.707666 0.009944
Al 1.105883 -2.450747 -0.453071
Al -0.015248 -2.152021 1.968463
Al -1.497839 0.094313 2.254608
Al -0.539773 2.462055 1.020589
Al 0.509050 0.025494 0.447584
Sn 2.035015 2.350892 -0.287158

15

Total energy
0.45508
Magnetic moment
0

Geometry

Al 2.552526 0.049065 -0.375021
Al 1.342430 2.323369 0.163342
Al -1.257761 2.271201 -0.178105
Al -2.552526 -0.049065 -0.375021
Al -1.342430 -2.323369 0.163342
Al 1.257761 -2.271201 -0.178106
Al 0.000000 0.000000 0.787064
Al -2.159365 0.931811 2.100194
Al 2.159365 -0.931811 2.100194
Al 0.000000 0.000000 3.376093
Sn 0.000000 0.000000 -1.894669

16

Total energy

0.48136

Magnetic moment

0

Geometry

Al 1.504004 0.009664 -2.339129
Al -0.568617 -1.703144 -1.919035
Al 2.177487 1.594614 -0.232383
Al -2.004906 1.764808 0.537815
Al -1.958113 -1.671294 0.346945
Al 1.884095 -1.779737 -0.404954
Al -1.406387 0.001937 2.435234
Al 0.762367 -1.413773 1.916810
Al 0.751772 1.594327 2.060940
Al 0.001420 0.095270 -0.015308
Sn -0.947045 1.516244 -2.083892

17

Total energy

0.51711

Magnetic moment

0

Geometry

Al 0.000000 0.000000 -1.528807
Al 2.526048 0.048050 -0.415383
Al 1.346530 2.320916 0.091526
Al -1.237205 2.247580 -0.244490
Al -2.526048 -0.048050 -0.415383
Al -1.346530 -2.320915 0.091525
Al 1.237205 -2.247581 -0.244491
Al 0.000000 0.000000 0.965371
Al -2.194340 0.972137 2.063090
Al 2.194339 -0.972139 2.063089
Sn 0.000000 0.000000 3.655033

18

Total energy

0.58048

Magnetic moment

0

Geometry

Al 2.405311 -0.021050 -1.137954
Al 0.682293 2.141638 -1.139634
Al -1.978362 1.416344 -1.130556
Al -1.869351 -1.314579 -1.342728

Al 0.676162 -2.155318 -1.349483
Al -2.454539 0.085045 1.143301
Al -0.754298 2.348579 1.195527
Al 1.979529 1.435921 1.193886
Al 1.996026 -1.403546 1.120370
Al -0.019139 -0.011528 0.081921
Sn -0.755057 -2.238085 1.443812

19

Total energy

0.6046

Magnetic moment

0

Geometry

Al -0.927021 1.447754 -2.067395
Al -0.927020 -1.447755 -2.067395
Al 1.896024 1.856346 -0.286856
Al -1.911303 1.787931 0.338149
Al -1.911303 -1.787931 0.338149
Al 1.896024 -1.856346 -0.286855
Al -1.410620 0.000000 2.242106
Al 0.831269 -1.435840 2.085999
Al 0.831269 1.435842 2.085998
Al 0.024383 0.000000 -0.031463
Sn 1.516822 0.000000 -2.460202

20

Total energy

0.74399

Magnetic moment

0

Geometry

Al 2.171383 -0.330775 0.865328
Al -1.880580 -1.215874 1.155649
Al -2.338672 0.006998 -1.093178
Al -0.527298 1.230228 -2.370290
Al 1.788333 1.033721 -1.338577
Al 2.321659 -1.684114 -1.519368
Al -0.140183 -1.499639 -0.849721
Al 0.380953 -1.445325 2.276814
Al 4.258059 -0.020838 -0.938036
Al -0.110676 0.917029 0.493005
Sn -2.729388 1.451359 1.265258

21

Total energy

0.78874

Magnetic moment

0

Geometry

Al 1.859390 -0.047144 -1.968588
Al 0.741473 2.180841 -1.309801
Al -1.894657 1.334482 -1.304472
Al -1.428865 -1.096526 -2.043085
Al 0.776148 -2.361146 -1.406557
Al 1.775573 0.022850 1.970846
Al 0.669691 2.264846 1.313523
Al -1.895626 1.415522 1.318953

Al -1.422066 -1.036723 2.004848
Al 0.014333 -0.090557 -0.015637
Sn 0.846039 -2.530630 1.285660

