# Planar Pentacoordinate Carbon Atoms embedded in a Metallocene Framework

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**Supplementary Information**

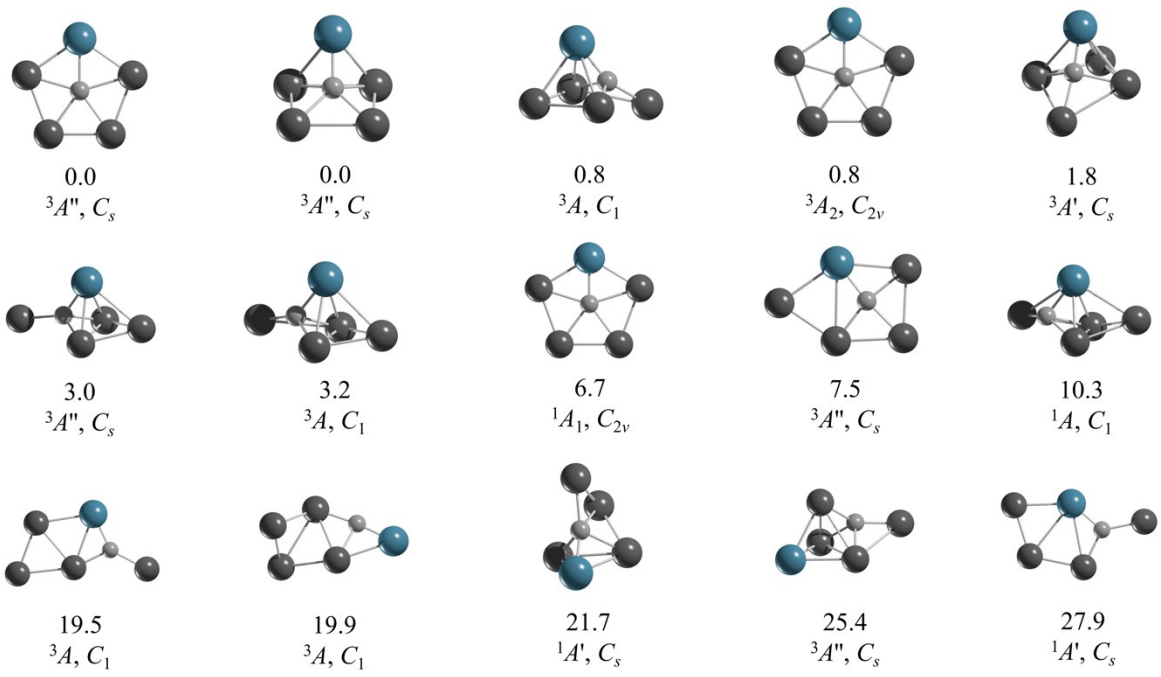


**Figure S1.** PBE0-D3/def2-TZVP structures of $CAl_4Ti$. Relative energies with respect to the lowest lying isomer are given in kcal·mol$^{-1}$.

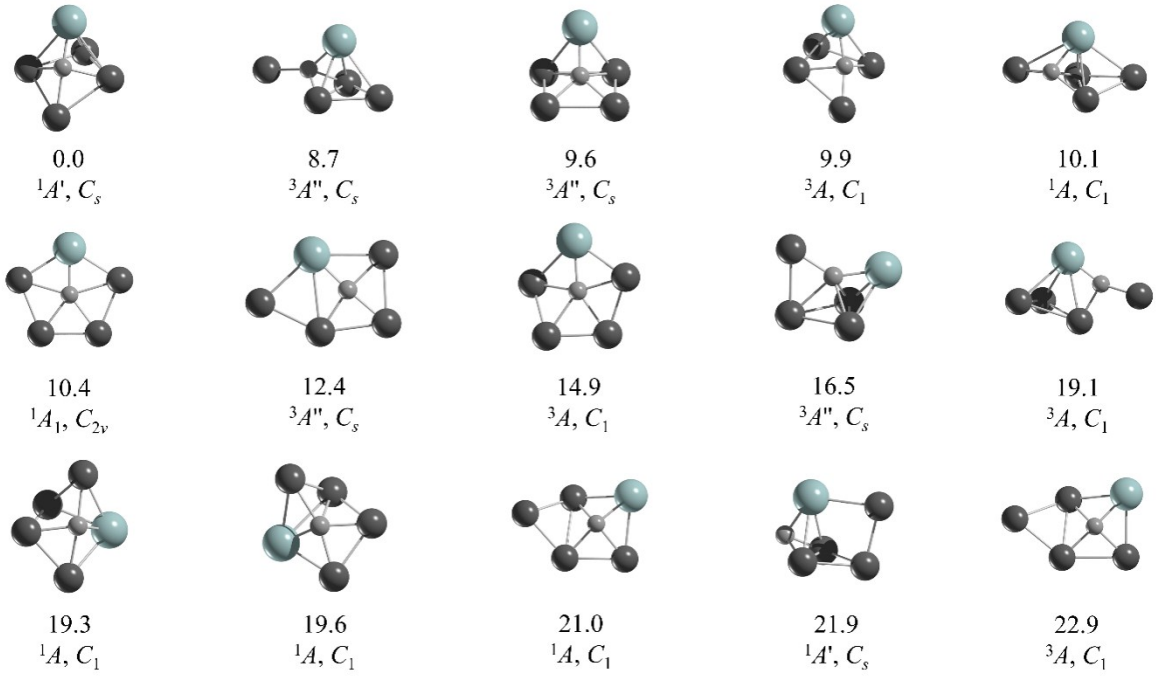


**Figure S2.** PBE0-D3/def2-TZVP structures of $CAl_4Zr$. Relative energies with respect to the lowest lying isomer are given in kcal·mol$^{-1}$.

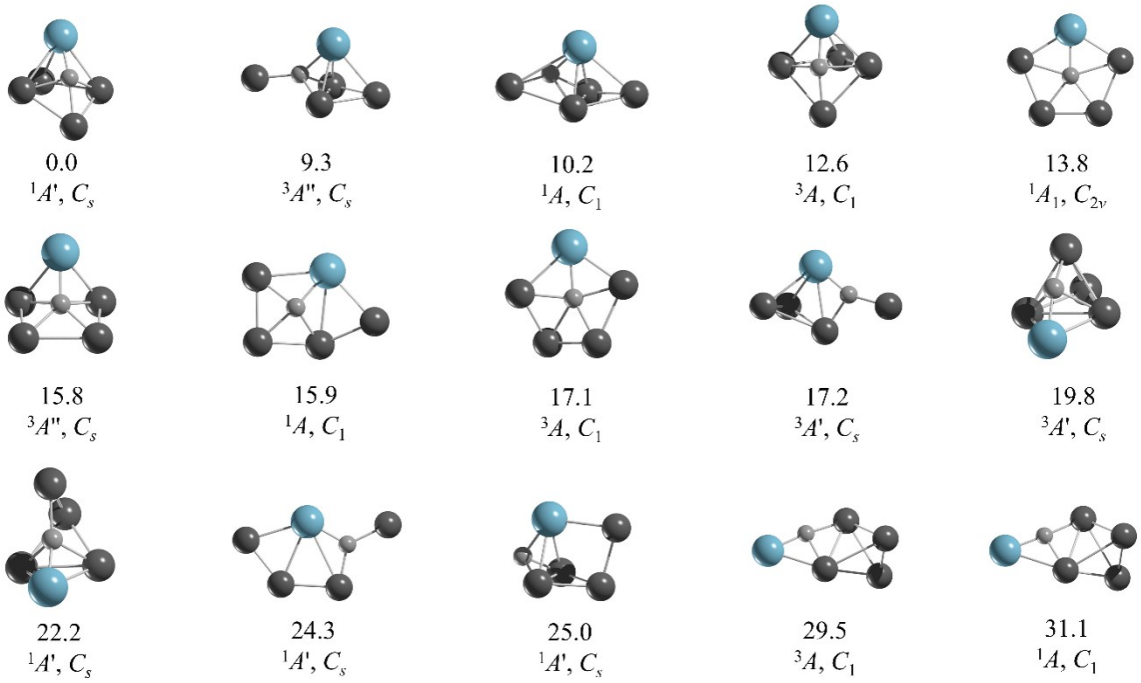


**Figure S3.** PBE0-D3/def2-TZVP structures of $CAl_4Hf$. Relative energies with respect to the lowest lying isomer are given in kcal·mol$^{-1}$.

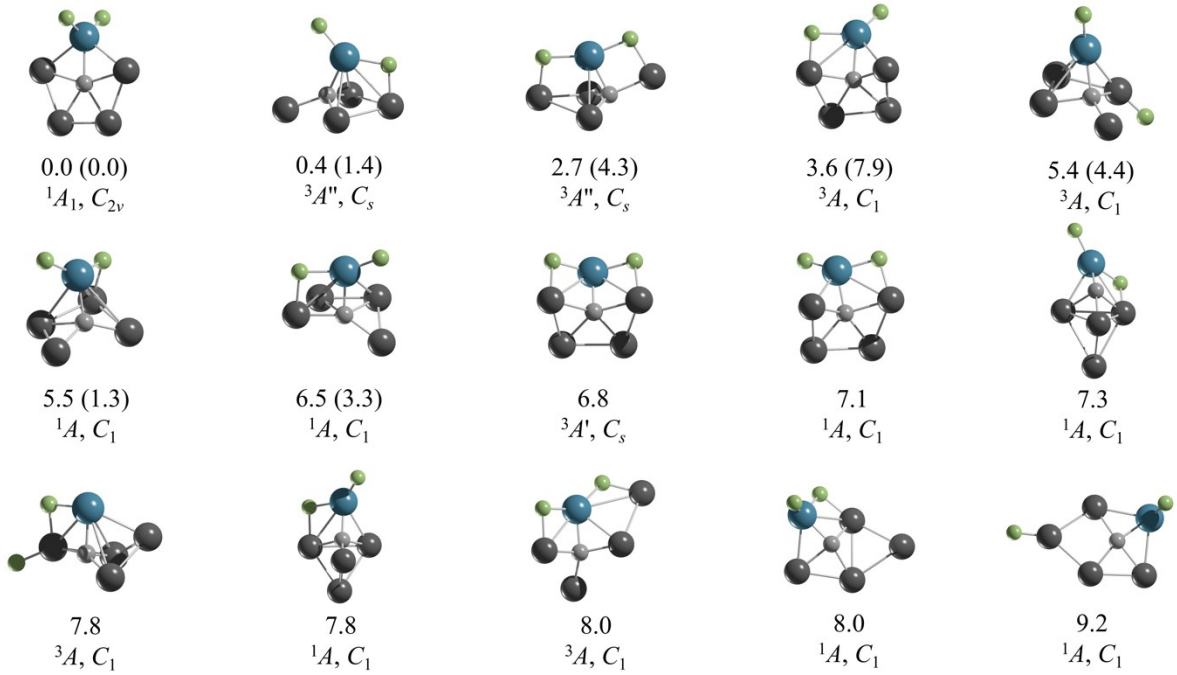


**Figure S4.** PBE0-D3/def2-TZVP structures of $CAl_4TiF_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

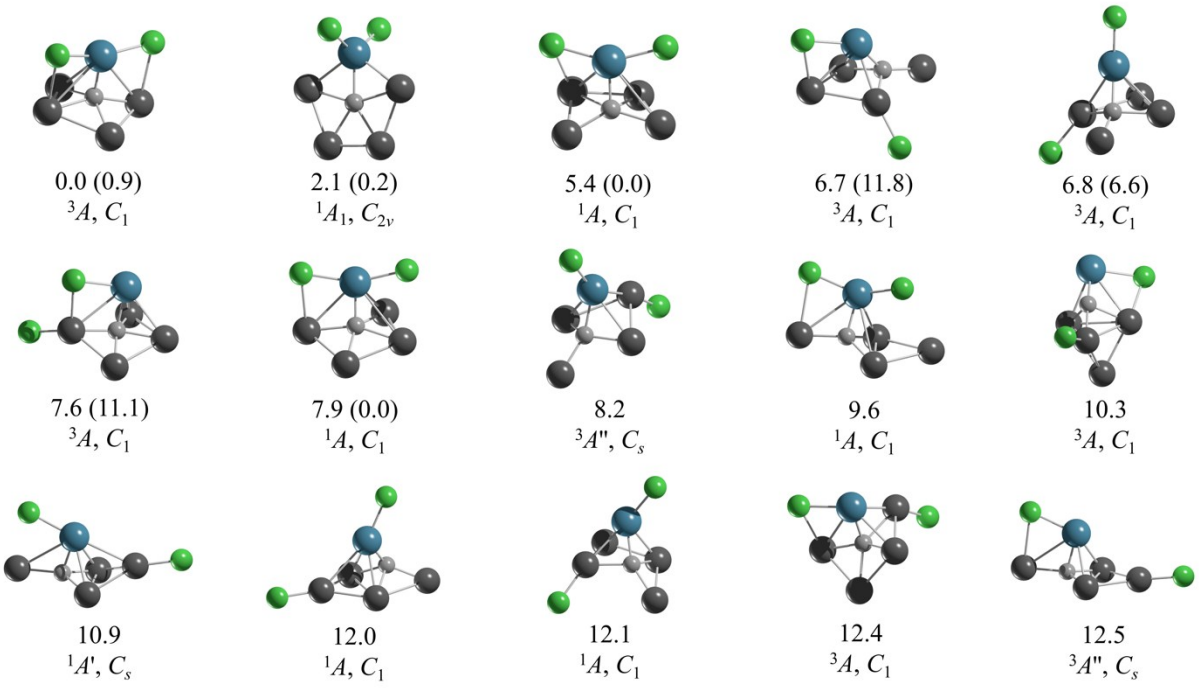


**Figure S5.** PBE0-D3/def2-TZVP structures of $CAl_4TiCl_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

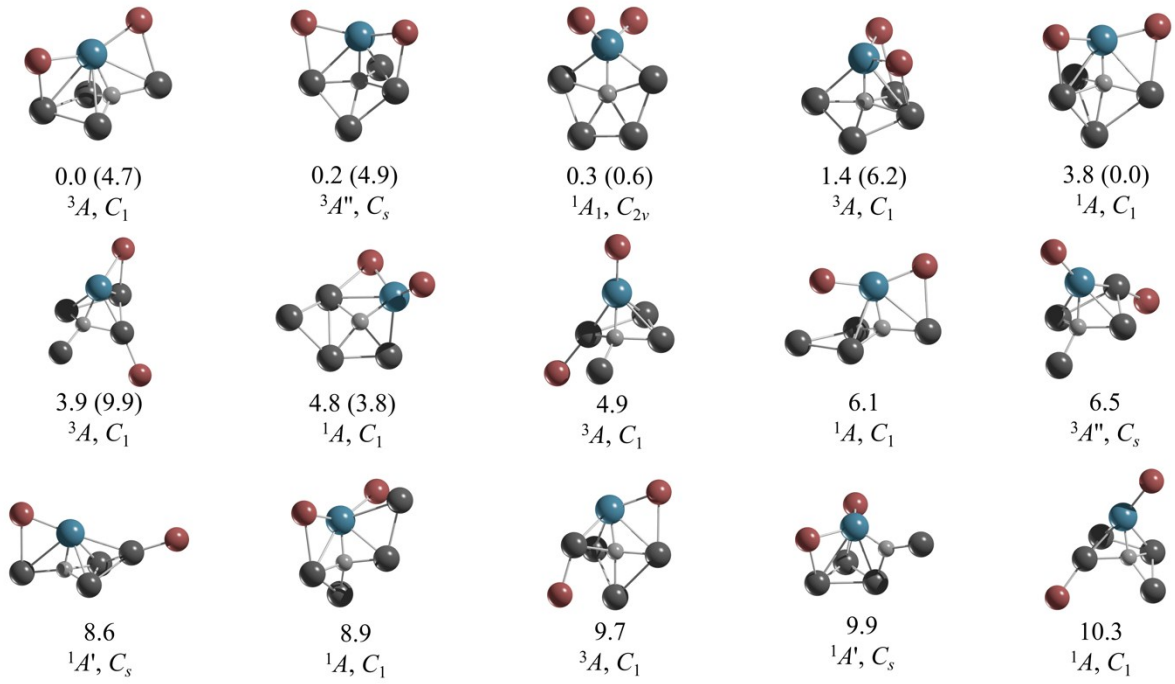


**Figure S6.** PBE0-D3/def2-TZVP structures of $CAl_4TiBr_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

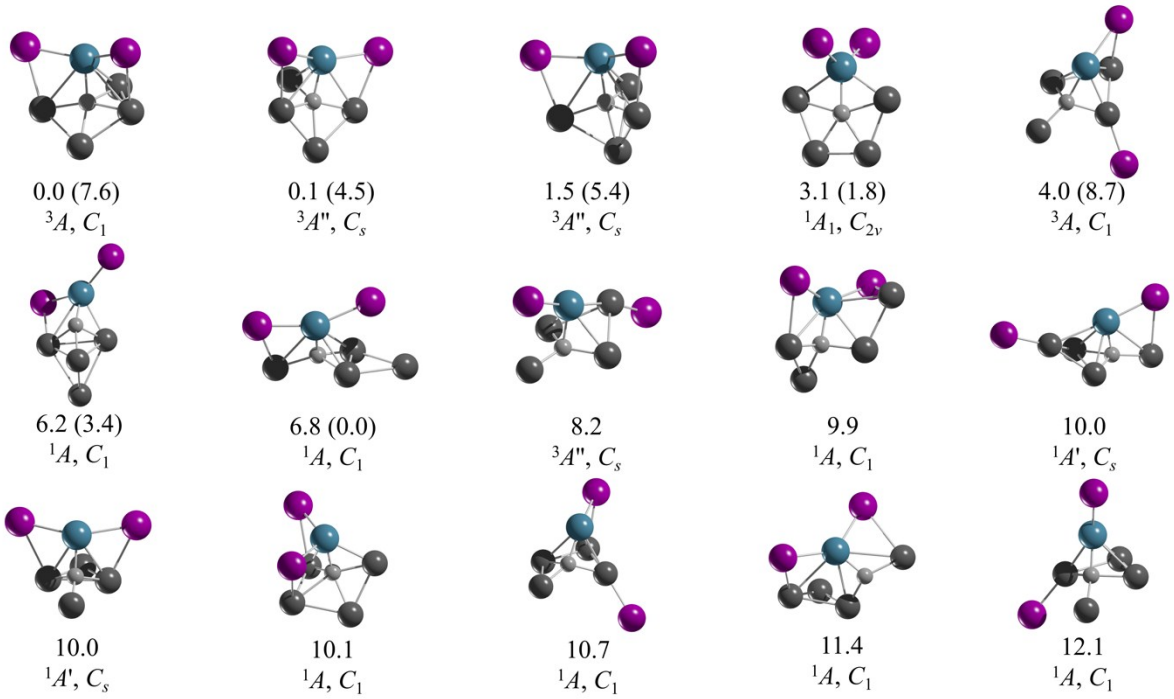


**Figure S7.** PBE0-D3/def2-TZVP structures of $CAl_4TiI_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

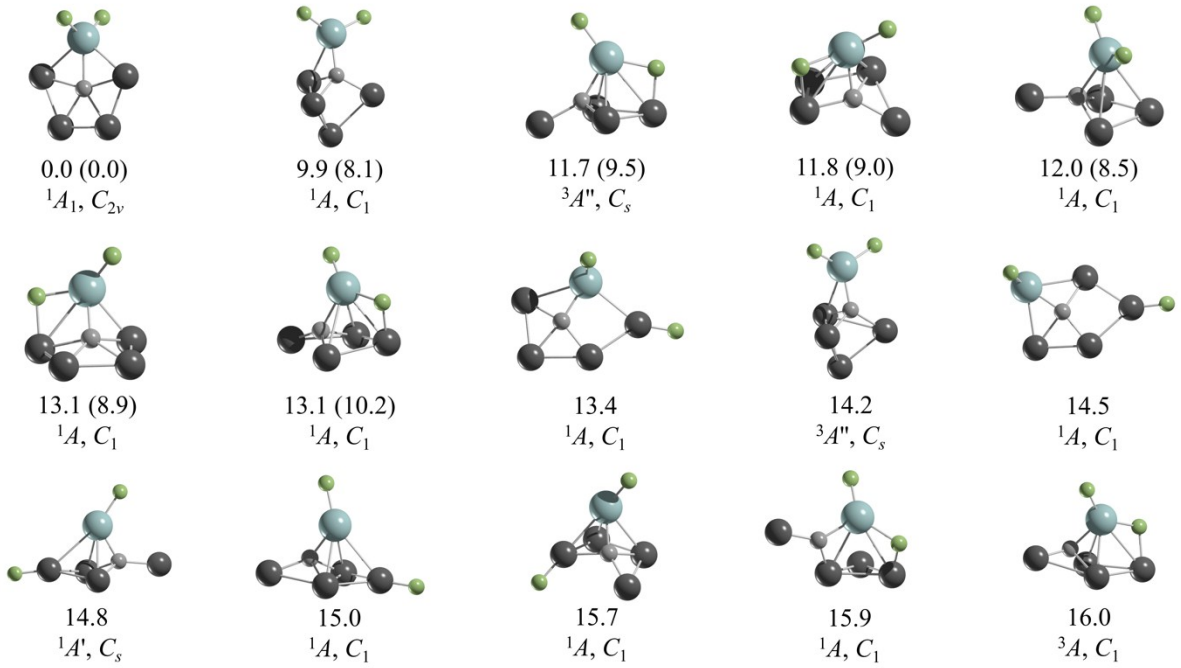


**Figure S8.** PBE0-D3/def2-TZVP structures of $CAl_4ZrF_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

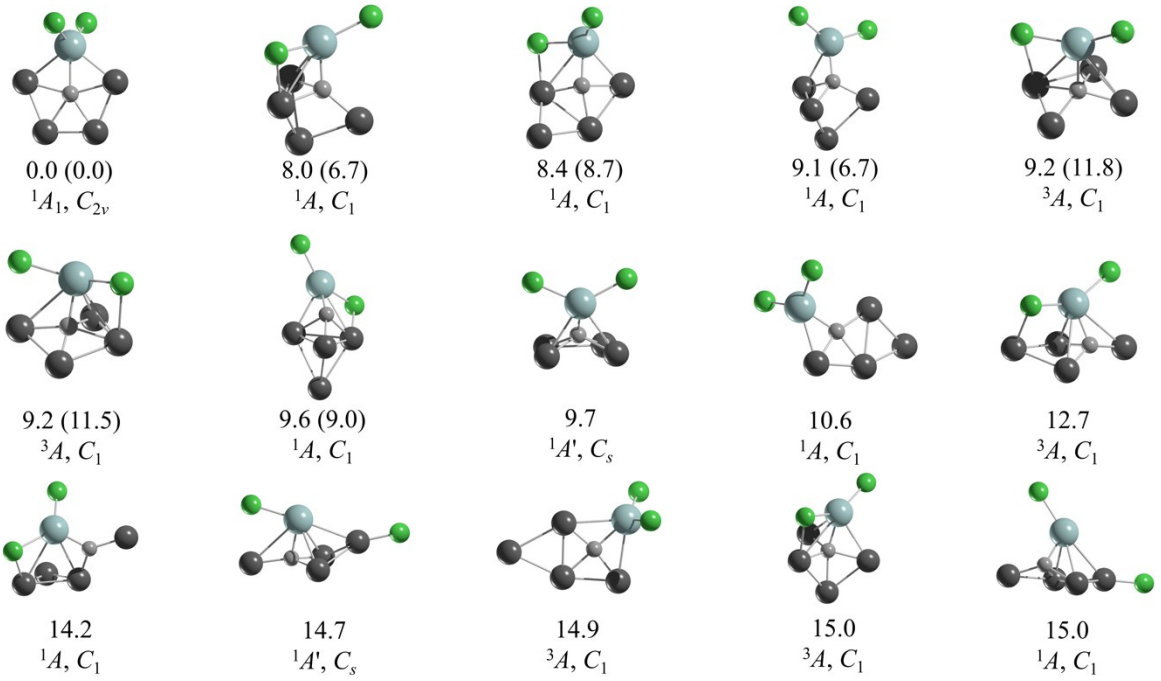


**Figure S9.** PBE0-D3/def2-TZVP structures of $CAl_4ZrCl_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

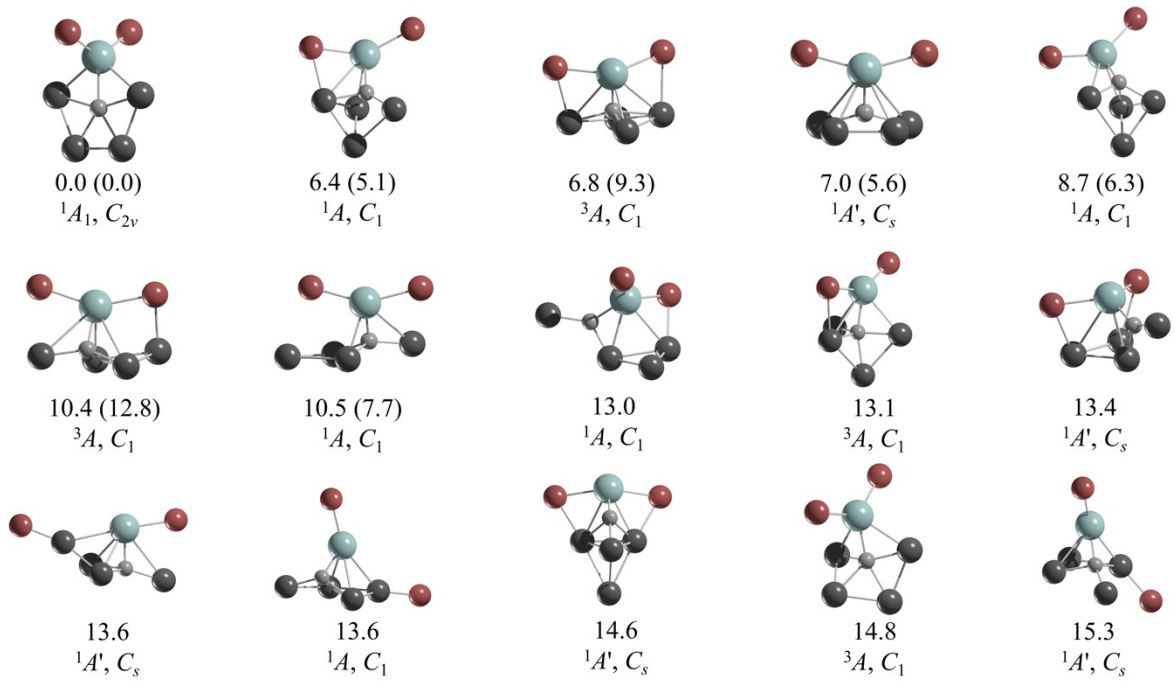


**Figure S10.** PBE0-D3/def2-TZVP structures of $CAl_4ZrBr_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

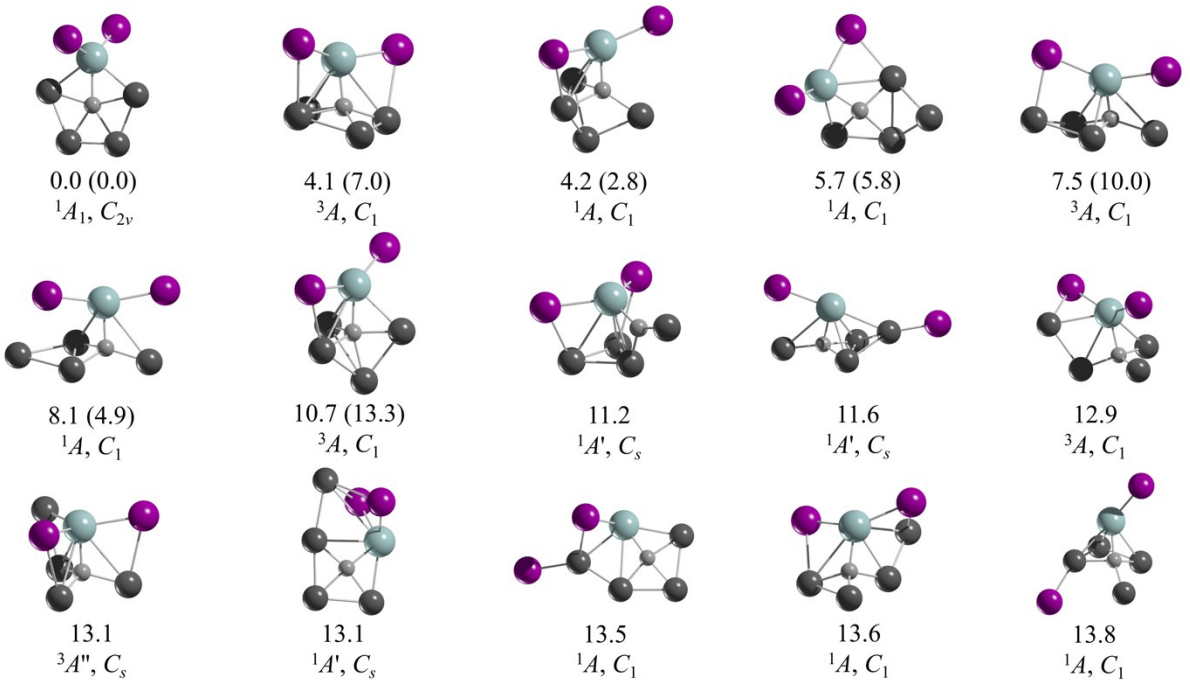


**Figure S11.** PBE0-D3/def2-TZVP structures of $CAl_4ZrI_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

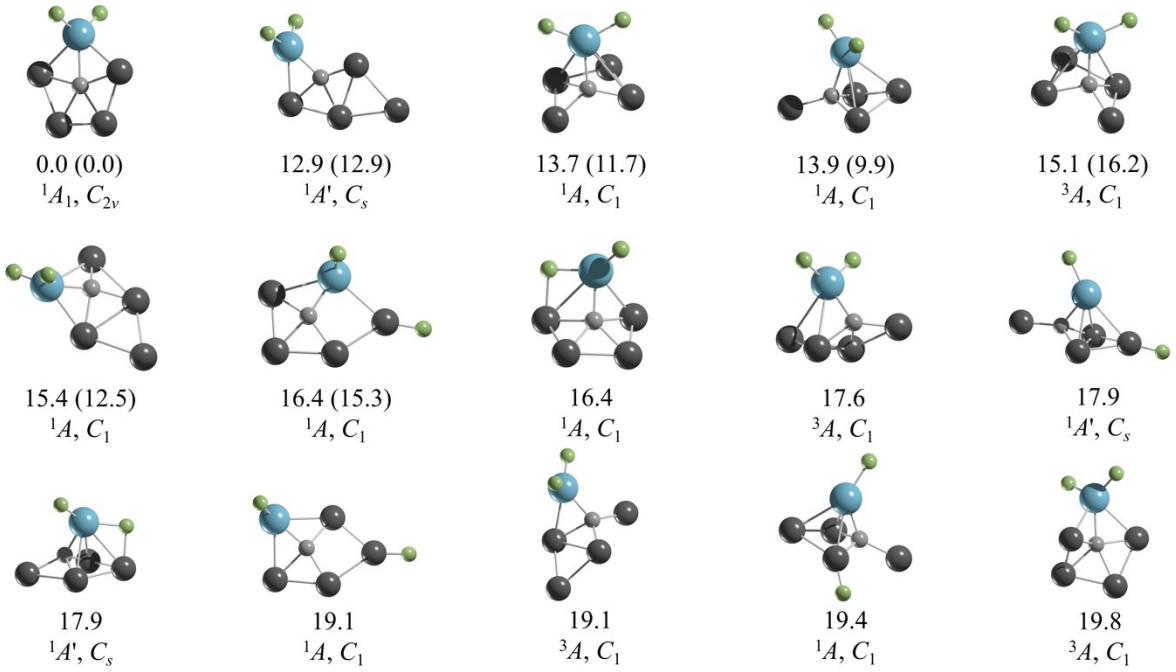


**Figure S12.** PBE0-D3/def2-TZVP structures of $CAl_4HfF_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

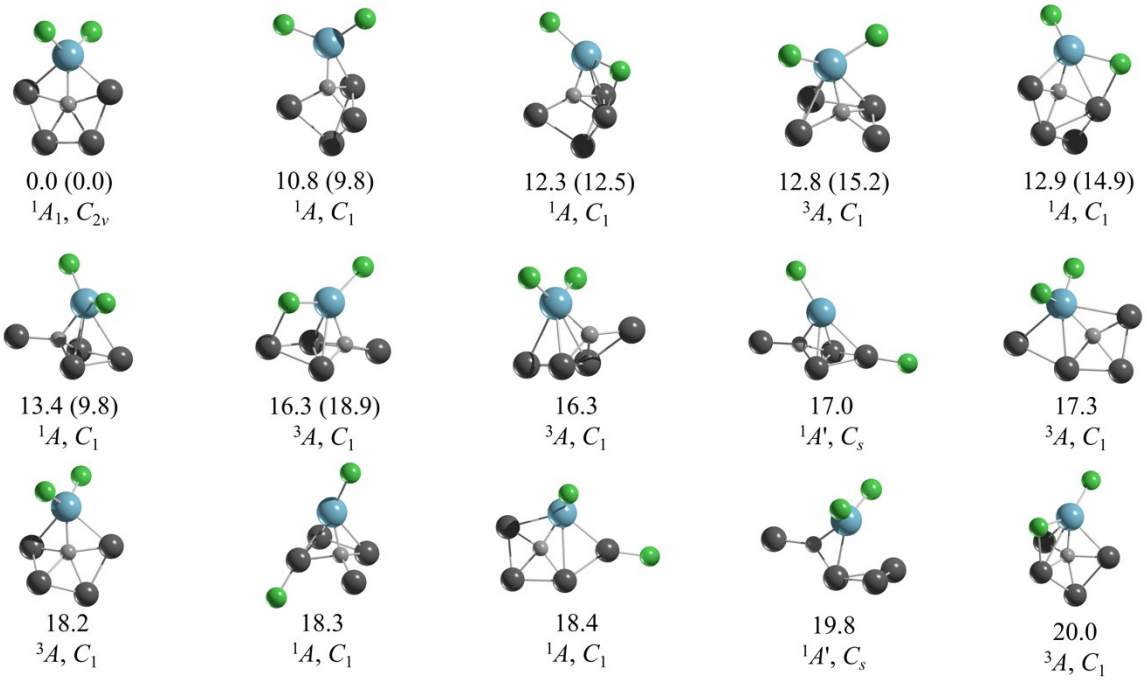


**Figure S13.** PBE0-D3/def2-TZVP structures of $CAl_4HfCl_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

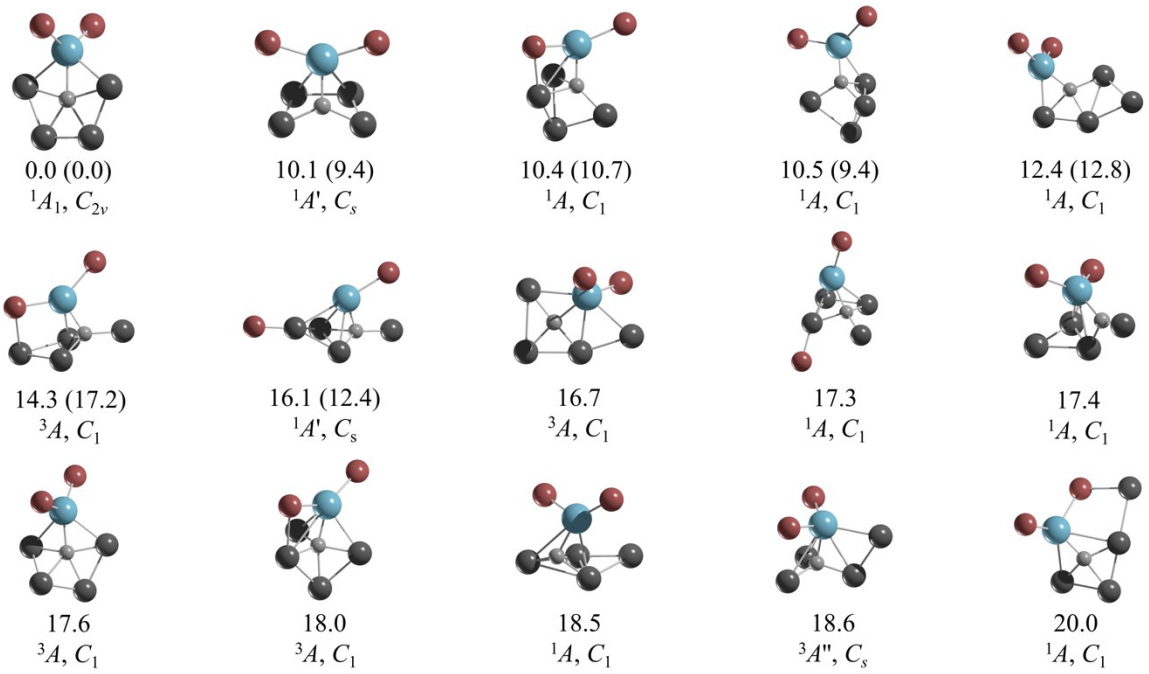


**Figure S14.** PBE0-D3/def2-TZVP structures of $CAl_4HfBr_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

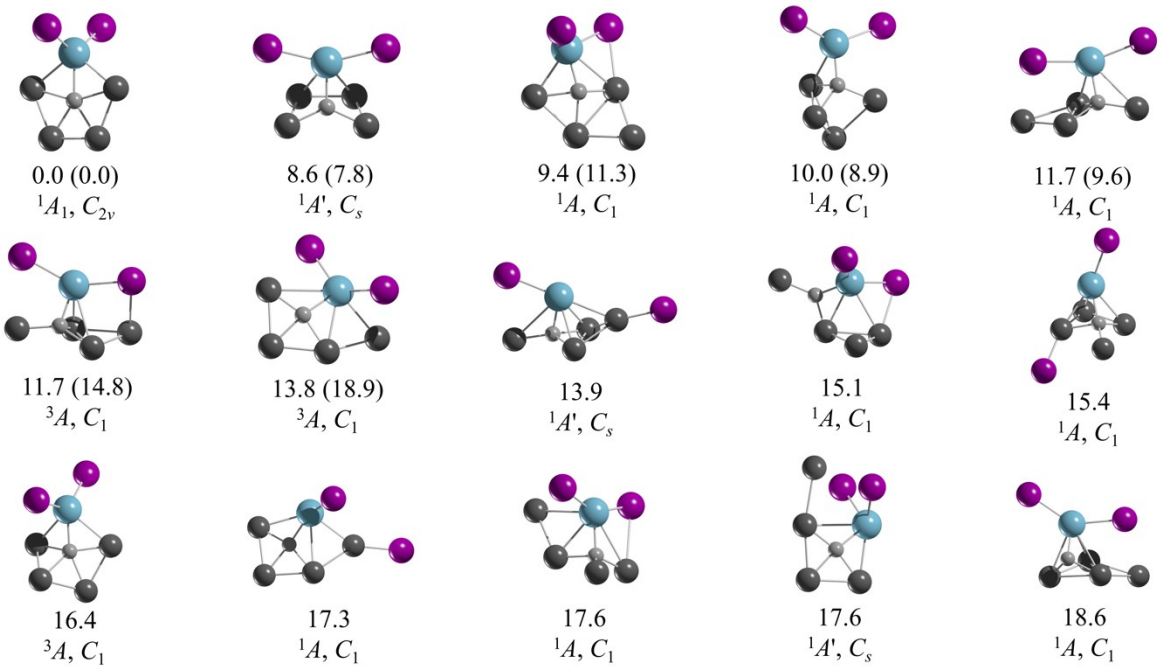


**Figure S15.** PBE0-D3/def2-TZVP structures of $CAl_4HfI_2$. The relative energies with respect to the lowest energy isomer obtained at the PBE0-D3/def2-TZVP and CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP levels are given in kcal·mol$^{-1}$ without and within parentheses, respectively.