22

Total energy

0.79504

Magnetic moment

0

Geometry

Al -0.008662 1.225449 -2.224392
Al -0.447577 -1.302195 -2.171361
Al 2.744934 0.021455 -0.527504
Al 1.507809 2.372698 -0.469129
Al -2.250061 1.140181 0.126296
Al -2.261038 -1.379923 -0.279387
Al 1.416862 -2.231081 -0.370941
Al -0.457303 -2.299897 1.481327
Al -0.536895 -0.003084 2.768745
Al 0.153637 0.040345 0.186549
Sn -0.360019 2.576980 1.496614

23

Total energy

0.83799

Magnetic moment

0

Geometry

Al 1.980415 -0.034074 1.599518
Al 0.369808 1.703176 2.567001
Al -1.780559 0.101925 2.213144
Al -0.296308 -1.471501 0.736603
Al 1.497524 -0.118963 -1.018919
Al -0.277597 1.104875 -2.523343
Al -2.131481 -0.288736 -1.307967
Al 0.286199 -1.044523 3.279686
Al 1.328957 -0.550411 -3.743037
Al -0.579245 1.412862 0.221975
Sn -0.249096 -2.170660 -1.989523

24

Total energy

0.86775

Magnetic moment

0

Geometry

Al -0.282946 1.309345 -2.065274
Al -0.287323 -1.306127 -2.065357
Al 2.131138 -0.003508 -1.898190
Al 1.557850 2.497739 -0.443239
Al -2.056075 1.319523 -0.151244
Al -2.061469 -1.303463 -0.150037
Al 1.532130 -2.512113 -0.442755
Al -0.359344 -2.455842 1.628663
Al -1.726054 0.010347 2.243049
Al -0.337343 2.458825 1.626291
Sn 0.575618 -0.001336 0.518060

25

Total energy

0.89198

Magnetic moment

0

Geometry

Al 1.998453 0.368302 2.351060
Al 0.193312 1.729083 0.975637
Al -1.716377 -0.182399 0.977462
Al -0.362909 -1.990630 2.347110
Al 1.300908 1.225395 -1.501608
Al -1.296304 1.314018 -1.221874
Al -1.219995 -1.280943 -1.500044
Al -0.498271 0.506168 3.282761
Al -0.529997 0.535912 -3.632554
Al 0.878375 -0.867821 0.212861
Sn 1.374955 -1.363331 -2.616924

26

Total energy

0.90137

Magnetic moment

2

Geometry

Al 0.000103 -1.046909 2.842035
Al -0.005606 -1.043083 -2.834863
Al 2.311697 -0.120970 1.620440
Al -2.310740 -0.119999 1.617154
Al 2.314465 -0.116649 -1.622391
Al -2.324520 -0.117289 -1.604062
Al 0.000686 1.530144 2.147310
Al -0.000586 1.532601 -2.143957
Al 1.478978 1.809049 0.001813
Al -1.466276 1.815606 0.002023
Sn 0.001369 -0.830109 0.000978

27

Total energy

0.9518

Magnetic moment

0

Geometry

Al 3.385607 -0.000272 0.267558
Al -2.252543 1.388091 0.995620
Al -2.259234 -1.365723 1.002660
Al -2.412348 0.001536 -1.344086
Al -0.549108 1.924775 -0.923084
Al 1.946055 1.371122 -1.534517
Al 1.943361 -1.388586 -1.529005
Al -0.554674 -1.923099 -0.918729
Al -1.330458 0.005236 3.113061
Al -0.051797 -0.002742 -2.762146
Sn 0.549195 -0.002578 0.897204

28

Total energy

0.95887

Magnetic moment

0

Geometry

Al 2.074994 1.980460 0.206568
Al -0.056493 2.349425 -0.961070
Al -2.409351 1.449293 -0.586156
Al -3.486546 0.000460 1.155107
Al -2.408670 -1.445559 -0.587580
Al -0.056807 -2.349092 -0.958649
Al 2.075792 -1.985271 0.203693
Al 1.877563 -0.003882 1.930321
Al 1.319019 -0.000472 -1.488687
Al -0.354930 0.000808 0.563958
Sn 3.928684 -0.000896 -0.430451

29

Total energy

1.24664

Magnetic moment

0

Geometry

Al -0.000843 -0.005818 -1.627879
Al 2.535241 0.059955 -0.482277
Al 1.343540 2.353469 -0.178632
Al -1.240794 2.240929 -0.422097
Al -2.537231 -0.061673 -0.476125
Al -1.342992 -2.353534 -0.177940
Al 1.243401 -2.245675 -0.411747
Al -2.268483 1.153320 2.077921
Al 2.267983 -1.158084 2.078311
Al -0.000584 -0.002985 3.845963
Sn 0.002206 0.000826 1.078440