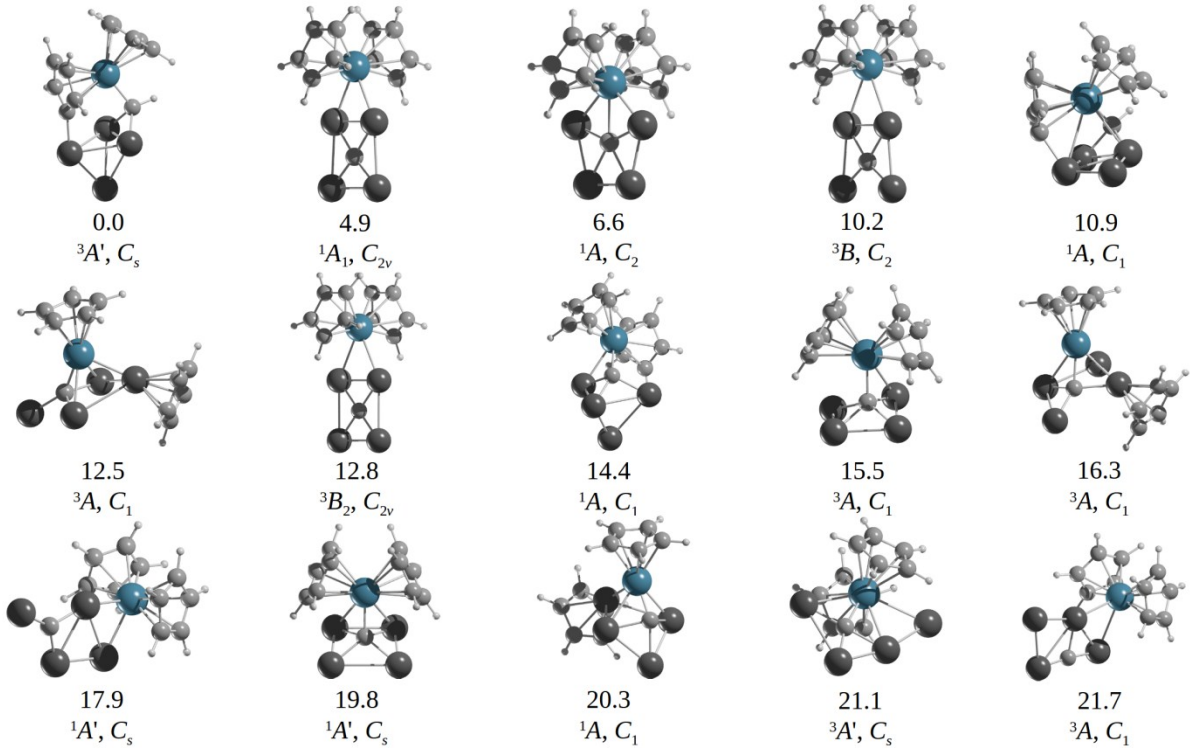


**Figure S16.**PBE0-D3/def2-TZVP structures of $CAl_4TiCp_2$. Relative energies with respect to the lowest lying isomer are given in kcal·mol$^{-1}$.

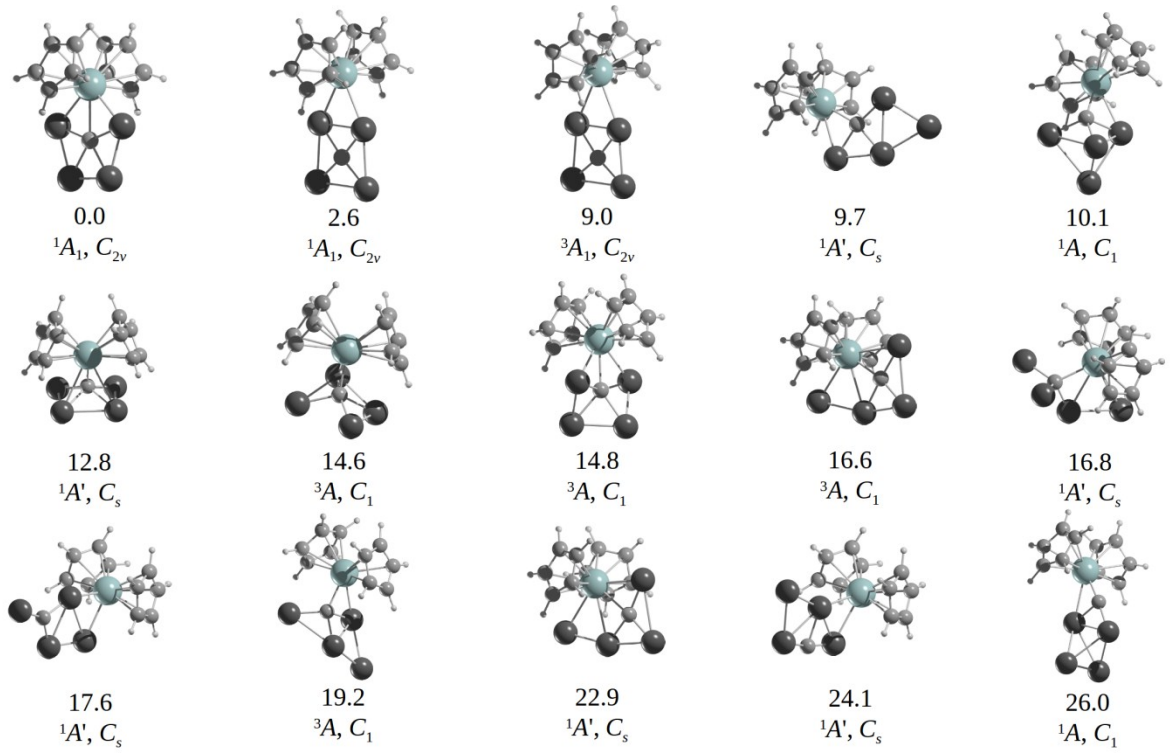


**Figure S17.** PBE0-D3/def2-TZVP structures of $CAl_4ZrCp_2$. Relative energies with respect to the lowest lying isomer are given in kcal·mol$^{-1}$.

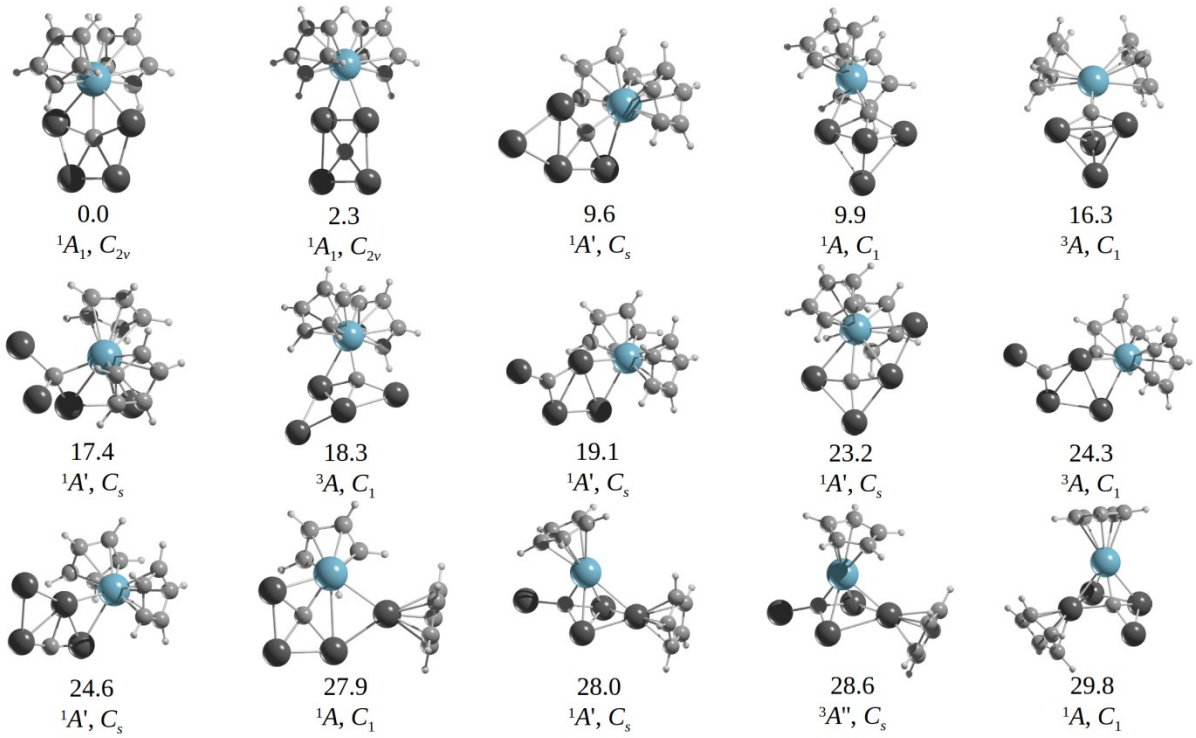


**Figure S18.** PBE0-D3/def2-TZVP structures of $CAl_4HfCp_2$. Relative energies with respect to the lowest lying isomer are given in kcal·mol$^{-1}$.

**Table S1.** NPA charges on carbon (q(C)), M (q(M)), sum of all Al (q(ΣAl)) atoms and $MX_2$ ($q(MX_2)$) fragment, and the Wiberg bond indices for the C-Al1 ($WBI_{C\text{-}Al1}$), C-Al2 ($WBI_{C\text{-}Al2}$), C-M ($WBI_{C\text{-}M}$) and M-X ($WBI_{M\text{-}X}$) bonds computed at the PBE0-D3/def2-TZVP level.

| System | q(C) | q(M) | q(ΣAl) | $q(MX_2)$ | Natural atomic orbital occupancies | $WBI_{C\text{-}Al1}$ | $WBI_{C\text{-}Al2}$ | $WBI_{C\text{-}M}$ | $WBI_{M\text{-}X}$ |
|---|---|---|---|---|---|---|---|---|---|
| $CAl_4ZrF_2$ | -2.32 | 1.56 | 1.98 | 0.34 | $2s^{1.57}2p_x^{1.62}2p_y^{1.65}2p_z^{1.45}$ | 0.41 | 0.53 | 0.75 | 0.66 |
| $CAl_4ZrCl_2$ | -2.24 | 0.85 | 2.16 | 0.08 | $2s^{1.55}2p_x^{1.60}2p_y^{1.64}2p_z^{1.42}$ | 0.36 | 0.51 | 0.95 | 0.96 |
| $CAl_4ZrBr_2$ | -2.22 | 0.63 | 2.20 | 0.02 | $2s^{1.55}2p_x^{1.59}2p_y^{1.64}2p_z^{1.41}$ | 0.35 | 0.50 | 1.01 | 1.05 |
| $CAl_4ZrI_2$ | -2.20 | 0.37 | 2.23 | -0.02 | $2s^{1.55}2p_x^{1.59}2p_y^{1.64}2p_z^{1.40}$ | 0.34 | 0.48 | 1.07 | 1.15 |
| $CAl_4HfF_2$ | -2.37 | 1.69 | 1.95 | 0.41 | $2s^{1.57}2p_x^{1.63}2p_y^{1.67}2p_z^{1.46}$ | 0.41 | 0.53 | 0.70 | 0.63 |
| $CAl_4HfCl_2$ | -2.29 | 0.98 | 2.11 | 0.18 | $2s^{1.55}2p_x^{1.61}2p_y^{1.67}2p_z^{1.43}$ | 0.36 | 0.51 | 0.89 | 0.96 |
| $CAl_4HfBr_2$ | -2.28 | 0.76 | 2.15 | 0.13 | $2s^{1.55}2p_x^{1.60}2p_y^{1.67}2p_z^{1.42}$ | 0.35 | 0.50 | 0.94 | 1.05 |
| $CAl_4HfI_2$ | -2.26 | 0.51 | 2.17 | 0.09 | $2s^{1.55}2p_x^{1.60}2p_y^{1.67}2p_z^{1.41}$ | 0.34 | 0.49 | 0.99 | 1.15 |
| $CAl_4ZrCp_2$ | -2.30 | 0.53 | 2.36 | -0.06 | $2s^{1.50}2p_x^{1.72}2p_y^{1.67}2p_z^{1.39}$ | 0.41 | 0.57 | 0.59 | - |
| $CAl_4HfCp_2$ | -2.30 | 0.65 | 2.27 | 0.03 | $2s^{1.49}2p_x^{1.70}2p_y^{1.69}2p_z^{1.40}$ | 0.41 | 0.56 | 0.61 | - |
| $CAl_4ZrCp^*_2$ | -2.31 | 0.61 | 2.27 | 0.05 | $2s^{1.48}2p_x^{1.70}2p_y^{1.72}2p_z^{1.39}$ | 0.38 | 0.56 | 0.63 | - |
| $CAl_4HfCp^*_2$ | -2.31 | 0.73 | 2.17 | 0.15 | $2s^{1.47}2p_x^{1.70}2p_y^{1.72}2p_z^{1.39}$ | 0.38 | 056 | 0.64 | - |

Al1 and Al2 are the adjacent and near adjacent Al atoms to the M atom, respectively.

Molecular coordinates Figure S1

1 TiAl4C

| | | | |
|---|---|---|---|
| Al | -1.220410000 | -1.708581000 | 0.082544000 |
| Al | 1.220208000 | -1.708736000 | 0.082785000 |
| Al | -2.081402000 | 0.607284000 | 0.069011000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Ti | 0.000113000 | 2.050705000 | 0.083675000 |
| Al | 2.081406000 | 0.607018000 | 0.068869000 |

2 TiAl4C

| | | | |
|---|---|---|---|
| Al | -1.468269000 | 0.081829919 | -1.523337577 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Ti | 0.000000000 | 1.860589223 | -0.338293066 |
| Al | -1.367118000 | -1.280527581 | 0.836334831 |
| Al | 1.468269000 | 0.081829919 | -1.523337577 |
| Al | 1.367118000 | -1.280527581 | 0.836334831 |

3 TiAl4C

| | | | |
|---|---|---|---|
| Al | 2.241808281 | -0.763276241 | -1.112672474 |
| C | 0.759174511 | 0.085707608 | -0.096899773 |
| Al | -0.518957265 | -0.189993270 | -1.695751812 |
| Al | -1.918311101 | -0.747169779 | 0.439891823 |
| Al | 0.439019287 | -0.883184901 | 1.636947056 |
| Ti | -0.350968330 | 1.503312552 | 0.458727898 |

4 TiAl4C

| | | | |
|---|---|---|---|
| Al | 1.227005000 | -1.703913000 | 0.000000000 |
| Al | -1.227005000 | -1.703913000 | 0.000000000 |
| Al | 2.093060000 | 0.620890000 | 0.000000000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Ti | 0.000000000 | 2.018624000 | 0.000000000 |
| Al | -2.093060000 | 0.620890000 | 0.000000000 |

5 TiAl4C

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.022644865 | 0.452206173 | -2.265272507 |
| Al | -1.413287148 | -0.124177887 | -1.461843491 |
| Ti | 0.248217337 | 1.752327764 | -0.181825444 |
| Al | -0.459361774 | -1.879876664 | 0.641875665 |
| Al | 1.986021260 | -0.453273447 | 0.007059801 |

6 TiAl4C

| | | | |
|---|---|---|---|
| Al | 0.812458438 | -0.243295843 | -1.445653609 |
| Al | -2.681350395 | -0.175542936 | -1.090976111 |
| C | -0.890999095 | -0.034735708 | -0.353643572 |
| Al | -0.175694517 | -1.216436535 | 1.139565502 |
| Al | 2.323329408 | -0.594340985 | 0.664325672 |

| | | | |
|---|---|---|---|
| Ti | 0.078287446 | 1.326972999 | 0.529429551 |

| | | | |
|---|---|---|---|
| 7 | TiAl4C | | |
| Ti | 0.114441763 | 1.380743462 | 0.532798301 |
| Al | 0.668681629 | -0.404494186 | -1.353749409 |
| C | -0.974945498 | 0.026787246 | -0.154319316 |
| Al | 2.187056169 | -0.701669712 | 0.768396985 |
| Al | -0.294319525 | -1.126061512 | 1.336770335 |
| Al | -2.305114516 | -0.116781596 | -1.581853807 |

| | | | |
|---|---|---|---|
| 8 | TiAl4C | | |
| Al | 1.245215000 | -1.688800000 | 0.000000000 |
| Al | -2.104655000 | 0.658117000 | 0.000000000 |
| Al | -1.245215000 | -1.688800000 | 0.000000000 |
| Ti | 0.000000000 | 1.922847000 | 0.000000000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 2.104655000 | 0.658117000 | 0.000000000 |

| | | | |
|---|---|---|---|
| 9 | TiAl4C | | |
| Al | -0.618463601 | -1.668734753 | 0.000000000 |
| C | 0.580557958 | -0.102368032 | 0.000000000 |
| Al | -2.807118525 | -0.189861405 | 0.000000000 |
| Al | 2.122805743 | 1.136968761 | 0.000000000 |
| Ti | -0.568292276 | 1.369506804 | 0.000000000 |
| Al | 1.996552035 | -1.548752655 | 0.000000000 |

| | | | |
|---|---|---|---|
| 10 | TiAl4C | | |
| Ti | -0.134722490 | 1.282808360 | 0.362738103 |
| Al | -0.060328678 | -1.172743692 | 1.314817831 |
| Al | 0.633440971 | -0.548277837 | -1.191993189 |
| Al | 2.392936896 | -0.298480336 | 0.824413667 |
| Al | -2.178785567 | -0.090113373 | -1.599996345 |
| C | -1.211755984 | -0.132797443 | 0.084271090 |

| | | | |
|---|---|---|---|
| 11 | TiAl4C | | |
| Al | -0.221487000 | -1.031226000 | -0.008661000 |
| C | 1.475787000 | -0.205660000 | 0.000020000 |
| Ti | 0.689899000 | 1.472982000 | 0.004825000 |
| Al | 3.183742000 | -1.096221000 | 0.000215000 |
| Al | -1.970061000 | 1.049553000 | -0.008595000 |
| Al | -2.840848000 | -1.319925000 | 0.008865000 |

| | | | |
|---|---|---|---|
| 12 | TiAl4C | | |
| Al | -0.661656000 | 1.291386000 | -0.706132000 |
| C | 1.116295000 | 0.678928000 | -0.420687000 |
| Al | -2.495890000 | 0.588896000 | 0.994896000 |
| Al | -2.145980000 | -1.181451000 | -0.752897000 |
| Ti | 2.682831000 | -0.075173000 | 0.110098000 |
| Al | 0.248138000 | -0.884968000 | 0.471976000 |

13 TiAl4C

| | | | |
|---|---|---|---|
| Al | 0.516379879 | 1.226321717 | -1.648843375 |
| Al | -0.368570413 | 2.273640084 | 0.628788032 |
| C | -0.195408951 | 0.284030636 | 0.493747080 |
| Al | 1.591770802 | -0.577738784 | -0.184559170 |
| Al | -1.036217525 | -0.742292192 | -1.129970804 |
| Ti | -0.362329989 | -1.365603736 | 1.244869099 |

14 TiAl4C

| | | | |
|---|---|---|---|
| Al | 0.935266000 | -0.862128632 | 0.723411817 |
| C | 0.929585000 | 0.696969450 | -0.584826808 |
| Al | -0.563427000 | 1.544345428 | 0.425036558 |
| Al | -0.563427000 | -0.150406529 | -1.594690175 |
| Al | 2.843617000 | 0.654552803 | -0.549235015 |
| Ti | -1.820631000 | -0.891115753 | 0.747734900 |

15 TiAl4C

| | | | |
|---|---|---|---|
| C | 1.370642000 | -0.097126000 | 0.000000000 |
| Al | 0.546954000 | -1.786286000 | 0.000000000 |
| Al | -1.873778000 | -1.285616000 | 0.000000000 |
| Al | -2.587118000 | 1.007027000 | 0.000000000 |
| Ti | 0.000000000 | 1.087279000 | 0.000000000 |
| Al | 3.281337000 | 0.269692000 | 0.000000000 |

Molecular coordinates Figure S2

1 ZrAl4C

| | | | |
|---|---|---|---|
| Zr | 0.001981417 | 1.374004125 | 0.490335219 |
| C | -0.271146608 | -0.523176206 | 0.596788343 |
| Al | 0.648650026 | 0.149565046 | -1.825537803 |
| Al | 1.692206610 | -0.985219206 | 0.294474765 |
| Al | -1.686157723 | -0.564272951 | -0.871437692 |
| Al | -0.535652080 | -2.586313679 | 0.618338726 |

2 ZrAl4C

| | | | |
|---|---|---|---|
| Al | -2.718699183 | -0.091040955 | -1.303254620 |
| Al | 2.012237738 | -1.280452215 | 0.594619235 |
| C | -0.954279239 | -0.069485244 | -0.467751765 |
| Al | 0.682648322 | -0.653140145 | -1.576302710 |
| Zr | 0.334013102 | 1.117143374 | 0.463700512 |
| Al | -0.563481971 | -1.380662933 | 1.074052582 |

3 ZrAl4C

| | | | |
|---|---|---|---|
| Al | 1.449157000 | -0.368046863 | -1.262640134 |
| C | 0.000000000 | -0.508452892 | 0.340562243 |
| Al | 1.404629000 | -1.755838863 | 1.141086121 |
| Al | -1.449157000 | -0.368046863 | -1.262640134 |
| Al | -1.404629000 | -1.755838863 | 1.141086121 |
| Zr | 0.000000000 | 1.456794149 | 0.027926518 |

4 ZrAl4C
Zr 0.131244020 1.313720389 0.439541860
C 0.410344492 -0.650739400 0.561890767
Al 0.303551254 -2.529890032 1.255948794
Al 1.563953644 -0.610582181 -1.099877861
Al -1.662327495 -0.812404142 0.250082922
Al -0.798394835 0.210999955 -2.017924423

5 ZrAl4C
Al 0.403671113 -1.628589327 0.894950427
Zr 0.078034413 1.100394766 0.466492212
C -1.110985492 -0.424323557 0.571175092
Al 0.030667698 -0.574563739 -1.554784027
Al 2.488793169 -0.656590223 -0.428401773
Al -2.650476123 -0.330244865 -0.610745120