30

Total energy

1.28892

Magnetic moment

0

Geometry

Al 2.346396 -0.292765 -0.406683
Al 1.894611 1.531033 1.334692
Al 0.006154 3.148578 0.773373
Al -1.485154 2.802209 -1.251916
Al -2.985794 1.074702 -0.157548
Al -2.360989 -1.412945 -0.309744
Al -1.105167 -1.603468 1.892577
Al 0.104763 -2.189693 -0.547245
Al 1.329033 -1.036640 1.948004
Al -0.398981 0.542364 0.263313
Sn 2.578653 -2.985175 -0.109013

31

Total energy

1.37702

Magnetic moment

0

Geometry

Al 2.953772 -0.000259 0.579072
Al -2.054579 1.365387 1.049160

Al -2.050439 -1.380408 1.049851
Al -2.464361 -0.001215 -1.173318
Al -0.621853 1.804055 -1.135073
Al 1.876489 1.499582 -1.215260
Al 1.875574 -1.499861 -1.215453
Al -0.623256 -1.808301 -1.136343
Al 4.292214 -0.000372 -1.719399
Al 0.273247 -0.002599 0.727998
Sn -1.387692 -0.003725 3.310507

32

Total energy

1.42737

Magnetic moment

0

Geometry

Al 2.378000 0.000000 1.238657
Al -1.902258 1.383808 1.195701
Al -1.902258 -1.383799 1.195699
Al -2.366635 0.000001 -1.155379
Al -0.675969 2.158040 -1.131524
Al 1.879929 1.466895 -1.237418
Al 1.879931 -1.466890 -1.237416
Al -0.675962 -2.158033 -1.131523
Al 0.052552 -0.000001 2.525631
Al 0.076183 0.000005 -0.015199
Sn 4.222784 0.000003 -0.851855

33

Total energy

1.71778

Magnetic moment

0

Geometry

Al 1.452143 0.000000 -2.425295
Al -0.859776 1.515703 -2.141414
Al -0.859776 -1.515703 -2.141414
Al 2.071067 1.776706 -0.339352
Al -2.071067 1.776706 0.339352
Al -2.071067 -1.776706 0.339352
Al 2.071067 -1.776706 -0.339352
Al -1.452143 0.000000 2.425295
Al 0.859776 -1.515703 2.141414
Al 0.859776 1.515703 2.141414
Sn 0.000000 0.000000 0.000000

34

Total energy

1.76147

Magnetic moment

0

Geometry

Al 2.476618 0.000000 -1.216411
Al 0.764334 2.355459 -1.216780
Al -1.998770 1.455095 -1.220285
Al -1.998770 -1.455095 -1.220285
Al 0.764334 -2.355459 -1.216780
Al -2.476618 0.000000 1.216411

Al -0.764334 2.355459 1.216780
Al 1.998770 1.455095 1.220285
Al 1.998770 -1.455095 1.220285
Al -0.764334 -2.355459 1.216780
Sn 0.000000 0.000000 0.000000

35

Total energy

1.88305

Magnetic moment

0

Geometry

Al 2.441007 -0.199926 1.197916
Al -1.965823 1.383768 1.311254
Al -1.986811 -1.285071 1.137916
Al -2.465380 -0.056990 -1.173930
Al -1.021135 2.175988 -1.049256
Al 1.981852 -1.509475 -1.107649
Al -0.598647 -2.099338 -1.118237
Al 0.111922 -0.049138 2.446950
Al 4.332158 -0.126940 -0.792826
Al 0.097043 0.116976 -0.089367
Sn 1.999652 1.608740 -1.342136

36

Total energy

2.16745

Magnetic moment

0

Geometry

Al 1.994936 0.000004 1.768730
Al 0.000000 1.994927 1.768705
Al -1.994936 0.000004 1.768731
Al 0.000000 -1.994939 1.768828
Al 1.380602 1.380625 -1.678820
Al -1.380602 1.380625 -1.678820
Al -1.380628 -1.380577 -1.678847
Al 1.380628 -1.380578 -1.678846
Al 0.000000 -0.000005 3.561334
Al 0.000000 -0.000044 0.057945
Sn 0.000000 -0.000007 -3.763605

37

Total energy

2.21026

Magnetic moment

0

Geometry

Al 1.984218 -0.000003 1.730260
Al 0.000049 1.984265 1.730224
Al -1.983866 -0.000012 1.732696
Al 0.000001 -1.984065 1.732062
Al 1.944903 0.000256 -1.783142
Al 0.000329 1.945246 -1.782975
Al -1.943768 0.000242 -1.779772
Al 0.000206 -1.943618 -1.779634
Al 0.003270 0.002676 3.520039
Al -0.000049 0.000082 -0.014484