6 ZrAl4C
C 0.000000000 0.000000000 0.000000000
Al 1.249156000 -1.681872000 0.000000000
Al -1.249156000 -1.681872000 0.000000000
Al 2.180157000 0.642039000 0.000000000
Zr 0.000000000 2.021995000 0.000000000
Al -2.180157000 0.642039000 0.000000000

7 ZrAl4C
C 0.000000000 0.000000000 0.000000000
Al 1.535529182 -1.319146159 0.000000000
Al -1.081163862 -1.665851307 0.000000000
Zr -1.410736380 1.389048110 0.000000000
Al -3.445705788 -0.517944062 0.000000000
Al 1.416177159 1.382156097 0.000000000

8 ZrAl4C
Al 1.212013709 -1.756067000 0.037338915
C 0.000000000 0.000000000 0.000000000
Al 1.929719581 0.548856000 0.773485874
Al -1.815343683 0.300444000 -1.124825377
Al -1.261489550 -1.830071000 0.082288784
Zr -0.138114940 2.026044000 0.004595022

9 ZrAl4C
Al -1.672163498 -1.502773250 -0.546964732
Al 0.622482902 -1.943682358 0.772411601
Zr 1.953727249 0.249792447 0.090917016
C 0.000000000 0.000000000 0.000000000
Al 0.622482902 -0.992450463 -1.841076551
Al -1.635290579 1.060373599 0.385944427

10 ZrAl4C
Al 0.371990255 -1.599047000 0.139492240

| | | | |
|---|---|---|---|
| Al | -1.234976058 | -0.699862000 | -1.946653828 |
| Al | -2.282796117 | -0.739478000 | 0.256030900 |
| C | 1.302661231 | 0.025910000 | 0.627451973 |
| Al | 2.974578226 | -0.497627000 | 1.462725831 |
| Zr | -0.139757862 | 1.145318000 | -0.065386297 |

| | | | |
|---|---|---|---|
| 11 | ZrAl4C | | |
| C | -0.062985249 | -0.009500000 | 0.939505021 |
| Al | -2.063437986 | -0.234723000 | 1.110676295 |
| Al | 0.146098429 | 1.980446000 | 0.883047842 |
| Al | -0.415608383 | -2.031849000 | 0.453337926 |
| Zr | 1.167980136 | -0.170719000 | -0.588766578 |
| Al | -1.231766048 | 0.815801000 | -1.069092849 |

| | | | |
|---|---|---|---|
| 12 | ZrAl4C | | |
| C | 0.359877568 | 0.104445213 | 0.642825380 |
| Al | 2.364436520 | 0.195396148 | 0.539462276 |
| Al | 0.904990758 | -1.862125843 | 0.964703662 |
| Zr | -1.132697162 | -0.556585664 | -0.444587891 |
| Al | 0.832288836 | 1.411699791 | -1.137225303 |
| Al | -0.782590109 | 1.919395350 | 0.704334613 |

| | | | |
|---|---|---|---|
| 13 | ZrAl4C | | |
| C | -0.058768902 | -0.296622684 | 0.410385000 |
| Al | 1.169376131 | -1.822229139 | -0.210635000 |
| Al | -1.411973133 | -1.778681645 | 0.028657000 |
| Al | -1.043933087 | 0.807270304 | -1.010997000 |
| Al | -3.120732023 | 0.139401095 | 0.483093000 |
| Zr | 1.441175651 | 0.907121108 | 0.169154000 |

| | | | |
|---|---|---|---|
| 14 | ZrAl4C | | |
| Al | -0.943318773 | -1.459831169 | 0.870624229 |
| Al | -0.112851491 | -0.993762075 | -1.666926926 |
| Zr | -0.600303430 | 1.131824840 | 0.011418970 |
| Al | 1.548710541 | -1.619210132 | 0.209449820 |
| C | -1.638206954 | -0.379566586 | -0.605852429 |
| Al | 2.110640425 | 0.765450799 | 0.831341183 |

| | | | |
|---|---|---|---|
| 15 | ZrAl4C | | |
| Al | -1.086222746 | 0.753702662 | -0.851968000 |
| Al | -3.422606765 | -0.088725047 | 0.318633000 |
| C | 0.051680981 | -0.423573909 | 0.377893000 |
| Zr | 1.439910426 | 0.995353075 | 0.162627000 |
| Al | 1.420054337 | -1.757031282 | -0.271965000 |
| Al | -1.365570764 | -1.775073898 | 0.130496000 |

Molecular coordinates Figure S3

| | | | |
|---|---|---|---|
| 1 | HfAl4C | | |
| Al | -1.982260224 | -0.517191000 | -0.018288081 |

| | | | |
|---|---|---|---|
| Al | -1.182010873 | -0.128915000 | -2.534830498 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.190250063 | -2.037195000 | 0.407992576 |
| Al | 1.260162829 | -0.517191000 | -1.530254781 |
| Hf | -0.361048698 | 1.753782000 | -0.774271431 |

| | | | |
|---|---|---|---|
| 2 | HfAl4C | | |
| Al | 0.211475705 | -0.908132487 | -1.809914153 |
| Hf | 0.282034362 | 0.849312409 | 0.281065807 |
| C | -1.134437335 | -0.425430658 | -0.317654357 |
| Al | -3.038815375 | -0.586050189 | -0.700447040 |
| Al | 2.093095112 | -1.318160862 | 0.014472211 |
| Al | -0.304205766 | -1.695185584 | 1.085827112 |

| | | | |
|---|---|---|---|
| 3 | HfAl4C | | |
| Al | -0.149929000 | -1.696154416 | 0.805741924 |
| Al | -2.788650000 | -0.797099177 | -0.058872479 |
| C | -1.100269000 | -0.257684506 | -0.838191335 |
| Al | 0.465938000 | -1.016009766 | -1.753877608 |
| Al | 2.386012000 | -1.107660602 | 0.087145760 |
| Hf | 0.107330000 | 0.855084700 | 0.235935513 |

| | | | |
|---|---|---|---|
| 4 | HfAl4C | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.564574201 | 0.081353778 | -1.403833014 |
| Hf | 0.127170857 | 1.959294553 | -0.346893357 |
| Al | 2.101188154 | 0.079619022 | -0.070282420 |
| Al | 0.172889356 | -1.967583228 | -0.473726052 |
| Al | 0.902135079 | 0.425020733 | -2.478183503 |

| | | | |
|---|---|---|---|
| 5 | HfAl4C | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Hf | 0.000000000 | 2.027840000 | 0.000000000 |
| Al | 2.193288000 | 0.661758000 | 0.000000000 |
| Al | -2.193288000 | 0.661758000 | 0.000000000 |
| Al | -1.254350000 | -1.649319000 | 0.000000000 |
| Al | 1.254350000 | -1.649319000 | 0.000000000 |

| | | | |
|---|---|---|---|
| 6 | HfAl4C | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Hf | 0.000000000 | 1.959681686 | -0.414064247 |
| Al | -1.391350000 | -1.279123743 | 0.808729312 |
| Al | -1.508552000 | 0.090928257 | -1.564270361 |
| Al | 1.391350000 | -1.279123743 | 0.808729312 |
| Al | 1.508552000 | 0.090928257 | -1.564270361 |

| | | | |
|---|---|---|---|
| 7 | HfAl4C | | |
| Al | 0.962375063 | -1.489946289 | -0.969362000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Hf | 1.265413530 | 1.454940773 | -0.474610000 |

| | | | |
|---|---|---|---|
| Al | 3.134753223 | -0.566693738 | -0.110140000 |
| Al | -1.552516386 | 1.215362941 | -0.464813000 |
| Al | -1.509020802 | -1.377900245 | -0.227405000 |

| | | | |
|---|---|---|---|
| 8 | HfAl4C | | |
| Al | 1.965455558 | 0.534831000 | 0.660379207 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.914734620 | -1.772732000 | 0.671288336 |
| Hf | -0.153186717 | 2.025243000 | -0.043393228 |
| Al | -2.111781765 | 0.194771000 | 0.240741736 |
| Al | -1.016455835 | -1.747292000 | -0.926326954 |

| | | | |
|---|---|---|---|
| 9 | HfAl4C | | |
| Al | 0.317895613 | -1.925359000 | 0.148237159 |
| Al | -2.310001215 | -0.855526000 | 0.286601644 |
| Hf | -0.071460556 | 0.841548000 | -0.033322605 |
| C | 1.339405996 | -0.366052000 | 0.624575273 |
| Al | -1.265290562 | -0.855526000 | -1.953787580 |
| Al | 3.034990045 | -0.855526000 | 1.415239100 |

| | | | |
|---|---|---|---|
| 10 | HfAl4C | | |
| C | -0.123425493 | 1.067776000 | 0.339108755 |
| Hf | -0.354953293 | -0.788474000 | 0.975226158 |
| Al | 0.324425943 | 2.495922000 | -0.891352953 |
| Al | 1.720021715 | 0.169577000 | -0.383397633 |
| Al | 1.049581839 | 1.039037000 | -2.883702403 |
| Al | -1.071169829 | 0.169577000 | -1.399308273 |

| | | | |
|---|---|---|---|
| 11 | HfAl4C | | |
| C | -0.012478311 | 0.854920059 | -0.064276327 |
| Hf | -0.161998311 | -0.863027177 | 0.891261032 |
| Al | -0.085400559 | 2.849307416 | -0.006853927 |
| Al | 0.441309645 | 1.771813434 | -2.344377771 |
| Al | 1.650801650 | -0.075948282 | -0.986670637 |
| Al | -1.103730882 | -0.159908128 | -1.568642950 |

| | | | |
|---|---|---|---|
| 12 | HfAl4C | | |
| Hf | -0.184485439 | 0.688509031 | 0.000000000 |
| Al | -2.819322689 | -0.105928844 | 0.000000000 |
| Al | 3.280692993 | 0.556836574 | 0.000000000 |
| Al | 1.178434822 | -2.132071189 | 0.000000000 |
| C | 1.532558441 | -0.285642728 | 0.000000000 |
| Al | -1.325374728 | -2.000279078 | 0.000000000 |

| | | | |
|---|---|---|---|
| 13 | HfAl4C | | |
| Al | -0.891460522 | -1.735058013 | 0.841405796 |
| Al | 1.626629540 | -1.860886290 | 0.273053518 |
| Hf | -0.424032536 | 0.846507718 | -0.007453941 |
| Al | 0.043395449 | -1.289043421 | -1.688068653 |
| Al | 2.259177049 | 0.494296726 | 0.922115939 |

| | | | |
|---|---|---|---|
| C | -1.493385824 | -0.644924819 | -0.665650738 |

| | | | |
|---|---|---|---|
| 14 | HfAl4C | | |
| Al | 0.837800000 | -0.844599000 | 0.452442000 |
| Hf | -1.705283000 | -0.031049000 | 0.035261000 |
| Al | 3.273814000 | -1.146468000 | -0.798785000 |
| Al | 3.544958000 | 0.515695000 | 1.079537000 |
| Al | 1.793001000 | 1.306858000 | -0.701178000 |
| C | -0.010676000 | 0.737701000 | -0.492501000 |

| | | | |
|---|---|---|---|
| 15 | HfAl4C | | |
| Al | 0.973586000 | -0.911766000 | 0.385183000 |
| Al | 1.761887000 | 1.397701000 | -0.688756000 |
| C | 0.020573000 | 0.637120000 | -0.386746000 |
| Al | 3.290663000 | -1.249221000 | -0.669311000 |
| Hf | -1.735783000 | -0.028914000 | 0.036525000 |
| Al | 3.577936000 | 0.629368000 | 0.949090000 |

Molecular coordinates Figure S4

| | | | |
|---|---|---|---|
| 1 | TiAl4CF2 | | |
| Al | 1.835257653 | 0.569305000 | 1.059586500 |
| F | -0.786773500 | 2.874126000 | 1.362731676 |
| Al | 1.047551257 | -1.720151000 | 0.604804000 |
| Al | -1.047551257 | -1.720151000 | -0.604804000 |
| F | 0.786773500 | 2.874126000 | -1.362731676 |
| Ti | 0.000000000 | 2.055991000 | 0.000000000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.835257653 | 0.569305000 | -1.059586500 |

| | | | |
|---|---|---|---|
| 2 | TiAl4CF2 | | |
| Al | -0.293766246 | -1.574273487 | 1.338719823 |
| Al | 2.066974448 | -0.960391337 | 0.048106576 |
| C | -0.699217796 | -0.483258209 | -0.282697060 |
| F | 1.987169934 | 0.842567987 | 0.628025299 |
| Al | 0.297398320 | -0.470316679 | -2.011955998 |
| F | -1.050587506 | 2.549475887 | 0.655659324 |
| Al | -2.511542416 | -1.113817320 | -0.810385899 |
| Ti | 0.068101652 | 1.177978108 | 0.400214666 |

| | | | |
|---|---|---|---|
| 3 | TiAl4CF2 | | |
| F | -2.124255000 | 0.919043954 | 0.298615482 |
| Ti | -0.105285000 | 0.984583161 | 0.319910461 |
| Al | -2.306716000 | -0.841176202 | -0.273314716 |
| F | 1.683857000 | 1.726132388 | 0.560854411 |
| Al | -0.105285000 | -1.721528731 | 1.194808454 |
| Al | -0.105285000 | -0.690455211 | -1.978509544 |
| Al | 2.647893000 | 0.085282189 | 0.027709863 |
| C | 0.763665000 | -0.714168310 | -0.232047350 |

4 TiAl4CF2

| | | | |
|---|---|---|---|
| Al | -0.979214000 | -1.606004000 | -1.009031000 |
| Al | 1.539268000 | -1.351899000 | -0.495555000 |
| Ti | 0.132250000 | 2.027426000 | -0.303809000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.967781000 | 0.290619000 | 0.435037000 |
| Al | 1.436897000 | 0.459829000 | 1.366395000 |
| F | -1.850583000 | 2.087653000 | 0.090907000 |
| F | 1.201124000 | 3.025793000 | -1.346608000 |

5 TiAl4CF2

| | | | |
|---|---|---|---|
| Al | 1.197462776 | -0.393657531 | -1.122110536 |
| Al | -1.346136742 | 0.262101739 | -1.882758379 |
| Ti | -0.148999840 | 1.340666748 | 0.309956257 |
| C | 0.096870037 | -0.632730653 | 0.526214991 |
| F | 2.327010508 | -1.459826789 | -1.688413274 |
| F | -0.244055644 | 2.778302659 | 1.396960254 |
| Al | -1.881407657 | -0.894368013 | 0.535270559 |
| Al | 0.795479143 | -1.863657029 | 1.903965366 |

6 TiAl4CF2

| | | | |
|---|---|---|---|
| Ti | -0.024464162 | 1.116286416 | 0.463716769 |
| F | 0.972138341 | 1.712585481 | -1.100152286 |
| Al | 0.557364515 | 0.118281435 | -2.077031926 |
| Al | -1.496663716 | -0.869040188 | -0.774831186 |
| Al | 2.024648748 | -1.174559126 | -0.136795695 |
| Al | -0.901473582 | -1.968613806 | 1.669303455 |
| F | -1.333601449 | 1.705094969 | 1.525211679 |
| C | 0.233499512 | -0.782718978 | 0.520719683 |

7 TiAl4CF2

| | | | |
|---|---|---|---|
| F | -1.836419439 | 0.980026434 | 0.980435848 |
| Al | -1.977120740 | -0.826192167 | 0.273556917 |
| Al | 1.423756590 | -0.115322497 | -1.486611503 |
| C | 0.035681889 | -0.833730216 | 0.162832168 |
| F | 1.556391555 | 1.554275991 | 1.453379488 |
| Al | 1.596575356 | -1.988447753 | 0.416987760 |
| Al | -0.979248336 | -0.121316965 | -2.036937714 |
| Ti | 0.067029717 | 0.993649465 | 0.633988279 |

8 TiAl4CF2

| | | | |
|---|---|---|---|
| F | 1.741567388 | 1.623429447 | -0.094618446 |
| Ti | -0.031255121 | 1.150689218 | -0.584643522 |
| C | 0.010677415 | -0.537287878 | 0.194740105 |
| F | -1.747907006 | 1.617389060 | 0.080040694 |
| Al | -1.818053657 | -0.042456738 | 1.242872328 |
| Al | -1.338461120 | -1.934544636 | -0.628763625 |
| Al | 1.275658419 | -1.930019514 | -0.759608508 |
| Al | 1.933210617 | -0.035963184 | 1.055109783 |

9 TiAl4CF2

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.166530000 | -1.492203000 | -0.991509000 |
| Al | 1.985757000 | 0.579738000 | 0.577861000 |
| F | 1.477271000 | 2.359085000 | -0.053591000 |
| Ti | -0.346240000 | 1.850515000 | -0.290994000 |
| F | -1.723517000 | 2.272548000 | -1.350846000 |
| Al | -1.432524000 | 0.279537000 | 1.471821000 |
| Al | -1.353025000 | -1.596992000 | -0.315860000 |

10 TiAl4CF2

| | | | |
|---|---|---|---|
| Ti | -0.155569602 | 1.647218674 | -0.508150373 |
| Al | -1.478105074 | -0.590906799 | -0.105570091 |
| Al | 1.350482530 | -0.691365623 | -0.382518807 |
| Al | -0.020334835 | -3.202536758 | 0.169766625 |
| F | -0.923957357 | 3.217739559 | -0.119036208 |
| C | 0.065531651 | 0.367134542 | 0.823183428 |
| F | 1.209364657 | 0.720755196 | -1.608254346 |
| Al | 0.183394491 | -1.198889585 | 1.994154704 |

11 TiAl4CF2

| | | | |
|---|---|---|---|
| Al | 0.928696571 | -1.513045135 | 1.793996775 |
| Al | -1.392993730 | -0.285617800 | -1.001389745 |
| Al | 2.446837352 | 0.130447790 | 0.530036708 |
| F | -1.563655077 | 1.454419775 | -0.600379929 |
| Al | 1.071408062 | -0.640504406 | -1.445321085 |
| F | -2.880580289 | -0.920218515 | -1.318959592 |
| C | -0.048456242 | -0.557744128 | 0.398589040 |
| Ti | 0.026706084 | 1.297818957 | 0.748968506 |

12 TiAl4CF2

| | | | |
|---|---|---|---|
| Al | -0.020280965 | -2.672554221 | -0.224017204 |
| Al | 0.151614629 | -1.268668070 | 2.186894038 |
| Al | 1.356124312 | -0.536806229 | -1.160699023 |
| C | 0.099807633 | -0.291193102 | 0.438239673 |
| F | -1.441180339 | 1.254350028 | -1.165289974 |
| F | 0.829678483 | 2.630653929 | 1.190376786 |
| Ti | 0.167582339 | 1.498961735 | -0.027276019 |
| Al | -1.393775305 | -0.613896927 | -0.975651260 |

13 TiAl4CF2

| | | | |
|---|---|---|---|
| F | 0.726689428 | 2.009949647 | -1.320638118 |
| Ti | -0.417665542 | 0.828588740 | -0.162840951 |
| Al | 2.494738812 | 1.552664762 | -0.979409596 |
| F | -1.924914003 | 0.876238684 | 1.089300450 |
| Al | -0.552110966 | -2.708973891 | -0.879150775 |
| Al | 1.569510746 | -0.727346985 | 0.674052946 |
| Al | -1.852249919 | -1.011086968 | 1.542345465 |
| C | -0.267648454 | -1.095496071 | 0.168774326 |

14 TiAl4CF2

| | | | |
|---|---|---|---|
| Ti | -1.281678104 | 0.890114387 | 0.495269111 |
| Al | 0.970697946 | -2.036223163 | -0.427644361 |
| C | 0.033200091 | -0.417165801 | 0.342471456 |
| Al | 3.205114557 | -0.530187423 | -0.280660648 |
| Al | 0.960101696 | 0.637476115 | -1.092449911 |
| Al | -1.511224476 | -1.653609159 | 0.047332724 |
| F | -0.487620388 | 1.834029931 | -1.058111964 |
| F | -1.637186878 | 1.443030468 | 2.151862051 |

15 TiAl4CF2

| | | | |
|---|---|---|---|
| F | -4.754803319 | 0.389367713 | 0.209333000 |
| Al | -3.135267045 | 0.198450486 | -0.053040000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.242230002 | -1.595555225 | -0.426178000 |
| F | 2.229631934 | 1.741183384 | 1.122847000 |
| Al | -1.037911009 | 1.551206428 | -0.771408000 |
| Ti | 1.498627687 | 1.054420475 | -0.336573000 |
| Al | -1.236724172 | -1.523094548 | 0.286036000 |

Molecular coordinates Figure S5

1 TiAl4CCl2

| | | | |
|---|---|---|---|
| Al | -1.373732781 | 0.375028304 | -1.462848517 |
| Al | -1.856064166 | -0.561135718 | 1.069875554 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Cl | -1.460801190 | 1.660641547 | 2.362533609 |
| Al | 0.638725804 | -1.585784586 | 1.207755833 |
| Cl | 2.354112221 | 2.186446699 | 0.076542037 |
| Al | 1.816924564 | -0.249945790 | -0.991109102 |
| Ti | 0.277622802 | 1.639442466 | 0.851336770 |

2 TiAl4CCl2

| | | | |
|---|---|---|---|
| Al | 1.853767214 | -0.434316000 | 1.070273000 |
| Al | 1.052187957 | -2.734161000 | 0.607481000 |
| C | 0.000000000 | -1.010538000 | 0.000000000 |
| Cl | 0.998326500 | 1.955557000 | -1.729152221 |
| Al | -1.052187957 | -2.734161000 | -0.607481000 |
| Cl | -0.998326500 | 1.955557000 | 1.729152221 |
| Al | -1.853767214 | -0.434316000 | -1.070273000 |
| Ti | 0.000000000 | 0.997940000 | 0.000000000 |

3 TiAl4CCl2

| | | | |
|---|---|---|---|
| Cl | 2.155170453 | 1.337100419 | 0.880466645 |
| Al | -1.621426570 | -2.010178139 | 0.508968528 |
| Al | -1.413344117 | -0.346867413 | -1.610352376 |
| C | 0.055191237 | -1.033680015 | 0.173017895 |
| Cl | -2.201939318 | 1.417681329 | 0.143421670 |
| Ti | -0.010627891 | 0.799155185 | 0.520917814 |
| Al | 1.136155792 | -0.497279645 | -1.762754076 |

| | | | |
|---|---|---|---|
| Al | 1.952286853 | -1.623415542 | 0.563799588 |

| | | | |
|---|---|---|---|
| 4 | TiAl4CCl2 | | |
| Cl | 1.658974976 | -2.875998775 | 0.759629058 |
| Al | 0.698300982 | -1.009620347 | 0.570136476 |
| Al | -0.666636999 | 0.384650413 | -2.028054129 |
| Al | -1.998801417 | -0.524118428 | 0.262226414 |
| C | 0.959483651 | 0.330764425 | -0.868798082 |
| Al | 2.576358160 | 0.390103510 | -1.950855535 |
| Ti | -0.107332701 | 1.389206301 | 0.401402198 |
| Cl | -2.324590353 | 1.541861803 | 1.433728246 |

| | | | |
|---|---|---|---|
| 5 | TiAl4CCl2 | | |
| Cl | -2.368272353 | -2.320335614 | -1.239419390 |
| Al | -1.051935583 | -0.706679331 | -0.924443736 |
| C | 0.208693495 | -0.620423065 | 0.621216103 |
| Ti | 0.258947018 | 1.295993331 | 0.120777781 |
| Cl | 0.294220726 | 3.317195210 | 1.120227790 |
| Al | -0.317758663 | -1.829200137 | 2.111610819 |
| Al | 1.342438945 | 0.017488449 | -2.015215172 |
| Al | 2.204941088 | -0.692064549 | 0.492803986 |

| | | | |
|---|---|---|---|
| 6 | TiAl4CCl2 | | |
| Al | -1.907291675 | 0.003290963 | 0.548150557 |
| Al | 0.521859616 | 0.682131170 | -1.896319877 |
| Ti | 0.394475254 | 1.831152649 | 0.435319505 |
| Al | -0.085067342 | -1.527660742 | 1.396666685 |
| Cl | -3.650494562 | -0.055250111 | -0.636119730 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Cl | -1.802165879 | 2.100550357 | 1.512398512 |
| Al | 2.009148180 | -0.360804875 | 0.381442301 |

| | | | |
|---|---|---|---|
| 7 | TiAl4CCl2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.943773000 | -0.651362000 | 0.568497000 |
| Al | 1.214464000 | 0.568839000 | -1.639058000 |
| Al | -2.039618000 | -0.196674000 | -0.395114000 |
| Ti | -0.021515000 | 1.827918000 | 0.322674000 |
| Cl | -2.272900000 | 2.188549000 | 0.543933000 |
| Al | -0.421569000 | -1.597281000 | 1.324628000 |
| Cl | 2.128521000 | 2.319019000 | 0.857549000 |

| | | | |
|---|---|---|---|
| 8 | TiAl4CCl2 | | |
| Al | 1.231335695 | 0.622856247 | -1.289470992 |
| Al | 1.264856250 | -1.330432766 | 0.810053565 |
| C | -0.673827839 | -1.057756991 | 0.391168179 |
| Cl | 2.393838799 | 0.142426509 | -2.975544419 |
| Cl | -1.237394884 | 2.041995373 | 2.466101386 |
| Al | -1.672534382 | -2.677459717 | 0.948141570 |
| Al | -1.450688620 | -0.391832447 | -1.329687676 |

| | | | |
|---|---|---|---|
| Ti | -0.339326510 | 0.832302073 | 0.795729560 |

| | | | |
|---|---|---|---|
| 9 | TiAl4CCl2 | | |
| Al | -2.699968207 | -0.795439067 | -0.129086743 |
| Ti | -0.202646429 | 0.965991521 | -0.004961521 |
| C | -0.675689132 | -0.861046441 | -0.011668645 |
| Cl | -2.257702307 | 1.878192305 | -0.360774855 |
| Al | 0.491223935 | -2.079463795 | 0.933880072 |
| Al | 0.609873238 | -0.903600999 | -1.592838148 |
| Cl | 1.722870775 | 1.198993137 | 1.161983312 |
| Al | 2.953061925 | -1.482856024 | -0.245907947 |

| | | | |
|---|---|---|---|
| 10 | TiAl4CCl2 | | |
| Al | 0.205523036 | -2.591448283 | -0.667000340 |
| Al | -0.493741183 | -1.138133164 | 1.376722815 |
| C | -0.415500018 | 0.455681824 | 0.213503141 |
| Cl | -1.409416299 | -0.997392895 | 3.279714638 |
| Cl | 2.046564886 | 1.657056184 | -1.435612365 |
| Al | -1.253169421 | -0.403599844 | -1.449668893 |
| Ti | -0.283361016 | 1.991351468 | -0.821218323 |
| Al | 1.379495282 | -0.309752198 | -0.380357918 |

| | | | |
|---|---|---|---|
| 11 | TiAl4CCl2 | | |
| Al | -0.012824826 | -1.706899832 | 0.881962614 |
| Ti | -0.578575079 | 0.832655339 | 0.233815019 |
| Cl | 4.130436960 | -0.178472892 | 0.686229070 |
| Al | 2.098816045 | -0.439022713 | 0.206396610 |
| Cl | -2.581608222 | 1.908555928 | 0.305196489 |
| Al | -3.091394391 | -0.550836596 | -0.793195917 |
| C | -1.109860838 | -0.745603717 | -0.508572775 |
| Al | 0.471385129 | -0.630640763 | -1.752603165 |

| | | | |
|---|---|---|---|
| 12 | TiAl4CCl2 | | |
| Al | 3.072165112 | -0.719535639 | -0.716226564 |
| Ti | 0.394831437 | 1.077651779 | 0.200455003 |
| Cl | 1.244752643 | 3.036163785 | 0.879369870 |
| Al | -0.354394760 | -0.466404190 | -1.970234732 |
| Al | 0.793138657 | -1.503448368 | 0.582957765 |
| Cl | -3.622678732 | -1.483216054 | 0.745692103 |
| Al | -1.654159030 | -1.156337102 | 0.091167965 |
| C | 1.266784640 | -0.019001918 | -0.979283361 |

| | | | |
|---|---|---|---|
| 13 | TiAl4CCl2 | | |
| C | 0.483376650 | -0.559018818 | 0.130757960 |
| Ti | 0.255008554 | 1.303861312 | 0.135963924 |
| Cl | 1.507994954 | 2.793092470 | 1.246790424 |
| Al | 1.487449302 | -2.122117360 | 0.876554735 |
| Cl | -2.700413323 | -2.228435159 | 0.681497846 |
| Al | 1.626365063 | -0.372754415 | -1.567876183 |
| Al | -0.684968693 | 0.387403173 | -2.247348447 |

| | | | |
|---|---|---|---|
| Al | -1.524178219 | -0.579453883 | 0.126619769 |

| | | | |
|---|---|---|---|
| 14 | TiAl4CCl2 | | |
| Cl | -2.760715760 | 1.017238606 | 0.423806881 |
| Al | 1.396637963 | 0.936948942 | -0.543344167 |
| Al | 1.345825880 | -0.909489382 | 1.656709814 |
| C | 0.008415429 | -0.572949273 | 0.037736298 |
| Al | -1.732030949 | -0.851550043 | -1.007850151 |
| Al | -0.163231732 | -2.607274066 | 0.335420761 |
| Ti | -0.505568988 | 0.968270162 | 1.026561356 |
| Cl | 2.764152255 | 0.555908649 | -2.102804004 |

| | | | |
|---|---|---|---|
| 15 | TiAl4CCl2 | | |
| Cl | 4.232502548 | -0.828053443 | 0.904392442 |
| Al | -3.010372615 | -0.435514202 | -0.927439168 |
| Al | -0.204457341 | -1.326065620 | 1.207859898 |
| Al | 2.212235798 | -0.972237320 | 0.323066786 |
| Cl | -2.712383091 | 2.093244414 | -0.146111893 |
| C | -1.047665421 | -0.610468936 | -0.450066051 |
| Al | 0.556179659 | -0.538596252 | -1.630876032 |
| Ti | -0.625120272 | 1.122542962 | 0.143894536 |

Molecular coordinates Figure S6

| | | | |
|---|---|---|---|
| 1 | TiAl4CBr2 | | |
| Al | -2.098211556 | -1.846650243 | -0.379380777 |
| Al | -0.195650854 | -1.160570938 | -2.133923269 |
| Al | 0.210418624 | -2.516074663 | 0.945390961 |
| C | 0.789242039 | -1.217382985 | -0.378026749 |
| Ti | -0.042145290 | 0.534265292 | -0.011109299 |
| Al | 2.753113977 | -0.763961144 | -0.652715735 |
| Br | 1.953957277 | 1.965809964 | -0.251777161 |
| Br | -2.311498710 | 0.242327801 | 1.148369867 |

| | | | |
|---|---|---|---|
| 2 | TiAl4CBr2 | | |
| C | 0.094967147 | -1.185574419 | -0.436965721 |
| Al | 0.996463758 | -0.609858427 | -2.200678586 |
| Br | 2.074451655 | 0.907165513 | 1.504644776 |
| Ti | 0.122342060 | 0.744355873 | -0.105079267 |
| Al | -1.943677263 | -1.269546894 | -0.857932142 |
| Al | -0.365540662 | -3.237441450 | 0.109714216 |
| Br | -2.296201764 | 1.329622530 | -0.591452641 |
| Al | 1.658901007 | -1.617763584 | 0.869808378 |

| | | | |
|---|---|---|---|
| 3 | TiAl4CBr2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.053753731 | -1.724050000 | 0.608385000 |
| Al | 1.858267948 | 0.579779000 | 1.072871500 |
| Br | 1.077197000 | 2.985546000 | -1.865759934 |
| Al | -1.053753731 | -1.724050000 | -0.608385000 |

| | | | |
|---|---|---|---|
| Al | -1.858267948 | 0.579779000 | -1.072871500 |
| Br | -1.077197000 | 2.985546000 | 1.865759934 |
| Ti | 0.000000000 | 1.994886000 | 0.000000000 |

| | | | |
|---|---|---|---|
| 4 | TiAl4CBr2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.506865068 | -1.622406305 | 1.238106324 |
| Al | -2.050541189 | 0.011011863 | -0.188760203 |
| Br | 1.429172156 | 1.610511407 | 2.506197096 |
| Al | 1.891395276 | -0.586983260 | 0.900665287 |
| Al | 1.262340165 | 0.267513824 | -1.657926153 |
| Br | 0.599603477 | 2.953144854 | -1.544905293 |
| Ti | -0.030133096 | 1.804668415 | 0.538694585 |

| | | | |
|---|---|---|---|
| 5 | TiAl4CBr2 | | |
| Br | -1.950535807 | 0.918692264 | 1.370214369 |
| Al | -1.686243116 | -1.609760518 | 0.706702048 |
| C | 0.062679928 | -1.025725671 | -0.255766602 |
| Ti | 0.000915668 | 0.803255030 | -0.173206359 |
| Al | -0.323200521 | -3.206301832 | -0.886778844 |
| Al | 2.035239500 | -1.504743212 | -0.201961125 |
| Al | -1.164364211 | -0.774562994 | -1.911457799 |
| Br | 2.362111777 | 1.387665480 | -0.365625766 |

| | | | |
|---|---|---|---|
| 6 | TiAl4CBr2 | | |
| Al | -2.188342115 | 0.098424454 | -1.065263775 |
| Al | -2.482047372 | -1.963773399 | 1.469891593 |
| Ti | -0.612637929 | 1.222432337 | 0.797714942 |
| Al | 0.536071972 | -0.986985774 | 0.314972688 |
| C | -1.383607877 | -0.580215544 | 0.632807453 |
| Br | 0.592479205 | 3.142301389 | -0.470847297 |
| Br | 1.410660344 | -3.077428873 | 0.223029484 |
| Al | 0.416608811 | 0.876740123 | -1.694442483 |

| | | | |
|---|---|---|---|
| 7 | TiAl4CBr2 | | |
| Br | 2.685349372 | 1.601754634 | 1.726021080 |
| Ti | 1.489270777 | 1.074111160 | -0.248361487 |
| Br | 0.452424241 | 2.561813737 | -2.001238201 |
| Al | -1.337420863 | 1.040115285 | -1.041908811 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.284192312 | -1.582232997 | -0.192558457 |
| Al | -3.054352479 | 0.177864956 | 0.744185825 |
| Al | 1.244600885 | -1.480134802 | -0.551184619 |

| | | | |
|---|---|---|---|
| 8 | TiAl4CBr2 | | |
| Al | 1.726962749 | 0.189991245 | -1.893188851 |
| Al | 2.419208685 | -0.893121211 | 0.537107290 |
| Al | -0.733535750 | -0.665737965 | -1.088888304 |
| C | 0.420116115 | -0.822477807 | 0.534309671 |
| Br | 0.533902492 | 3.138100241 | 1.688378562 |

| | | | |
|---|---|---|---|
| Br | -2.098856367 | -2.363673799 | -1.726289326 |
| Ti | 0.504326613 | 1.141673753 | 0.334478016 |
| Al | -0.246674750 | -2.268583800 | 1.734392532 |

| | | | |
|---|---|---|---|
| 9 | TiAl4CBr2 | | |
| Ti | 0.222803037 | 0.604764504 | -0.108985102 |
| Al | -0.794461977 | -2.230942551 | 0.953098128 |
| C | 0.591199720 | -1.227965774 | 0.034372512 |
| Al | -0.540207309 | -1.303099320 | -1.665588861 |
| Al | 2.604586093 | -1.366170380 | 0.180067093 |
| Br | -2.031804424 | 0.846186654 | 0.796744752 |
| Al | -3.087196135 | -1.879184759 | -0.636965434 |
| Br | 2.465397714 | 1.502244679 | -0.299787919 |

| | | | |
|---|---|---|---|
| 10 | TiAl4CBr2 | | |
| Br | -1.683040989 | 1.903593079 | 2.473479304 |
| Ti | -0.550718168 | 0.590918457 | 0.803679856 |
| Al | -1.442649733 | -3.010106800 | 1.295080333 |
| Al | -1.481331799 | -0.947471243 | -1.203272956 |
| Al | 1.318267128 | -1.339750391 | 1.003569692 |
| C | -0.636005627 | -1.352765374 | 0.566374328 |
| Br | 2.346148952 | -0.217672394 | -3.015015335 |
| Al | 1.045948444 | 0.382651066 | -1.258870952 |

| | | | |
|---|---|---|---|
| 11 | TiAl4CBr2 | | |
| Al | 1.968443603 | -0.408257138 | 0.212039068 |
| Al | 0.008235189 | -1.901879710 | 0.861338973 |
| Br | -3.105571516 | 1.378145184 | -0.065461652 |
| Al | -3.088030996 | -1.336769015 | -1.057401920 |
| Ti | -0.846460029 | 0.494714104 | 0.025808556 |
| Br | 4.058627880 | 0.211242267 | 0.823175597 |
| Al | 0.498049365 | -0.924734505 | -1.804420129 |
| C | -1.126984389 | -1.180153679 | -0.639665616 |

| | | | |
|---|---|---|---|
| 12 | TiAl4CBr2 | | |
| Ti | -0.299252997 | 0.266548033 | -0.290177135 |
| Al | -1.547166648 | -2.130533995 | 1.203197854 |
| Br | -1.916989038 | 0.580552486 | 1.494864236 |
| Al | -0.323199317 | -3.021750705 | -1.593010237 |
| Br | 1.308459885 | 1.550442481 | -1.642942449 |
| C | -0.138920757 | -1.621298275 | -0.200909238 |
| Al | 1.742301757 | -1.439216420 | 0.387494305 |
| Al | 2.336956621 | 1.151419474 | 0.984788487 |

| | | | |
|---|---|---|---|
| 13 | TiAl4CBr2 | | |
| Br | -2.239112431 | -2.226732863 | 0.908895324 |
| Al | 0.232377891 | -2.324304886 | -0.909547358 |
| Al | -1.608272981 | -0.004843216 | 0.575033764 |
| Al | 2.137446031 | -0.434284885 | 0.286499343 |
| C | 0.229664386 | -0.280818658 | -0.438153043 |

| | | | |
|---|---|---|---|
| Br | 2.180104719 | 2.365889671 | 0.358451762 |
| Al | -0.695221265 | -0.177597706 | -2.340044327 |
| Ti | -0.007953821 | 1.593082441 | -0.485612461 |

| | | | |
|---|---|---|---|
| 14 | TiAl4CBr2 | | |
| C | 1.715305340 | -0.406139536 | 0.903324485 |
| Br | 0.310602653 | 1.607206294 | -1.834867657 |
| Al | -0.131528347 | -1.024537786 | -2.217110597 |
| Br | -1.873094347 | 0.008748166 | 1.593036860 |
| Al | 3.303233066 | -0.209143959 | 2.006751425 |
| Al | -1.430963347 | -1.975719400 | -0.177295043 |
| Ti | 0.265711316 | 0.578095166 | 0.438837755 |
| Al | 1.224618811 | -1.932110777 | -0.120832348 |

| | | | |
|---|---|---|---|
| 15 | TiAl4CBr2 | | |
| Ti | 0.390902105 | 1.231694021 | -0.113211178 |
| C | 0.641562271 | -0.622413363 | -0.163426458 |
| Al | 1.738479861 | -0.384432620 | -1.889396131 |
| Br | -2.615281708 | -2.465910667 | 0.514140700 |
| Br | 1.693797752 | 2.872749554 | 1.061172944 |
| Al | -0.611737747 | 0.326334944 | -2.474500678 |
| Al | -1.359635417 | -0.688175249 | -0.101489059 |
| Al | 1.756179857 | -2.146199187 | 0.491171987 |

Molecular coordinates Figure S7

| | | | |
|---|---|---|---|
| 1 | TiAl4CI2 | | |
| Ti | -0.116141488 | 1.889150564 | 0.458267596 |
| I | 1.644144027 | 2.138866777 | 2.515814614 |
| Al | 1.365083076 | 0.679183833 | -1.387265213 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.315724332 | -1.906264710 | 0.857668921 |
| Al | 1.868788615 | -0.407775627 | 1.077103893 |
| I | -2.676110323 | 2.396779865 | -0.417682876 |
| Al | -1.939365061 | -0.296556258 | -0.437278483 |

| | | | |
|---|---|---|---|
| 2 | TiAl4CI2 | | |
| Ti | 0.393051228 | 1.845796064 | 0.561335328 |
| I | 2.925689255 | 2.228722639 | -0.390822655 |
| Al | -1.040752064 | 0.984762581 | -1.486347985 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.123026124 | -2.179558171 | 0.175699514 |
| Al | 1.864704233 | -0.403214498 | -0.817350026 |
| I | -1.367897823 | 2.228722639 | 2.615579384 |
| Al | -1.405824197 | -0.403214498 | 1.472698635 |

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|---|---|---|---|
| 3 | TiAl4CI2 | | |
| Al | 1.304041887 | -0.542452928 | 1.491547229 |
| Al | -1.913770232 | -0.653182704 | -0.361011652 |
| I | 1.473741017 | 2.133019168 | 2.427660275 |

| | | | |
|---|---|---|---|
| Al | 0.504817341 | -2.013595347 | -0.756490069 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Ti | -0.259354994 | 1.854424606 | 0.339646760 |
| Al | 0.958259458 | 0.661882223 | -1.704015456 |
| I | -2.945755842 | 1.980937604 | -0.116732577 |