Sn -0.001568 -0.001294 -3.85677

38

Total energy

2.38838

Magnetic moment

0

Geometry

Al 2.443724 -0.000005 -1.353951
Al 0.753598 2.329226 -1.356750
Al -1.978588 1.433996 -1.355491
Al -1.978576 -1.433985 -1.355502
Al 0.753615 -2.329150 -1.357014
Al 2.443818 0.000212 1.354158
Al 0.753551 2.329155 1.356742
Al -1.978597 1.433998 1.355494
Al -1.978573 -1.433984 1.355497
Al 0.753672 -2.329091 1.357050
Sn 0.000213 0.000000 0.000002

39

Total energy

2.57439

Magnetic moment

0

Geometry

Al 2.799939 -0.002712 0.200238
Al 1.497827 2.095510 0.365559
Al 0.000491 4.047001 1.059676
Al -1.497963 2.095809 0.369237
Al -2.800455 -0.001837 0.200262
Al -1.498146 -2.100116 0.370749
Al -0.003712 -4.054045 1.070278
Al 1.495340 -2.099535 0.381794
Al 0.000521 0.008725 -3.211920
Al 0.000140 -0.002196 -0.595769
Sn -0.000248 0.003540 2.161788

40

Total energy

2.92054

Magnetic moment

0

Geometry

Al 1.951081 0.000023 2.070077
Al 0.000037 1.951047 2.070048
Al -1.950960 0.000025 2.069975
Al 0.000036 -1.950971 2.069985
Al 1.951081 0.000020 -2.070078
Al 0.000036 1.951046 -2.070048
Al -1.950962 0.000021 -2.069976
Al 0.000035 -1.950975 -2.069988
Al -0.000099 -0.000060 3.935969
Al -0.000098 -0.000057 -3.935969
Sn 0.000110 0.000068 -0.000002

41

Total energy

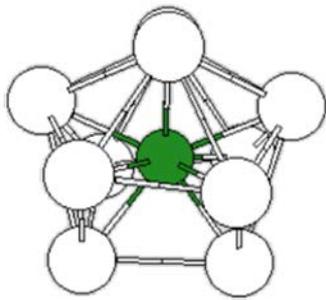
2.93495
Magnetic moment
0
Geometry
Al 1.955634 0.000184 2.050798
Al 0.000173 1.955645 2.050823
Al -1.953700 0.000325 2.053088
Al 0.000330 -1.953606 2.053234
Al 1.383957 1.383685 -2.053669
Al -1.384188 1.382792 -2.053576
Al -1.383289 -1.383436 -2.053211
Al 1.382579 -1.384029 -2.053878
Al 0.000429 0.000445 3.915299
Al -0.000013 0.000134 -3.911365
Sn -0.000030 -0.000066 -0.002152

42
Total energy
2.98085
Magnetic moment
0
Geometry
Al 2.535576 0.000015 1.281129
Al -2.044350 1.380395 1.213821
Al -2.044333 -1.380373 1.213825
Al -2.501150 0.000005 -1.132230
Al -0.798409 2.254421 -1.147654
Al 2.028897 1.513660 -1.301345
Al 2.028883 -1.513682 -1.301217
Al -0.798390 -2.254410 -1.147610
Al -0.044685 0.000030 2.635925
Al 4.374823 0.000013 -0.873189
Sn 0.124442 0.000031 -0.033583

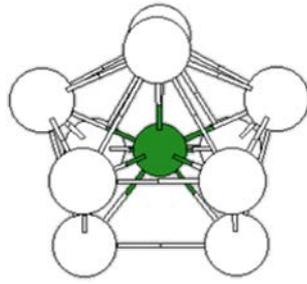
43
Total energy
4.24044
Magnetic moment
0
Geometry
Al 2.910344 -0.000023 0.000000
Al 1.709450 2.204046 0.000000
Al -0.000145 4.115634 0.000000
Al -1.709377 2.204026 0.000000
Al -2.910469 0.000087 0.000000
Al -1.709476 -2.203893 0.000000
Al -0.000152 -4.115646 0.000000
Al 1.709487 -2.204097 0.000000
Al -0.000001 0.000000 2.806825
Al -0.000001 0.000000 -2.806825
Sn 0.000038 -0.000033 0.000000