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|---|---|---|---|
| 4 | TiAl4CI2 | | |
| Ti | 0.000000000 | 1.980259000 | 0.000000000 |
| I | -1.003537914 | 3.011219000 | 2.152094001 |
| Al | 1.949085588 | 0.585349000 | 0.908873536 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.105000362 | -1.724150000 | -0.515270131 |
| Al | 1.105000362 | -1.724150000 | 0.515270131 |
| I | 1.003537914 | 3.011219000 | -2.152094001 |
| Al | -1.949085588 | 0.585349000 | -0.908873536 |

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|---|---|---|---|
| 5 | TiAl4CI2 | | |
| C | -1.707477985 | -0.521158000 | 0.476989990 |
| Al | 0.346248143 | 1.044762000 | -1.530054322 |
| I | 0.735297256 | 3.339302000 | 0.047189892 |
| Al | 0.186285126 | -1.071966000 | 0.218850762 |
| Ti | -0.807884206 | 1.162035000 | 0.924849157 |
| I | 0.975450238 | -3.407108000 | -0.141308957 |
| Al | -2.347402254 | 0.428745000 | -1.159482014 |
| Al | -3.004462484 | -1.851085000 | 1.069121798 |

| | | | |
|---|---|---|---|
| 6 | TiAl4CI2 | | |
| Al | 1.483229845 | -0.738497806 | -1.230365584 |
| Al | 0.205640191 | -3.464519620 | -1.154876463 |
| Ti | 0.271270181 | 1.568147256 | -0.924255348 |
| Al | 0.104954348 | -1.750584345 | 0.936536227 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| I | 1.753480206 | 3.405826047 | 0.169946756 |
| Al | -1.365013103 | -0.980579627 | -1.106720819 |
| I | -1.598120723 | 1.107051777 | -2.851514110 |

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|---|---|---|---|
| 7 | TiAl4CI2 | | |
| C | -0.228204907 | -1.074630871 | -0.980626728 |
| I | -2.917286667 | 0.219488123 | 0.852235475 |
| I | 2.117284997 | 1.290781907 | 0.095781007 |
| Al | 1.066037623 | -1.937755909 | 0.387156299 |
| Ti | -0.335861411 | 0.226449638 | 0.333292476 |
| Al | -2.103420036 | -1.639715337 | -1.469731136 |
| Al | 1.322658832 | -0.879284149 | -2.148937694 |
| Al | 3.649974664 | -1.587740111 | -0.744914459 |

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|---|---|---|---|
| 8 | TiAl4CI2 | | |
| C | -0.757315760 | -1.301454134 | 0.175431433 |
| Al | -1.343737586 | -0.480619254 | -1.544318479 |
| Al | -2.162568543 | -2.243532535 | 1.267230875 |

| | | | |
|---|---|---|---|
| I | 2.790441238 | 0.199464097 | -3.037493778 |
| Al | 1.146364792 | -1.631439214 | 0.667681805 |
| Al | 1.265345967 | 0.606536990 | -1.108872430 |
| Ti | -0.512153297 | 0.494351316 | 0.833735654 |
| I | -2.223629995 | 0.662247428 | 2.847736478 |

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|---|---|---|---|
| 9 | TiAl4CI2 | | |
| Al | 1.376181876 | -2.006370988 | 0.390898382 |
| I | 1.667566355 | 0.834488431 | -2.005524823 |
| I | -1.668943505 | 1.004175997 | 1.728072514 |
| Al | -1.942032455 | -1.876274145 | 1.457977501 |
| Al | -1.287574297 | -3.295809982 | -1.077825852 |
| C | -0.544856649 | -1.775679037 | -0.029735366 |
| Al | 2.532400399 | 0.378387934 | 0.886528059 |
| Ti | -0.249296442 | 0.072986931 | -0.302961179 |

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|---|---|---|---|
| 10 | TiAl4CI2 | | |
| Al | 0.322502600 | -2.155106071 | 0.518332106 |
| I | 3.239173071 | 1.528872660 | -0.523320307 |
| Al | 3.037567283 | -1.264690149 | -1.802098159 |
| C | 1.173185251 | -1.216239068 | -1.049698258 |
| Ti | 0.898564285 | 0.362191233 | -0.175266387 |
| Al | -1.794824696 | -0.758897577 | 0.332858736 |
| Al | -0.629777703 | -0.971328156 | -1.917566149 |
| I | -3.974429878 | -0.278315882 | 1.418494014 |

| | | | |
|---|---|---|---|
| 11 | TiAl4CI2 | | |
| I | 2.582906680 | 0.789994479 | 0.329361778 |
| Ti | -0.044878522 | 0.355427205 | 0.655582542 |
| Al | 0.229803139 | -1.040153218 | -3.078758363 |
| C | -0.111572265 | -1.466679195 | 0.791412469 |
| Al | -0.275351468 | -2.746189328 | 2.264733067 |
| Al | 1.335488600 | -1.646485535 | -0.673415094 |
| I | -2.549305766 | 0.945376623 | -0.106209841 |
| Al | -1.299485599 | -1.566709426 | -0.897045739 |

| | | | |
|---|---|---|---|
| 12 | TiAl4CI2 | | |
| Al | -1.073831314 | 0.272470255 | -1.761489254 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.811285446 | -1.910516961 | 0.415525440 |
| I | -1.838688085 | 0.289817905 | 2.859408765 |
| I | -1.549788502 | 3.024601222 | -0.752737442 |
| Al | 1.907346833 | 0.406437946 | 0.600443402 |
| Ti | -0.358954864 | 1.520922543 | 1.044111300 |
| Al | -1.816179688 | -1.364640607 | 0.326661732 |

| | | | |
|---|---|---|---|
| 13 | TiAl4CI2 | | |
| C | -1.326754869 | -0.405205132 | 1.244346264 |
| Al | 0.446251905 | -0.861289401 | 0.504816108 |
| I | 1.700952644 | -2.971479395 | 0.831239449 |

| | | | |
|---|---|---|---|
| Al | -0.395559371 | 0.330657263 | -1.724149359 |
| Al | -2.508329790 | -0.297312327 | -0.406150995 |
| Ti | -0.769658932 | 1.350649454 | 0.728610717 |
| Al | -2.615128945 | -1.473431939 | 2.251217329 |
| I | 0.012990485 | 3.021193329 | -1.428031879 |

| | | | |
|---|---|---|---|
| 14 | TiAl4CI2 | | |
| Al | -0.498769485 | -1.848160323 | -2.624452665 |
| Ti | 0.229467702 | 0.003734504 | 0.193022055 |
| I | 1.500022583 | 2.096717671 | -0.772120642 |
| Al | 3.349598756 | -0.278496230 | 0.129817129 |
| I | -2.209851338 | -0.307552056 | 1.517003708 |
| C | 1.583283907 | -1.151886371 | 0.442763830 |
| Al | -1.867060177 | -2.076268427 | -0.549280587 |
| Al | 0.791073283 | -2.566045080 | -0.523922319 |

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|---|---|---|---|
| 15 | TiAl4CI2 | | |
| Al | 2.633855920 | -0.781465895 | 0.329550576 |
| Al | 0.373210230 | -2.320823430 | 1.594671593 |
| I | -2.112372241 | -2.519765289 | -1.832449999 |
| I | 0.714586868 | 3.043833226 | 2.001216176 |
| Al | 1.896468187 | 0.030069130 | -1.948110057 |
| C | 0.588536219 | -0.719402019 | 0.414510122 |
| Ti | 0.659733583 | 1.137166464 | 0.205472626 |
| Al | -0.592977763 | -0.656769680 | -1.203192505 |

Molecular coordinates Figure S8

| | | | |
|---|---|---|---|
| 1 | ZrAl4CF2 | | |
| Al | -1.888450264 | 0.406899088 | -1.055723556 |
| Al | -0.909472778 | -1.790766021 | -0.607628191 |
| Zr | -0.173415804 | 2.241455467 | 0.013100275 |
| Al | 1.174632518 | -1.636509549 | 0.587597343 |
| F | -1.077700060 | 3.063394883 | 1.483813613 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| F | 0.592363791 | 3.209733680 | -1.447150065 |
| Al | 1.804342297 | 0.680223643 | 1.062077288 |

| | | | |
|---|---|---|---|
| 2 | ZrAl4CF2 | | |
| Al | -1.086414627 | -0.829999000 | -1.108238259 |
| Al | -0.894273228 | -1.904997000 | 1.356578129 |
| Al | -0.065248709 | -3.356923000 | -0.547803203 |
| Al | 1.911116877 | -1.448767000 | 0.116649348 |
| F | 1.509581809 | 2.253795000 | -0.888328128 |
| F | -1.322492287 | 2.430521000 | 1.008469132 |
| Zr | -0.029783555 | 1.474946000 | -0.043045378 |
| C | 0.210033194 | -0.521294000 | 0.502855302 |

| | | | |
|---|---|---|---|
| 3 | ZrAl4CF2 | | |
| Al | 2.029006632 | -1.191120121 | -0.390858953 |

| | | | |
|---|---|---|---|
| Zr | 0.123856513 | 1.089757170 | 0.133160195 |
| Al | 0.094853101 | -1.471301993 | 1.581634321 |
| F | -0.989767198 | 2.624938061 | 0.466742685 |
| F | 2.178988187 | 0.677340698 | -0.155476938 |
| C | -0.878168860 | -0.702320047 | 0.004666968 |
| Al | -2.624036600 | -1.650698190 | 0.074443495 |
| Al | -0.298918053 | -1.002023805 | -1.892588197 |

| | | | |
|---|---|---|---|
| 4 | ZrAl4CF2 | | |
| F | 1.357848230 | 2.728758633 | 1.287651534 |
| Zr | -0.255883025 | 1.915275776 | 0.619232951 |
| F | -2.062379407 | 1.241759026 | 1.403300746 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.904067046 | -0.450913857 | 0.435713909 |
| Al | -1.698050701 | 0.643450489 | -1.934222162 |
| Al | 0.720137068 | 1.088901411 | -1.920616573 |
| Al | 1.673299198 | -0.919957905 | -0.420923850 |

| | | | |
|---|---|---|---|
| 5 | ZrAl4CF2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Zr | 1.180761268 | 1.698295208 | 0.514534508 |
| F | 1.871355225 | 1.661997780 | 2.299763035 |
| Al | -1.956581719 | -0.044266161 | -0.082555898 |
| Al | 0.907736852 | -0.093820233 | -1.825621743 |
| Al | 2.922031419 | -0.643545565 | -0.493337180 |
| F | 0.634548277 | 3.343093001 | -0.304973343 |
| Al | 0.870783266 | -1.453686813 | 1.067656033 |

| | | | |
|---|---|---|---|
| 6 | ZrAl4CF2 | | |
| Al | -1.036885585 | -1.081028943 | 1.520282861 |
| Al | -1.953126752 | -0.401016520 | -0.960857133 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| F | -2.081104813 | 1.621609546 | -1.160943527 |
| Zr | -0.134210066 | 1.920545458 | -0.679317399 |
| Al | 1.568791476 | -0.089584727 | -1.367840274 |
| F | 0.832981387 | 3.189258657 | 0.397921354 |
| Al | 1.517964243 | -1.015948423 | 1.032921936 |

| | | | |
|---|---|---|---|
| 7 | ZrAl4CF2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.244505088 | -0.378957424 | -1.531122515 |
| Zr | 0.938551052 | 1.771503580 | 0.398311906 |
| F | 2.571551580 | 1.189481105 | 1.579210907 |
| Al | 1.471385996 | -0.199501387 | -1.637268374 |
| Al | 2.755127427 | -0.479326766 | 0.625321191 |
| Al | 0.243353671 | -1.126256114 | 1.562363486 |
| F | 0.433688113 | 3.170571658 | -0.817270054 |

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|---|---|---|---|
| 8 | ZrAl4CF2 | | |
| Zr | 0.035718000 | 1.198815000 | -0.211939000 |

| | | | |
|---|---|---|---|
| F | 0.142118000 | 2.158511000 | 1.418022000 |
| Al | -2.341842000 | -2.045830000 | 0.183855000 |
| C | -1.014235000 | -0.492998000 | 0.179691000 |
| Al | -2.594568000 | 0.396406000 | -0.649105000 |
| Al | 2.286574000 | -0.636741000 | -0.211603000 |
| Al | 0.200899000 | -2.037483000 | 0.494669000 |
| F | 3.912645000 | -0.912644000 | -0.332711000 |

| | | | |
|---|---|---|---|
| 9 | ZrAl4CF2 | | |
| Al | 1.588965147 | -0.955463444 | -0.707115618 |
| Al | -0.495187045 | -2.629792996 | -1.109187645 |
| Al | -1.076365413 | -1.227569200 | 1.127938156 |
| Al | -1.158398814 | -0.251084475 | -1.719751941 |
| F | -1.666967343 | 2.716933199 | 0.976513454 |
| F | 1.111065657 | 3.000544839 | -0.936134837 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Zr | -0.378020298 | 1.999698964 | -0.252537261 |

| | | | |
|---|---|---|---|
| 10 | ZrAl4CF2 | | |
| C | -0.092955396 | -0.386023022 | 0.151462000 |
| Zr | -1.721731184 | 0.727947643 | -0.214673000 |
| F | 4.652297242 | -0.025992827 | 0.306234000 |
| Al | 3.033053736 | -0.203371931 | 0.023069000 |
| Al | 1.140974084 | -1.920071267 | 0.378481000 |
| Al | 0.945475937 | 1.155007993 | -0.680069000 |
| F | -2.439433032 | 1.377097303 | 1.426454000 |
| Al | -1.310950473 | -2.028620137 | -0.330407000 |

| | | | |
|---|---|---|---|
| 11 | ZrAl4CF2 | | |
| F | -3.767291496 | -1.169270862 | 0.497409772 |
| F | 1.218525249 | 2.724475612 | 0.173948049 |
| Al | -2.145041823 | -0.978298249 | 0.238616877 |
| Zr | 0.155465475 | 1.114597287 | 0.131650199 |
| Al | 3.073921303 | -0.716099775 | -0.644209076 |
| C | 1.154821594 | -0.570371388 | -0.285023280 |
| Al | 0.162338583 | -1.476769599 | 1.252530033 |
| Al | -0.338038933 | -1.071792855 | -1.585251874 |

| | | | |
|---|---|---|---|
| 12 | ZrAl4CF2 | | |
| Al | -0.504679969 | -1.464552585 | 1.092331895 |
| Al | 1.888007206 | -1.241502525 | 0.211468371 |
| F | -0.468584778 | 3.014688595 | -0.238471310 |
| Zr | -0.081289742 | 1.176870871 | 0.215364660 |
| C | -1.184769858 | -0.264590482 | -0.595765565 |
| F | 3.485053845 | -1.517711375 | 0.539276567 |
| Al | -2.971360660 | -0.919577900 | -0.177482520 |
| Al | 0.296646695 | -0.909759156 | -1.722259253 |

| | | | |
|---|---|---|---|
| 13 | ZrAl4CF2 | | |
| Al | -1.720840610 | -0.772248456 | -0.096840413 |

| | | | |
|---|---|---|---|
| Al | 1.743659752 | -0.792237780 | -0.995989316 |
| F | -2.777095699 | -1.988147366 | 0.276840764 |
| Zr | 0.100764012 | 1.270373530 | 0.173125034 |
| F | 1.095816933 | 2.423172872 | 1.365367531 |
| Al | 1.027802299 | -2.188017115 | 1.532196889 |
| C | 0.229989443 | -0.727994048 | 0.431186824 |
| Al | -0.302850660 | -0.121512753 | -2.307983781 |

| | | | |
|---|---|---|---|
| 14 | ZrAl4CF2 | | |
| Al | -0.945429070 | -1.550011178 | -0.376568492 |
| C | -1.368260330 | -0.133751700 | 0.787338869 |
| Al | -3.093294772 | 0.210535991 | 1.594428350 |
| Al | 1.798588443 | -1.615579456 | -0.431661520 |
| Al | 0.437575679 | -1.174314605 | -2.529104303 |
| F | 2.096166496 | -0.275620428 | 0.822891120 |
| F | 0.012675909 | 2.524155905 | -0.527130608 |
| Zr | 0.316581975 | 0.856187238 | 0.381797687 |

| | | | |
|---|---|---|---|
| 15 | ZrAl4CF2 | | |
| Al | -2.761704350 | -0.796706249 | 0.755838555 |
| C | -1.198672892 | -0.368048515 | -0.367239106 |
| Zr | 0.213896788 | 0.958068523 | 0.301919704 |
| F | -0.432645477 | 2.315171759 | 1.505362478 |
| Al | -0.000740328 | -1.647628279 | 0.937399099 |
| F | 1.937105249 | 0.641114605 | -0.838211440 |
| Al | 2.084211386 | -1.308426431 | -0.893956448 |
| Al | -0.468226340 | -1.071932333 | -2.020644247 |

Molecular coordinates Figure S9

| | | | |
|---|---|---|---|
| 1 | ZrAl4CCl2 | | |
| Zr | 0.000000000 | 2.186496000 | 0.000000000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.134379078 | -1.723512000 | 0.412880219 |
| Al | -1.134379078 | -1.723512000 | -0.412880219 |
| Al | -2.034769994 | 0.543628000 | -0.740595711 |
| Cl | -0.724180797 | 3.221668000 | 1.989670387 |
| Cl | 0.724180797 | 3.221668000 | -1.989670387 |
| Al | 2.034769994 | 0.543628000 | 0.740595711 |

| | | | |
|---|---|---|---|
| 2 | ZrAl4CCl2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.953259289 | -2.148915619 | -0.981465475 |
| Al | -1.307231882 | 0.439399594 | -1.568563885 |
| Al | 1.525107326 | -1.304541590 | -0.051484634 |
| Cl | 2.012520141 | 3.007451214 | 0.258641167 |
| Cl | -1.900522787 | 1.488669014 | 2.077217824 |
| Al | -1.698747428 | -0.636252878 | 0.934131636 |
| Zr | -0.104016076 | 1.941576715 | 0.378837268 |

3 ZrAl4CCl2

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Cl | -2.006434568 | 1.934986659 | -1.594337539 |
| Al | -1.804806267 | -0.345759554 | -0.762269734 |
| Al | -1.938335897 | -2.305629613 | 0.966545504 |
| Al | 0.362869656 | -1.987067784 | -0.351705402 |
| Cl | 0.481383338 | 3.106493582 | 1.820530819 |
| Zr | 0.076964320 | 1.985053488 | -0.218234205 |
| Al | 1.837678707 | 0.014944699 | -0.868475296 |

4 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Al | -1.039684788 | -1.388129000 | 0.933737133 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Zr | -0.178025095 | 1.953741000 | -0.597522800 |
| Al | 1.712613481 | -0.870171000 | -0.502269715 |
| Al | -1.408294250 | -0.303378000 | -1.514812371 |
| Al | -0.313865250 | -2.817726000 | -1.035872566 |
| Cl | -1.690588308 | 3.239814000 | 0.696250974 |
| Cl | 1.706252823 | 2.551941000 | -1.903121117 |

5 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Zr | 0.005556583 | 1.963350198 | 0.469631531 |
| Al | 0.659879893 | 0.908932464 | -2.025296304 |
| Al | -1.140729229 | -1.495652850 | 0.658721826 |
| Cl | 1.900055970 | 2.481567482 | 1.813935916 |
| Al | 1.954004585 | -0.542170583 | -0.089379263 |
| Cl | -2.374396962 | 2.386098707 | 0.096060881 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.795744017 | 0.216191541 | -1.328561225 |

6 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Al | 2.040660601 | -0.647738598 | 0.497409121 |
| Zr | 0.303244286 | 1.951292844 | 0.301922002 |
| Cl | 2.188847851 | 1.744594637 | 1.821877404 |
| Cl | -1.995928818 | 2.649613292 | 0.007828852 |
| Al | -0.379919709 | -1.564814993 | 1.287256993 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.982219328 | -0.093655549 | -0.511973504 |
| Al | 1.057646806 | 0.373991339 | -1.835565476 |

7 ZrAl4CCl2

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.078686278 | -1.598474107 | 1.183853103 |
| Al | -0.329979990 | -3.637469287 | -0.568151064 |
| Cl | 1.375501559 | 0.441747430 | -2.845757451 |
| Al | 1.232026312 | -1.186355806 | -1.076916576 |
| Zr | -0.297765773 | 1.471535725 | -1.292087894 |
| Al | -1.601584997 | -0.930249977 | -0.966573087 |
| Cl | -1.283830759 | 3.456525358 | -0.419814468 |

8 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Al | -1.439689861 | -0.550019979 | -1.353120961 |
| Cl | -2.049781101 | 2.378278326 | 1.782435715 |
| Cl | 2.190945252 | 2.540687353 | 1.333999292 |
| Zr | 0.100268366 | 1.423145231 | 1.463624050 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.713552506 | -0.848281854 | 0.947763973 |
| Al | -1.408643618 | -0.967854020 | 1.277921202 |
| Al | 1.162729196 | -0.450353952 | -1.628314263 |