AlSn10 isomers

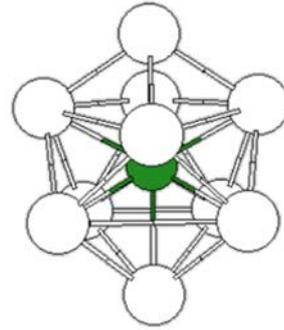
Number of isomers: 15



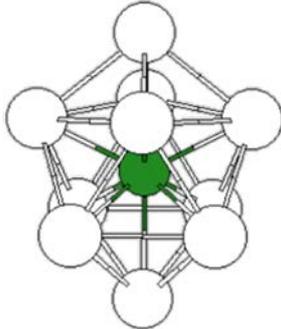
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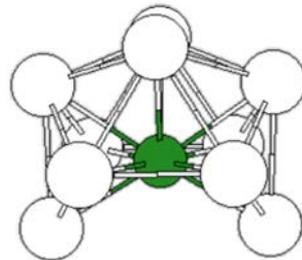
2



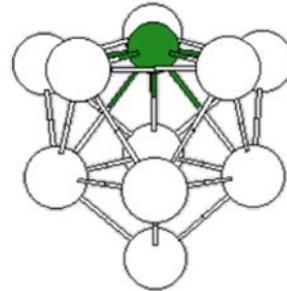
3



4



5



6

1

Total energy 0
Magnetic moment 1
Geometry

| | | | |
|----|-----------|-----------|-----------|
| Al | -0.195634 | -0.117139 | 0.744945 |
| Sn | 0.473077 | 1.035421 | -1.755972 |
| Sn | 2.609636 | -0.542012 | 0.188173 |
| Sn | 1.652248 | 2.307261 | 0.934296 |
| Sn | -1.429895 | 2.387459 | 0.602166 |
| Sn | -2.363308 | -0.168959 | -1.093085 |
| Sn | -1.930840 | -2.669558 | 0.872296 |
| Sn | 0.322715 | -2.114561 | -1.154561 |
| Sn | -2.727786 | 0.035651 | 2.147111 |
| Sn | 0.827894 | -2.123891 | 2.250479 |
| Sn | 0.084466 | 0.889762 | 3.254548 |

2

Total energy 0.01387
Magnetic moment 1
Geometry

| | | | |
|----|-----------|-----------|-----------|
| Al | 0.000018 | -0.117400 | 0.000010 |
| Sn | 0.000006 | -2.252517 | 1.664059 |
| Sn | 0.000005 | -2.252515 | -1.664057 |
| Sn | 2.532967 | -0.427591 | 1.556047 |
| Sn | -2.532947 | -0.427687 | 1.556025 |
| Sn | 2.532967 | -0.427599 | -1.556037 |
| Sn | -2.532949 | -0.427687 | -1.556022 |
| Sn | -0.000005 | 1.004231 | 2.562241 |
| Sn | -0.000003 | 1.004217 | -2.562233 |
| Sn | 1.572967 | 2.257292 | 0.000001 |
| Sn | -1.572905 | 2.257289 | 0.000000 |

3

Total energy 0.03357

Magnetic moment 1

Geometry

Al -0.039790 -0.000007 -0.315655
Sn 2.882508 -0.000022 -1.336074
Sn -1.517199 2.131253 -1.383983
Sn -1.517154 -2.131236 -1.384013
Sn 1.917813 0.000006 1.746476
Sn -0.795728 1.658421 1.824479
Sn -0.795730 -1.658430 1.824469
Sn 1.369874 2.480673 -0.312376
Sn 1.369905 -2.480721 -0.312283
Sn -3.019659 -0.000015 0.326986
Sn 0.225410 0.000052 -2.991095

4

Total energy 0.11498

Magnetic moment 1

Geometry

Al 0.000042 -0.000002 -0.045250
Sn 2.450969 0.000192 1.393364
Sn 0.000020 2.472887 1.190946
Sn -2.450829 0.000421 1.393627
Sn 0.000129 -2.472861 1.190830
Sn 1.943000 1.614301 -1.235913
Sn -1.943195 1.614208 -1.235718
Sn -1.943447 -1.614163 -1.235358
Sn 1.943317 -1.614163 -1.235704
Sn 0.000199 -0.000084 3.184009
Sn -0.000165 -0.000289 -3.080654

5

Total energy 0.14813

Magnetic moment 1

Geometry

Al 0.063792 0.044834 0.049610
Sn -2.093306 1.522547 1.407525
Sn -2.202523 -1.602084 1.281957
Sn 0.802496 -2.460316 1.407055
Sn -2.691736 0.004019 -1.343415
Sn -0.719200 2.521534 -1.341728
Sn 2.108164 1.531791 -1.230127
Sn 2.175812 -1.462835 -1.343668
Sn -0.828407 -2.560967 -1.344272
Sn 0.052667 0.038969 2.882258
Sn -0.059056 -0.041605 -3.008047