9 ZrAl4CCl2

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.915738600 | -1.456095874 | 1.053281524 |
| Zr | -1.654063094 | 1.103501897 | 0.571345865 |
| Al | 1.485969099 | 1.001519586 | -0.723037062 |
| Cl | -1.112347707 | 2.767639274 | 2.160226832 |
| Al | 3.077897342 | -0.676833714 | -2.249516544 |
| Al | 1.233979118 | -1.599116016 | -0.251557350 |
| Cl | -3.251673041 | 1.360824569 | -1.146077844 |

10 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Cl | 0.907137751 | 3.339733867 | -0.698129307 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Zr | -0.737124016 | 1.883821802 | 0.207029240 |
| Al | -1.451188145 | 0.048625286 | -1.617217961 |
| Al | 1.558156120 | -0.102098733 | -1.223657931 |
| Al | -3.446712487 | -0.152283986 | 0.270103144 |
| Cl | -2.667464111 | 1.793310349 | 1.762511233 |
| Al | -1.045636192 | -1.144493517 | 1.162181210 |

11 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Cl | 0.025694468 | 2.580167280 | -1.057151155 |
| Al | 3.422239494 | 0.316057882 | 1.020429492 |
| Zr | -0.123603783 | 0.686974149 | 0.365944326 |
| Cl | -2.142023998 | -0.370695136 | 1.502440919 |
| C | 1.612350756 | -0.239003199 | 0.598603665 |
| Al | -1.606421243 | -1.981168383 | -0.205729777 |
| Al | -0.503387785 | -1.477759139 | -2.406246472 |
| Al | 1.091232940 | -1.749895600 | -0.393015978 |

12 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Al | 0.364172479 | -1.640185548 | 1.118942990 |
| Al | 2.292937110 | -0.269069370 | 0.138249158 |
| Al | -2.896607220 | -1.319821279 | -0.559288968 |
| Zr | -0.594077955 | 0.815127791 | 0.136930836 |
| C | -0.932630884 | -1.068682266 | -0.329261820 |
| Al | 0.606055830 | -0.999457010 | -1.645796359 |
| Cl | -2.889592793 | 1.528964941 | 0.101531121 |
| Cl | 4.336278580 | 0.163852019 | 0.417347934 |

13 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Cl | 2.079527830 | 2.686287871 | -1.631098283 |
| Zr | 1.520183455 | 1.389349046 | 0.263868180 |
| Al | -1.410732987 | 1.217812297 | 0.611751226 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -3.963641959 | -0.142692974 | 0.524050815 |
| Al | -1.473026614 | -1.316754288 | -0.251064896 |
| Al | 1.119089606 | -1.489675195 | -0.681955172 |
| Cl | 2.638558946 | 1.329613381 | 2.344534232 |

14 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Zr | 0.538681575 | 1.900548266 | 0.656150045 |
| Al | -0.986420190 | 0.844214994 | -1.600862758 |
| Al | -0.050631886 | -2.084287475 | -0.371908070 |
| Cl | -1.144353357 | 1.681991406 | 2.463436030 |
| Al | -1.437984309 | -0.516721597 | 1.370011426 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 2.019868548 | -0.511256195 | 0.359531906 |
| Cl | 1.927059489 | 3.413622803 | -0.550389632 |

15 ZrAl4CCl2

| | | | |
|---|---|---|---|
| Al | -0.700805691 | -1.259942743 | -1.157811367 |
| Cl | 3.705777778 | -1.462322187 | -1.239749221 |
| Al | 0.373536934 | -1.470030391 | 1.610026319 |
| C | -1.200138547 | -0.544902333 | 0.920930091 |
| Zr | -0.241055569 | 1.053856403 | 0.269783649 |
| Al | 1.730264266 | -1.280012671 | -0.537681212 |
| Al | -2.991815289 | -1.084681310 | 0.358543807 |
| Cl | -1.500028855 | 3.070900389 | 0.071106358 |

Molecular coordinates Figure S10

1 ZrAl4CBr2

| | | | |
|---|---|---|---|
| Al | 0.990095150 | -1.723034000 | 0.693272088 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Br | 1.308002633 | 3.226397000 | -1.868021354 |
| Zr | 0.000000000 | 2.167764000 | 0.000000000 |
| Al | 1.783084297 | 0.546115000 | 1.248529066 |
| Al | -1.783084297 | 0.546115000 | -1.248529066 |
| Br | -1.308002633 | 3.226397000 | 1.868021354 |
| Al | -0.990095150 | -1.723034000 | -0.693272088 |

2 ZrAl4CBr2

| | | | |
|---|---|---|---|
| Br | -2.988739658 | 1.454103393 | -0.125683824 |
| Br | 1.426005117 | 3.400135934 | -0.703244269 |
| Al | 1.450321169 | -0.459308732 | 1.311083428 |
| Al | -1.834841880 | -0.818720907 | 0.349756988 |
| Zr | -0.454140634 | 1.715879548 | -0.874433974 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.036452394 | -2.539761247 | 0.119851729 |

| | | | |
|---|---|---|---|
| Al | -0.252884849 | -0.810330223 | -1.907696835 |

| | | | |
|---|---|---|---|
| 3 | ZrAl4CBr2 | | |
| Br | 2.237604017 | 1.453697159 | -0.167845347 |
| Zr | -0.030389037 | 0.460168821 | 0.562767154 |
| C | 0.011814199 | -1.200902285 | -0.543017006 |
| Al | 0.200184778 | -1.551452668 | -2.567635115 |
| Al | 2.191715835 | -1.369947020 | -0.752906274 |
| Br | -2.590114596 | 0.732582662 | 0.652568167 |
| Al | 0.602386912 | -2.117770385 | 1.318460808 |
| Al | -1.957169915 | -1.708611556 | -0.783911874 |

| | | | |
|---|---|---|---|
| 4 | ZrAl4CBr2 | | |
| Br | 2.458853000 | 1.195595608 | 0.063848541 |
| C | 0.000000000 | -1.237085226 | -0.809116040 |
| Al | 1.809453000 | -1.724281371 | -1.433881434 |
| Al | -1.809453000 | -1.724281371 | -1.433881434 |
| Al | -1.237382000 | -1.997496614 | 1.165587961 |
| Al | 1.237382000 | -1.997496614 | 1.165587961 |
| Br | -2.458853000 | 1.195595608 | 0.063848541 |
| Zr | 0.000000000 | 0.512426458 | 0.184023249 |

| | | | |
|---|---|---|---|
| 5 | ZrAl4CBr2 | | |
| Br | -3.300473700 | 1.216752049 | -0.830527812 |
| Al | 0.110914163 | -1.179262574 | -1.728457062 |
| Zr | -0.811042146 | 1.345446050 | -1.293976307 |
| Al | 1.661615603 | -0.944445085 | 0.472273657 |
| Al | 0.187905255 | -3.022005615 | 0.359992989 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.419789619 | -0.746810716 | 1.188926767 |
| Br | 0.799596378 | 3.072523539 | -2.200124708 |

| | | | |
|---|---|---|---|
| 6 | ZrAl4CBr2 | | |
| Al | 1.169205237 | -2.096862857 | 1.288543000 |
| C | -0.508668356 | -1.380883708 | 0.644117000 |
| Al | -2.493226838 | -1.670361313 | 0.653047000 |
| Br | -2.558898731 | 1.313601569 | -0.128459000 |
| Zr | -0.148107072 | 0.480849101 | -0.049932000 |
| Al | -0.148502960 | -1.811804337 | -1.441291000 |
| Al | 2.546623578 | -1.457048381 | -0.987838000 |
| Br | 2.416412759 | 0.986980126 | 0.256190000 |

| | | | |
|---|---|---|---|
| 7 | ZrAl4CBr2 | | |
| Al | -3.193963883 | -1.924277688 | 0.187801604 |
| Br | -2.162715750 | 1.159904114 | -0.156480951 |
| C | 0.430940240 | -1.220612335 | -0.630333447 |
| Br | 2.726348258 | 1.134632921 | 0.409034623 |
| Al | -1.115128291 | -1.812598989 | -1.657248754 |
| Zr | 0.248657374 | 0.485238640 | 0.415353629 |
| Al | -0.523485940 | -2.026208502 | 1.026965049 |

| | | | |
|---|---|---|---|
| Al | 2.351111170 | -1.344196602 | -1.224559233 |

| | | | |
|---|---|---|---|
| 8 | ZrAl4CBr2 | | |
| Br | 1.737349685 | 0.678659960 | -1.873650690 |
| Zr | -0.230207794 | 0.485832630 | -0.037048483 |
| C | -1.835803993 | -0.544447816 | -0.551187380 |
| Al | -0.942824927 | -2.200609074 | -0.549326331 |
| Al | 1.681314929 | -1.779239765 | -1.065588398 |
| Al | -3.746704758 | -0.241090223 | -0.388058959 |
| Al | 0.934928063 | -2.618374782 | 1.174680940 |
| Br | -0.389468077 | 1.399753394 | 2.318133346 |

| | | | |
|---|---|---|---|
| 9 | ZrAl4CBr2 | | |
| Br | -1.449194929 | 2.175548402 | 2.087938072 |
| Zr | 0.260489143 | 2.053528806 | 0.097492141 |
| Al | 2.079884760 | -0.116158256 | 0.357725995 |
| Br | 1.511710687 | 3.383399914 | -1.668699824 |
| Al | -1.103850911 | 0.225502104 | -1.727440179 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.267909986 | -2.104701913 | 0.129288497 |
| Al | -1.338705230 | -0.399148990 | 1.493390178 |

| | | | |
|---|---|---|---|
| 10 | ZrAl4CBr2 | | |
| Al | 0.876908327 | -2.125206960 | 0.423740312 |
| Br | 1.310834428 | 1.348974280 | -1.765029975 |
| Al | 0.589571044 | -1.325662217 | -2.095166857 |
| Zr | 0.120124422 | 0.618989306 | 0.452069244 |
| C | 1.182097323 | -0.624661217 | 1.541071947 |
| Br | -2.466586961 | 0.281805338 | 0.699917018 |
| Al | 2.242168592 | -0.636527981 | 3.160446342 |
| Al | -1.512205739 | -1.919440532 | -0.723657611 |

| | | | |
|---|---|---|---|
| 11 | ZrAl4CBr2 | | |
| Al | -0.315166862 | -1.703901036 | 1.242613823 |
| Br | 3.323037612 | 0.921543108 | -0.437731461 |
| Al | -0.802655334 | -1.259262976 | -1.522070687 |
| C | 0.862229470 | -1.435711544 | -0.382936613 |
| Al | -2.148751386 | -0.158411816 | 0.353405824 |
| Br | -4.210198779 | 0.649726005 | 0.846865627 |
| Zr | 0.821442485 | 0.507039899 | -0.063296374 |
| Al | 2.729613614 | -2.006248827 | -0.803965063 |

| | | | |
|---|---|---|---|
| 12 | ZrAl4CBr2 | | |
| Al | -1.224390191 | -1.291316226 | -1.329449046 |
| Br | -1.120027930 | 3.136485043 | 1.212163979 |
| Al | -0.061241763 | -1.900463142 | 1.364796613 |
| C | -1.590942358 | -0.797646520 | 0.896066359 |
| Al | 1.238149151 | -1.486595261 | -0.755668934 |
| Br | 3.324931891 | -1.704232855 | -1.606078401 |
| Zr | -0.574447333 | 0.798895183 | 0.343231486 |

| | | | |
|---|---|---|---|
| Al | -3.386984874 | -1.267685572 | 0.311192026 |

| | | | |
|---|---|---|---|
| 13 | ZrAl4CBr2 | | |
| Al | 0.133729162 | -1.719417565 | 2.551704412 |
| C | 0.070658698 | -0.184151819 | 1.348248273 |
| Al | 1.252481727 | -1.293593107 | -0.021089822 |
| Br | -2.548404501 | 0.825705997 | -0.594314183 |
| Al | -1.247824987 | -1.293593107 | 0.109945700 |
| Br | 2.472321326 | 0.825705997 | -0.857439274 |
| Al | 0.033543716 | -3.807766228 | 0.640052222 |
| Zr | 0.000096869 | 1.219807438 | 0.001848372 |

| | | | |
|---|---|---|---|
| 14 | ZrAl4CBr2 | | |
| Al | -1.026389286 | -3.071305629 | 0.126935382 |
| C | 0.425227543 | -1.535813936 | -0.242578505 |
| Br | -1.821804882 | 0.651314007 | 1.868853180 |
| Zr | 0.021060576 | 0.503663014 | 0.151114515 |
| Al | -0.907089201 | -1.280821935 | -1.817535681 |
| Al | 2.375431190 | -1.061991995 | 0.178846771 |
| Br | 1.015762197 | 2.309323638 | -1.314184070 |
| Al | 1.467102115 | -3.397721419 | -0.334594854 |

| | | | |
|---|---|---|---|
| 15 | ZrAl4CBr2 | | |
| Zr | -0.521201856 | 1.172215529 | -0.019355453 |
| Al | -2.271281692 | -1.103220267 | 0.187354096 |
| Br | -0.867614105 | 3.001072324 | 1.721814840 |
| C | -0.267194366 | -0.766373259 | 0.467505025 |
| Al | 0.249261149 | -2.148164692 | 1.829492392 |
| Al | -1.519985239 | -0.459105875 | -2.130885436 |
| Al | 0.979969247 | -0.813066494 | -1.135688548 |
| Br | 2.460692383 | -2.529190439 | -1.315653133 |

| | | | |
|---|---|---|---|
| 16 | ZrAl4CBr2 | | |
| Br | -0.782154258 | -3.111218218 | -2.148951163 |
| Al | 0.811455444 | -2.133670671 | 2.229455510 |
| Al | -1.332376054 | -0.886322288 | 1.542423932 |
| Br | 0.216956760 | 3.672389474 | 0.596083799 |
| Al | -0.458434886 | -1.048876237 | -1.259539497 |
| C | 0.571774708 | -0.208269817 | 1.570938100 |
| Al | 2.012110264 | -0.886322288 | 0.325130463 |
| Zr | 0.073136275 | 1.150653652 | 0.200940263 |

Molecular coordinates Figure S11

| | | | |
|---|---|---|---|
| 1 | ZrAl4CI2 | | |
| Al | 1.958674887 | 0.461662656 | 1.010258733 |
| I | 1.069724375 | 3.463327109 | -1.899366182 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.967669509 | 0.628952073 | -0.896023672 |
| Al | 1.102279160 | -1.761519961 | 0.348648579 |

| | | | |
|---|---|---|---|
| Al | -1.073988331 | -1.668795919 | -0.707952678 |
| I | -1.122837149 | 2.976695885 | 2.573918247 |
| Zr | -0.017629621 | 2.137624480 | 0.223902773 |

| | | | |
|---|---|---|---|
| 2 | ZrAl4CI2 | | |
| Al | 0.672168399 | -2.674103000 | 1.583560187 |
| Al | 1.748689198 | -2.082124000 | -0.901859880 |
| Al | -1.495727701 | -1.671722000 | -1.554233278 |
| Zr | -0.199407901 | 0.427130000 | -0.325675715 |
| C | -0.000651066 | -1.530183000 | 0.002265530 |
| I | -1.826663303 | 1.057015000 | 1.853331815 |
| Al | -1.860989147 | -1.902238000 | 1.110414380 |
| I | 2.206782935 | 0.837104000 | -1.666143185 |

| | | | |
|---|---|---|---|
| 3 | ZrAl4CI2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Zr | -0.081043779 | 1.943002393 | 0.340681377 |
| I | 2.421882616 | 3.046918495 | 0.106637931 |
| Al | -0.712029557 | -2.154694765 | -1.075208382 |
| Al | -1.274008793 | 0.420379181 | -1.596169330 |
| I | -2.125091971 | 1.575398440 | 2.296928422 |
| Al | -1.672388385 | -0.794059658 | 0.862611342 |
| Al | 1.668447827 | -1.117802530 | -0.040931592 |

| | | | |
|---|---|---|---|
| 4 | ZrAl4CI2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Zr | -1.662432733 | 1.081274675 | 0.214852427 |
| I | -3.011578443 | 0.453518109 | 2.503692193 |
| I | -0.374817772 | 3.517351460 | -0.491946856 |
| Al | 1.424912685 | 1.376681305 | -0.151925649 |
| Al | -1.088160210 | -1.066880251 | -1.347924763 |
| Al | 2.995231655 | -0.311115333 | 1.080232467 |
| Al | 1.389168252 | -1.275825378 | -0.820351855 |

| | | | |
|---|---|---|---|
| 5 | ZrAl4CI2 | | |
| I | -2.381714043 | 1.307478624 | -0.486625322 |
| Al | -1.224587798 | -1.719313309 | -1.973419149 |
| C | 0.378167388 | -1.473171427 | -0.913233916 |
| Al | 2.281365671 | -2.103909480 | -0.810836229 |
| Al | -2.935366275 | -1.512832861 | 0.133219301 |
| Zr | 0.147450399 | 0.209460259 | 0.175942995 |
| Al | -0.419882657 | -2.311606552 | 0.903065467 |
| I | 2.791395259 | 0.577054090 | 0.885971282 |

| | | | |
|---|---|---|---|
| 6 | ZrAl4CI2 | | |
| I | 2.918363183 | 0.988052979 | -0.387538259 |
| C | 0.301657780 | -1.543062695 | -0.210777392 |
| I | -2.259345523 | 0.759188542 | 1.058861476 |
| Al | 2.216628529 | -2.151330643 | -0.105571489 |
| Al | -1.177886534 | -2.486830420 | 0.651551061 |

| | | | |
|---|---|---|---|
| Zr | 0.212644976 | 0.456206460 | -0.205880601 |
| Al | -3.533778357 | -1.859582199 | -0.717308243 |
| Al | -0.985248497 | -1.317155908 | -1.834845937 |

| | | | |
|---|---|---|---|
| 7 | ZrAl4CI2 | | |
| Al | 2.087046882 | 0.050591751 | 0.342220867 |
| I | 1.367269429 | 3.637938143 | -1.503338169 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.053731246 | 0.332650082 | -1.752415600 |
| Al | 0.488474750 | -2.069078580 | -0.167673375 |
| Al | -1.306149342 | -0.765521315 | 1.365885763 |
| I | -1.819937453 | 1.832138131 | 2.426692658 |
| Zr | 0.062910366 | 2.034174171 | 0.321703251 |

| | | | |
|---|---|---|---|
| 8 | ZrAl4CI2 | | |
| C | 1.457775483 | -0.793225215 | 1.523119473 |
| I | 1.368418760 | 1.367085938 | -1.896718043 |
| Al | 2.648511844 | -0.784623609 | 3.051561029 |
| Zr | 0.279528463 | 0.431148718 | 0.544656064 |
| Al | -1.365823179 | -2.196819134 | -0.544475195 |
| Al | 0.587013069 | -1.536327041 | -2.069554393 |
| I | -2.473229166 | 0.067756268 | 1.103439977 |
| Al | 1.101615421 | -2.292476917 | 0.417756434 |

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|---|---|---|---|
| 9 | ZrAl4CI2 | | |
| I | -3.427327151 | 1.441417366 | -0.104716624 |
| Al | -0.045284739 | -2.110891826 | 0.749105502 |
| Al | 1.993585759 | -0.716286778 | 0.105734119 |
| I | 4.374094394 | -0.305428015 | 0.696620647 |
| Al | -3.144777929 | -1.527567128 | -1.141974254 |
| Zr | -0.827561307 | 0.480208716 | 0.023214167 |
| Al | 0.439398504 | -1.148888766 | -1.872446960 |
| C | -1.205699323 | -1.311419007 | -0.704151980 |

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|---|---|---|---|
| 10 | ZrAl4CI2 | | |
| Al | 1.949989758 | -1.478714718 | -1.728178204 |
| Zr | 0.164569931 | 0.129768733 | -0.101059347 |
| I | 1.575300909 | 0.505197980 | 2.246067218 |
| Al | -1.191029494 | -2.558552124 | -0.578009784 |
| Al | 1.553810374 | -2.610963267 | 1.314139823 |
| C | 0.613015735 | -1.884621586 | -0.322300644 |
| I | -1.667783489 | 1.343699285 | -1.924110567 |
| Al | -2.725028473 | -0.419044771 | 0.139161767 |

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|---|---|---|---|
| 11 | ZrAl4CI2 | | |
| Al | -1.102385000 | -1.322507446 | -2.513280368 |
| Al | 1.827267371 | -2.009822523 | -0.966134927 |
| Al | -1.724221000 | 1.170532506 | -2.752062348 |
| Zr | -0.251008500 | 0.460770297 | -0.294954697 |
| I | -1.763869779 | 0.073751816 | 1.998630712 |