6

Total energy 0.28286

Magnetic moment 1

Geometry

Al -1.312264 0.000808 -0.473598
Sn 0.171158 1.621957 -2.122960
Sn 0.172877 -1.617121 -2.121143
Sn 2.639152 0.003698 -1.126696
Sn 1.361396 2.191657 0.665719
Sn -1.585591 2.494808 0.628214
Sn -1.581754 -2.492753 0.626287

Sn 1.365661 -2.187771 0.664934
Sn -3.072995 0.000136 1.768187
Sn -0.215419 -0.000583 2.513804
Sn 2.719664 0.003512 2.137718

7

Total energy

0.44742

Magnetic moment

1

Geometry

Al 0.007695 0.000000 0.014447
Sn 2.625118 0.000001 1.378753
Sn -1.950913 1.563757 1.269616
Sn -1.950913 -1.563756 1.269617
Sn -2.734276 0.000000 -1.382876
Sn -0.871250 2.534826 -1.412920
Sn 2.009860 1.564106 -1.172694
Sn 2.009860 -1.564110 -1.172690
Sn -0.871250 -2.534825 -1.412920
Sn 0.056064 0.000000 2.965420
Sn -0.014589 -0.000001 -3.063993

8

Total energy

0.78353

Magnetic moment

1

Geometry

Al 0.013305 0.000002 -0.017072
Sn 1.732056 0.000023 -2.205825
Sn -0.894052 1.644228 -2.025214
Sn -0.894020 -1.644137 -2.025300
Sn 2.009658 -0.000032 1.859690
Sn -0.905428 1.818647 1.855261
Sn -0.905403 -1.818643 1.855273
Sn 1.473231 2.433832 0.016814
Sn 1.473196 -2.433850 0.016787
Sn -2.771558 -0.000004 0.013063
Sn -0.068513 0.000011 4.151731

9

Total energy

0.99305

Magnetic moment

1

Geometry

Al 0.092683 -0.004858 -3.782381
Sn 1.869690 0.001957 -1.601637
Sn -0.945561 1.570992 -1.552258
Sn -0.947193 -1.569090 -1.553912
Sn 1.961521 0.000627 1.577916
Sn -0.908317 1.629487 1.506921
Sn -0.914305 -1.629516 1.510514
Sn 1.547634 2.546429 -0.025499
Sn 1.545383 -2.545278 -0.027397
Sn -2.993910 -0.001024 0.045777
Sn -0.012751 0.001892 3.822753

10

Total energy

1.00689

Magnetic moment

1

Geometry

Al -2.755562 0.000000 -3.191465
Sn 2.822828 0.000002 -1.476589
Sn -1.588122 2.480555 -1.555811
Sn -1.588119 -2.480554 -1.555812
Sn 1.843900 0.000001 1.608018
Sn -0.776738 1.606411 1.847340
Sn -0.776737 -1.606411 1.847340
Sn 1.153441 2.224325 -0.428469
Sn 1.153443 -2.224323 -0.428469
Sn -2.205960 0.000000 -0.205175
Sn 0.068010 0.000001 -2.615892

11

Total energy

1.01493

Magnetic moment

1

Geometry

Al -0.000002 0.000001 0.000001
Sn 2.473861 -0.000742 -1.390370
Sn 0.799950 2.518624 -1.421185
Sn -2.054978 1.511560 -1.387840
Sn -2.061088 -1.522587 -1.388292
Sn 0.796752 -2.519236 -1.415241
Sn -2.473868 0.000746 1.390381
Sn -0.796756 2.519244 1.415283
Sn 2.061085 1.522591 1.388293
Sn 2.054972 -1.511562 1.387849
Sn -0.799977 -2.518623 1.421194

12

Total energy

1.12911

Magnetic moment

1

Geometry

Al -2.870174 -0.000074 -2.856792
Sn 1.894471 0.000032 -1.658535
Sn -0.830634 1.566610 -1.647952
Sn -0.829182 -1.567260 -1.648062
Sn 1.765955 0.000018 1.414973
Sn -0.851873 1.634297 1.733043
Sn -0.851836 -1.634272 1.733046
Sn 1.300840 2.651555 0.023685
Sn 1.301093 -2.651786 0.023990
Sn -2.984513 -0.000276 -0.038931
Sn -2.967603 -0.000007 2.890726

13

Total energy

1.43725

Magnetic moment

1

Geometry

Al -1.577508 2.834319 -0.741400
Sn -0.202356 0.395673 -1.148496
Sn 2.833607 0.119733 -1.424235
Sn -1.534858 -2.389085 -1.442312
Sn 1.904929 -0.081824 1.620449
Sn -0.809687 1.382067 1.958178
Sn -0.940871 -1.683452 1.586060
Sn 1.292441 2.692024 0.133196
Sn 1.387908 -2.430063 -0.313754
Sn -2.954990 0.292061 0.031876
Sn 0.829289 -1.443611 -3.213727

14

Total energy

1.44358

Magnetic moment

1

Geometry

Al 2.547766 0.272065 -1.582761
Sn -0.275571 0.300221 -1.201051
Sn -1.487004 2.899713 -0.800431
Sn -1.504011 -2.557823 -1.408211
Sn 1.818142 -0.042433 1.582051
Sn -0.908049 1.473993 1.907111
Sn -0.968283 -1.613716 1.599414
Sn 1.514431 2.612513 0.089438
Sn 1.410617 -2.320377 -0.393793
Sn -2.981665 0.212612 -0.030013
Sn 0.758144 -1.365133 -3.294432

15

Total energy

1.50498

Magnetic moment

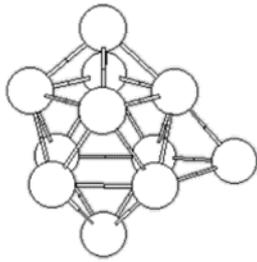
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Geometry

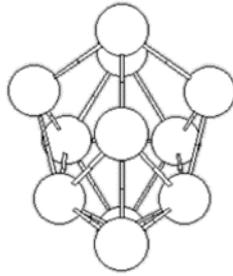
Al 0.046830 0.000000 0.134757
Sn 2.499168 -0.000001 1.398760
Sn -1.967454 1.634841 1.259094
Sn -1.967453 -1.634842 1.259095
Sn -2.121432 -0.000001 -1.655697
Sn -0.858984 2.664920 -1.322908
Sn 1.921410 1.664545 -1.153647
Sn 1.921409 -1.664546 -1.153647
Sn -0.858984 -2.664922 -1.322908
Sn -0.126490 0.000000 3.015949
Sn 4.293694 -0.000001 -1.270088

Sn11 isomers

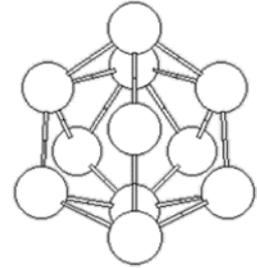
Number of isomers: 9



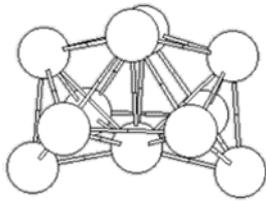
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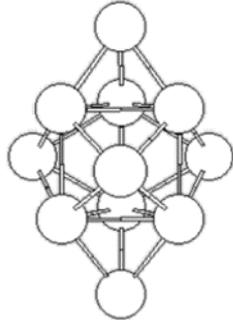
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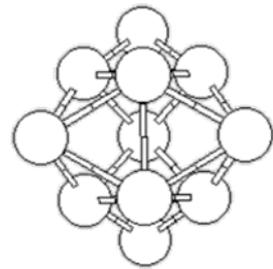
3



4



5



6

1

Total energy 0
Magnetic moment 0
Geometry

| | | | |
|----|-----------|-----------|-----------|
| Sn | 2.104228 | 0.000000 | 1.319490 |
| Sn | -0.042078 | 2.395057 | 1.287212 |
| Sn | -2.297541 | 0.000000 | 1.254933 |
| Sn | -0.042078 | -2.395057 | 1.287212 |
| Sn | 1.569819 | 1.678622 | -1.216049 |
| Sn | -1.510219 | 1.568409 | -1.240888 |
| Sn | -1.510219 | -1.568410 | -1.240887 |
| Sn | 1.569819 | -1.678622 | -1.216049 |
| Sn | -0.097076 | 0.000000 | 3.254419 |
| Sn | 0.039541 | 0.000000 | -3.315557 |
| Sn | 4.009806 | 0.000000 | -0.847401 |

2

Total energy 0.0018
Magnetic moment 0
Geometry

| | | | |
|----|-----------|-----------|-----------|
| Sn | 0.162371 | 1.561059 | -2.107505 |
| Sn | 0.162372 | -1.561059 | -2.107506 |
| Sn | 2.554469 | 0.000002 | -1.015936 |
| Sn | 1.098722 | 2.393192 | 0.673725 |
| Sn | -1.834663 | 1.694367 | 0.233196 |
| Sn | -1.834661 | -1.694368 | 0.233196 |
| Sn | 1.098724 | -2.393190 | 0.673726 |
| Sn | -3.233956 | -0.000001 | 2.237429 |
| Sn | -0.336429 | 0.000001 | 2.328973 |
| Sn | 2.572381 | 0.000001 | 1.965160 |
| Sn | -2.444911 | -0.000002 | -2.263624 |

3

Total energy 0.08671

Magnetic moment 0

Geometry

Sn 0.001197 -1.746088 2.767138
Sn 0.001098 -2.037182 -3.023447
Sn 2.391288 -0.405413 1.412757
Sn -2.390099 -0.407765 1.412774
Sn 2.514804 -0.754249 -1.608995
Sn -2.513801 -0.756327 -1.608975
Sn -0.000182 1.310831 2.489747
Sn -0.000214 0.758373 -1.816379
Sn 1.653415 2.272556 0.122193
Sn -1.654945 2.271093 0.122624
Sn 0.001223 -2.135924 -0.119632

4

Total energy 0.20874

Magnetic moment 0

Geometry

Sn 0.000779 -1.698575 2.883304
Sn 0.000238 -1.699479 -2.881330
Sn 2.469242 -0.367068 1.681546
Sn -2.469226 -0.370298 1.682531
Sn 2.469027 -0.367757 -1.680421
Sn -2.469142 -0.368480 -1.680961
Sn -0.000145 1.468151 2.598040
Sn -0.000205 1.466796 -2.597371
Sn 1.624455 2.088102 0.000155
Sn -1.625497 2.086829 0.000496
Sn -0.000101 -1.079582 0.000819

5

Total energy 0.2665

Magnetic moment 2

Geometry

Sn 1.906029 -0.000004 -1.579521
Sn -0.936067 1.643233 -1.574837
Sn -0.936066 -1.643241 -1.574831
Sn 1.920915 0.000002 1.551455
Sn -0.931087 1.650923 1.549674
Sn -0.931086 -1.650917 1.549684
Sn 1.507824 2.578269 -0.015791
Sn 1.507824 -2.578271 -0.015776
Sn -2.961560 -0.000002 -0.005236
Sn 0.013806 0.000008 3.825641
Sn 0.007100 -0.000007 -3.861596

6

Total energy 0.33609

Magnetic moment 0

Geometry

Sn 1.882642 0.000006 -1.561908
Sn -0.828738 1.571982 -1.690596
Sn -0.828744 -1.571973 -1.690603
Sn 1.882641 0.000006 1.561907
Sn -0.828739 1.571981 1.690595
Sn -0.828745 -1.571973 1.690602

Sn 1.304709 2.628166 -0.000001
Sn 1.304903 -2.627807 -0.000001
Sn -2.951794 -0.000060 -0.000001
Sn -3.015580 0.000014 2.895110
Sn -3.015577 0.000014 -2.895112

7

Total energy

0.73789

Magnetic moment

0

Geometry

Sn 2.708004 0.000001 1.481294
Sn -2.092598 1.558406 1.329181
Sn -2.092598 -1.558406 1.329182
Sn -2.799641 0.000000 -1.455214
Sn -0.877875 2.508756 -1.423706
Sn 2.125186 1.558614 -1.280447
Sn 2.125185 -1.558613 -1.280447
Sn -0.877875 -2.508756 -1.423706
Sn 0.115830 0.000000 3.084145
Sn -0.053269 0.000000 -3.156579
Sn 0.067591 0.000000 0.106692

8

Total energy

0.85956

Magnetic moment

0

Geometry

Sn 2.234370 -0.172123 1.698359
Sn 0.011301 2.200555 2.647783
Sn -2.200560 0.213408 1.100191
Sn -0.002761 -2.402936 1.156378
Sn 1.528026 1.483508 -2.743269
Sn -1.752764 1.478403 -1.733479
Sn -1.756411 -1.704812 -1.176388
Sn 1.664400 -1.391514 -1.151998
Sn -0.325963 -0.570515 3.491841
Sn -0.305110 -0.642174 -3.545331
Sn 0.631782 1.539692 -0.046022

9

Total energy

2.12837

Magnetic moment

2

Geometry

Sn 2.667090 -0.000056 1.421700
Sn -2.012858 1.664371 1.363548
Sn -2.012850 -1.664389 1.363545
Sn -2.572646 -0.000028 -1.467661
Sn -0.932110 2.560914 -1.336687
Sn 2.098847 1.671565 -1.373278
Sn 2.098893 -1.671700 -1.373225
Sn -0.932086 -2.560969 -1.336675
Sn -0.071357 -0.000011 3.019748
Sn 4.476512 -0.000005 -0.935340

Sn 0.072196 -0.000033 -0.016882