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|---|---|---|---|
| I | 2.486570779 | 0.913066854 | -0.307368401 |
| C | -0.152007000 | -1.495824812 | -0.824616525 |
| Al | -1.104566371 | -2.588758309 | 0.624478073 |

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|---|---|---|---|
| 12 | ZrAl4CI2 | | |
| I | 1.572006174 | 3.023502354 | 1.756128818 |
| I | 0.563546527 | 3.023502354 | -2.288581907 |
| Al | -0.963238455 | 4.012822319 | 0.240162320 |
| Al | -1.423723778 | -1.365450460 | 0.354974206 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.466455228 | 1.273003201 | 0.365628353 |
| Al | 1.135467196 | -1.566575607 | -0.283103768 |
| Zr | 1.506456343 | 1.219933245 | -0.375601751 |

| | | | |
|---|---|---|---|
| 13 | ZrAl4CI2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| I | -2.932692935 | 1.934476834 | 1.503022436 |
| Zr | -1.110281088 | 1.554937460 | -0.543470991 |
| Al | -1.278809133 | -1.510026600 | 0.266258431 |
| I | -5.702514996 | -0.592459938 | -1.172536512 |
| Al | 1.333941422 | -1.510026600 | 0.266258431 |
| Al | -3.279160237 | -0.202299283 | -0.728999125 |
| Al | 1.639777543 | 1.051639287 | -0.354905531 |

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|---|---|---|---|
| 14 | ZrAl4CI2 | | |
| Zr | -0.182696214 | 0.245503381 | 0.344569039 |
| Al | -2.178971948 | -2.287959956 | -0.237636557 |
| I | 2.312640298 | 1.302351980 | 1.060593416 |
| I | -2.334554496 | 0.499753946 | -1.372750479 |
| Al | 1.287451950 | -2.081284580 | -0.324251231 |
| C | -0.424536401 | -1.742028594 | 0.661801765 |
| Al | 2.168182155 | 0.000970289 | -1.784078156 |
| Al | -0.429238754 | -2.930155661 | 2.252949171 |

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|---|---|---|---|
| 15 | ZrAl4CI2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.988769249 | -0.017547797 | -0.399946073 |
| I | -3.253332468 | -2.091403175 | 0.183317308 |
| Al | 0.501089037 | -1.649115140 | 1.044648309 |
| Zr | -0.145942550 | 1.988971572 | -0.228644187 |
| Al | -0.749301369 | 0.701240363 | -2.698640437 |
| I | 1.378547558 | 3.777498586 | 1.229678662 |
| Al | 1.347378499 | -0.083150632 | -1.541998392 |

Molecular coordinates Figure S12

| | | | |
|---|---|---|---|
| 1 | HfAl4CF2 | | |
| Al | -1.764997880 | 0.497685169 | -1.222298566 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| F | 0.863988633 | 3.193578973 | -1.399527136 |

| | | | |
|---|---|---|---|
| Hf | -0.066036851 | 2.257064560 | -0.017601183 |
| F | -1.049852168 | 3.159025551 | 1.349987855 |
| Al | 1.038799077 | -1.672238642 | 0.702056361 |
| Al | -0.938939592 | -1.740845100 | -0.675440237 |
| Al | 1.732325928 | 0.619005038 | 1.213590322 |

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|---|---|---|---|
| 2 | HfAl4CF2 | | |
| Al | 1.645395147 | 0.566853366 | 0.810869267 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.880648077 | -1.836526026 | 0.037810438 |
| Al | -1.386779802 | -1.241497071 | -0.824818848 |
| Hf | -1.507604862 | 1.424305102 | -0.383111457 |
| F | -2.450616080 | 2.028221945 | 1.172186202 |
| Al | 3.507899827 | -1.507740393 | 1.225849063 |
| F | -1.149052693 | 2.589886841 | -1.861555259 |

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|---|---|---|---|
| 3 | HfAl4CF2 | | |
| Hf | -0.067910455 | 0.759450403 | 0.392000573 |
| F | -1.710402583 | 1.378277837 | 1.180718811 |
| F | 1.611207958 | 1.669103516 | 0.627546550 |
| Al | -1.305927836 | -2.654623411 | 0.490516046 |
| C | 0.097803520 | -1.324327363 | 0.255602848 |
| Al | -1.279103355 | -0.965880200 | -1.617044334 |
| Al | 1.968475654 | -1.687966955 | -0.131244306 |
| Al | 1.016208075 | -0.396214721 | -2.283157793 |

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|---|---|---|---|
| 4 | HfAl4CF2 | | |
| Hf | -0.019655548 | 0.794208413 | 0.204346542 |
| C | -0.668264289 | -1.197631548 | -0.247003701 |
| Al | 2.379739809 | -0.961904631 | -0.496637482 |
| Al | 0.500882534 | -2.299030109 | 0.946064807 |
| Al | -2.544870527 | -1.727485213 | -0.373345499 |
| F | -0.929090989 | 2.190554702 | -0.738203953 |
| F | 0.465500795 | 1.108204610 | 2.028406522 |
| Al | 0.402484733 | -1.141277134 | -1.987065580 |

| | | | |
|---|---|---|---|
| 5 | HfAl4CF2 | | |
| F | -1.165649668 | 1.384685767 | 1.691683600 |
| Hf | 0.053264314 | 0.807103265 | 0.328233000 |
| Al | 1.282114861 | -1.335065375 | -1.709857132 |
| Al | 0.992046647 | -2.836814633 | 0.667683847 |
| Al | -1.955549773 | -1.642224443 | 0.002008321 |
| C | 0.017503807 | -1.262407438 | -0.072210880 |
| F | 1.805800551 | 1.581017633 | 0.232419293 |
| Al | -1.064873185 | -0.126534662 | -2.076485282 |

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|---|---|---|---|
| 6 | HfAl4CF2 | | |
| Hf | -0.982329745 | 0.362505786 | 0.300047153 |
| Al | 0.907634065 | 1.457152770 | -2.226903038 |
| F | -2.383518957 | 0.914220937 | -0.885364069 |

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|---|---|---|---|
| C | 0.890512978 | 0.234205709 | -0.671987430 |
| Al | 2.761912161 | -0.304829284 | -0.545943246 |
| F | -0.943342255 | 0.786143289 | 2.169160722 |
| Al | 3.085381922 | -2.663354112 | 0.796292629 |
| Al | 0.577874305 | -1.781963842 | -0.263879116 |

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|---|---|---|---|
| 7 | HfAl4CF2 | | |
| F | 0.215773000 | 1.906478000 | 1.487789000 |
| Hf | 0.064670000 | 0.947572000 | -0.136186000 |
| Al | 2.225130000 | -0.992068000 | -0.185101000 |
| Al | -2.581075000 | 0.217225000 | -0.624140000 |
| Al | -2.433748000 | -2.230746000 | 0.172332000 |
| C | -1.030964000 | -0.732514000 | 0.236398000 |
| Al | 0.095250000 | -2.337421000 | 0.482574000 |
| F | 3.846147000 | -1.281029000 | -0.332973000 |

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|---|---|---|---|
| 8 | HfAl4CF2 | | |
| Al | -1.951970695 | -1.051025387 | -0.869634644 |
| C | 0.009633687 | -1.081597631 | 0.090125656 |
| Al | -1.130441177 | -2.407683999 | 1.340106670 |
| Al | 1.413338323 | -2.497659108 | 0.771608790 |
| F | -1.829954861 | 1.043791715 | -0.630575400 |
| Al | 1.631347886 | -0.935038875 | -1.248062443 |
| F | 1.114739213 | 1.856877290 | 1.279150576 |
| Hf | 0.095410492 | 0.971831327 | -0.087502277 |

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|---|---|---|---|
| 9 | HfAl4CF2 | | |
| C | 0.878403336 | -0.847164795 | 0.729199902 |
| Al | 0.773793923 | -1.966884980 | -1.124506736 |
| Al | -0.656212687 | -1.958461340 | 1.189483156 |
| F | 0.839864560 | 1.784942058 | -1.217147878 |
| Al | -1.818144236 | -1.567306098 | -1.111585840 |
| F | -1.213510067 | 1.782552009 | 1.355276587 |
| Al | 2.769649130 | -1.047776415 | 0.382619862 |
| Hf | -0.219524001 | 0.805570505 | 0.041854563 |

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|---|---|---|---|
| 10 | HfAl4CF2 | | |
| Al | -0.433678156 | -1.841162814 | 0.948458824 |
| Al | -3.092591571 | -0.452712265 | -0.979193168 |
| C | -1.209655946 | -0.628845598 | -0.504058943 |
| F | 3.566699808 | -1.876665228 | 0.486556647 |
| Al | 0.320758137 | -1.112433314 | -1.771196695 |
| Hf | -0.022855769 | 0.845686241 | 0.220260722 |
| F | -0.830997319 | 2.577084019 | 0.460007748 |
| Al | 1.996450909 | -1.472162986 | 0.159353427 |

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|---|---|---|---|
| 11 | HfAl4CF2 | | |
| C | -0.827918921 | -0.708950604 | -0.798977903 |
| Al | -0.316621632 | -1.891943651 | 1.048820153 |
| Al | -2.587048367 | -1.616088849 | -0.459078288 |

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|---|---|---|---|
| Hf | 0.063805278 | 0.830292867 | 0.243357721 |
| F | -1.007658120 | 1.644243745 | 1.612306879 |
| F | 2.066847796 | 0.648174534 | -0.175998851 |
| Al | 1.933522868 | -1.350875657 | -0.192877655 |
| Al | 0.265595503 | -0.999489549 | -2.370298990 |

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|---|---|---|---|
| 12 | HfAl4CF2 | | |
| Al | 1.206998266 | 1.400681724 | -0.821212000 |
| F | -2.141109905 | 2.082289116 | 1.261721000 |
| Al | 3.115023994 | -0.231670387 | -0.215391000 |
| F | 4.740541240 | -0.288250209 | 0.077742000 |
| Al | -1.456728445 | -1.463755805 | -0.506828000 |
| Al | 1.001381523 | -1.688243173 | 0.142429000 |
| Hf | -1.489328138 | 1.325618820 | -0.358073000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |

| | | | |
|---|---|---|---|
| 13 | HfAl4CF2 | | |
| Al | -1.590366159 | -3.235445623 | 0.714610677 |
| Al | 0.310835690 | -1.498922553 | 1.202752541 |
| Al | -1.787542126 | -0.984282726 | -0.567856110 |
| Al | 1.578484233 | 0.316897983 | -1.135678554 |
| F | -1.748199782 | 1.722811217 | 2.302629793 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| F | -1.166113235 | 3.026510730 | -0.717132112 |
| Hf | -1.372274373 | 1.510780467 | 0.436206222 |

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|---|---|---|---|
| 14 | HfAl4CF2 | | |
| Al | -0.435340764 | -1.699836000 | 0.989380036 |
| Hf | 0.010039284 | 0.933604000 | 0.287027286 |
| C | 0.605764943 | -0.850218000 | -0.547008263 |
| Al | 2.336620515 | -1.695462000 | -0.961910476 |
| Al | -0.515483608 | -0.479588000 | -2.213724663 |
| Al | -2.356756307 | -0.452719000 | -0.431187266 |
| F | 1.031943264 | 2.574884000 | 0.305063533 |
| F | -0.113605066 | -3.225919000 | 1.544144335 |

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|---|---|---|---|
| 15 | HfAl4CF2 | | |
| Al | -1.195412682 | 0.241312000 | 1.662570414 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| F | -1.322382156 | 2.893879000 | -1.312206108 |
| Hf | -0.089726684 | 2.193805000 | -0.027576067 |
| F | 0.950234314 | 3.364102000 | 1.078762367 |
| Al | 0.894032143 | -1.989350000 | -0.093800086 |
| Al | -1.556429824 | -1.437215000 | -0.293531196 |
| Al | 1.907891985 | 0.270921000 | -0.637548765 |

Molecular coordinates Figure S13

| | | | |
|---|---|---|---|
| 1 | HfAl4CCl2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |

| | | | |
|---|---|---|---|
| Al | 1.046314572 | -1.713226000 | 0.604090000 |
| Al | -1.046314572 | -1.713226000 | -0.604090000 |
| Cl | -1.048159500 | 3.267954000 | 1.815465508 |
| Hf | 0.000000000 | 2.198114000 | 0.000000000 |
| Cl | 1.048159500 | 3.267954000 | -1.815465508 |
| Al | -1.874181165 | 0.553573000 | -1.082059000 |
| Al | 1.874181165 | 0.553573000 | 1.082059000 |

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|---|---|---|---|
| 2 | HfAl4CCl2 | | |
| Al | 1.140118129 | 0.046170978 | -1.775126858 |
| Cl | 1.723841924 | 3.161975858 | 0.981494136 |
| Hf | 0.061211433 | 2.045627308 | -0.272713710 |
| Cl | -1.997654315 | 2.880183610 | -1.073769510 |
| Al | 1.208271890 | -1.476393527 | 0.463266248 |
| Al | -1.747893597 | -0.885746115 | -0.311016957 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.194496726 | -2.547136143 | -1.596979666 |

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|---|---|---|---|
| 3 | HfAl4CCl2 | | |
| Cl | -1.114918876 | 3.473997526 | -0.047255861 |
| Al | 1.430805225 | 0.003282864 | -1.558969346 |
| Cl | 2.202196637 | 1.162883106 | 2.003703536 |
| Hf | 0.615050780 | 1.887836213 | 0.232880800 |
| Al | 1.467305392 | -0.980024993 | 1.007440510 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.774433507 | -0.917628205 | -0.045997011 |
| Al | 0.450255856 | -2.387148252 | -0.879090020 |

| | | | |
|---|---|---|---|
| 4 | HfAl4CCl2 | | |
| Al | 1.778613925 | -2.478121150 | 0.741473372 |
| Al | -1.502758670 | -2.241155824 | 0.172238621 |
| C | 0.302128329 | -1.371980009 | -0.014375259 |
| Cl | -1.887912892 | 1.035631400 | 1.726594447 |
| Cl | 1.806363719 | 1.904167482 | -0.184269141 |
| Al | -0.986566350 | -0.805301955 | -2.092927556 |
| Hf | -0.167334822 | 0.634838159 | 0.152615962 |
| Al | 1.604685907 | -1.202577995 | -1.676291928 |

| | | | |
|---|---|---|---|
| 5 | HfAl4CCl2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.295623000 | 0.168512089 | 1.574972878 |
| Al | -0.700222000 | -1.914462920 | 0.269660577 |
| Al | 0.742624000 | -2.303311600 | -1.938765955 |
| Hf | 0.478444000 | 1.897141830 | 0.474574639 |
| Al | 1.806611000 | -0.805008437 | -0.086294331 |
| Cl | 2.832188000 | 1.270213487 | 0.876384463 |
| Cl | -0.348696000 | 3.511144262 | -1.030982617 |

| | | | |
|---|---|---|---|
| 6 | HfAl4CCl2 | | |
| C | -1.026314292 | -1.067726861 | -0.109621051 |

| | | | |
|---|---|---|---|
| Cl | -0.534259306 | 2.435924396 | -1.258825768 |
| Cl | 1.137777963 | 0.615214576 | 2.201934739 |
| Al | 1.838278627 | -1.970727290 | -0.362523562 |
| Al | -2.976397005 | -0.928293135 | -0.321498976 |
| Al | -0.377199354 | -2.346715748 | 1.303792311 |
| Al | -0.067666335 | -1.566212383 | -1.880779789 |
| Hf | 0.228844949 | 0.598504336 | 0.014139194 |

| | | | |
|---|---|---|---|
| 7 | HfAl4CCl2 | | |
| Cl | 1.681274441 | 2.243365301 | -0.676086101 |
| Hf | 0.140859281 | 0.625045019 | 0.097624690 |
| Cl | -1.697600632 | 0.612798381 | 1.704240660 |
| Al | -0.224132086 | -2.397316957 | 1.050231690 |
| Al | 2.362133782 | -1.596518755 | -1.350679476 |
| Al | -0.655887207 | -1.199925373 | -1.707982973 |
| C | 0.845570698 | -1.289976514 | -0.127527753 |
| Al | -2.631171064 | -1.407634491 | 0.182088213 |

| | | | |
|---|---|---|---|
| 8 | HfAl4CCl2 | | |
| Al | 2.972580178 | -0.604310094 | -0.047064747 |
| C | 1.152251908 | -0.810415699 | 0.611590224 |
| Cl | -1.459658046 | 1.650352040 | 1.826892007 |
| Al | -0.053039356 | -2.178426929 | 1.298632610 |
| Hf | -0.312280497 | 0.543216635 | 0.084270590 |
| Cl | 0.542083631 | 1.627528084 | -1.833236539 |
| Al | -1.574866314 | -2.116641091 | -0.797604116 |
| Al | 1.052976068 | -2.021624949 | -1.194668584 |

| | | | |
|---|---|---|---|
| 9 | HfAl4CCl2 | | |
| Al | 1.943806380 | -1.385574907 | 0.164536752 |
| Al | -0.459536770 | -1.946910093 | 0.855289472 |
| Al | 0.324459239 | -1.163490755 | -1.809466358 |
| Hf | -0.239272564 | 0.751305554 | 0.150482292 |
| C | -1.288882409 | -0.788123061 | -0.610903819 |
| Cl | -1.453688309 | 2.778485896 | 0.389166519 |
| Cl | 3.963690161 | -1.715965960 | 0.661672762 |
| Al | -3.170968093 | -0.690802604 | -1.136019449 |

| | | | |
|---|---|---|---|
| 10 | HfAl4CCl2 | | |
| Hf | -1.450106728 | 1.492441538 | -0.087826000 |
| Al | -1.214734786 | -1.526086417 | -0.336722000 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Cl | -0.884002846 | 3.150117661 | -1.668511000 |
| Cl | -2.402208039 | 1.974277460 | 2.012087000 |
| Al | 1.299512724 | -1.631633864 | -0.036652000 |
| Al | 1.691270871 | 0.901911822 | 0.402248000 |
| Al | -3.556385728 | -0.362230253 | -1.088614000 |

| | | | |
|---|---|---|---|
| 11 | HfAl4CCl2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |

| | | | |
|---|---|---|---|
| Al | 0.847706479 | -1.978589000 | -0.249542226 |
| Al | -1.370230813 | -1.427793000 | 0.836112049 |
| Cl | -1.080005199 | 2.858802000 | 2.143178428 |
| Hf | -0.091818523 | 2.141055000 | 0.129348922 |
| Cl | 0.605289769 | 3.595759000 | -1.596623777 |
| Al | -1.705565598 | 0.238718000 | -1.154348992 |
| Al | 2.020301655 | 0.278630000 | -0.116806969 |

| | | | |
|---|---|---|---|
| 12 | HfAl4CCl2 | | |
| C | 0.526422984 | -1.020083143 | 0.218364616 |
| Cl | -2.471137703 | -3.021896161 | 0.339743397 |
| Al | 1.752354355 | -0.937947525 | -1.411809891 |
| Al | -1.446681429 | -1.261416428 | -0.219163921 |
| Hf | 0.124506670 | 0.977755292 | 0.046376055 |
| Cl | 0.985865580 | 2.818543584 | 1.303198832 |
| Al | 1.151409968 | -2.298948708 | 1.594899478 |
| Al | -0.447345808 | -0.180217599 | -2.470026657 |

| | | | |
|---|---|---|---|
| 13 | HfAl4CCl2 | | |
| Cl | 1.366148953 | 2.651135323 | 1.978261400 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.187763473 | -1.582379461 | -0.101322728 |
| Hf | 1.059631744 | 1.722293767 | -0.143793826 |
| Al | 3.256515393 | -0.095780163 | -0.621221314 |
| Cl | 5.322751049 | -0.389164738 | -0.914297708 |
| Al | -1.585122306 | 1.036697249 | -0.668610650 |
| Al | -1.357180250 | -1.512576520 | -0.317928661 |

| | | | |
|---|---|---|---|
| 14 | HfAl4CCl2 | | |
| Cl | 1.133235173 | 1.944814211 | -1.401248398 |
| Al | -3.332230309 | -0.340485590 | -1.318308591 |
| Hf | -0.008706435 | 0.525705155 | 0.122923508 |
| C | -1.513474213 | -0.582748249 | -0.701944015 |
| Al | 2.148287418 | -1.763453316 | -0.969724905 |
| Al | -0.486731442 | -2.117501593 | -0.690134796 |
| Al | 1.312210025 | -2.304381708 | 1.278506136 |
| Cl | -0.288072419 | 1.024680975 | 2.428116948 |

| | | | |
|---|---|---|---|
| 15 | HfAl4CCl2 | | |
| Cl | -1.464205977 | 1.442135469 | 2.476341153 |
| Al | -1.339341725 | -0.852296336 | 1.303151684 |
| Hf | 0.129612150 | 1.969564806 | 0.705690590 |
| Al | 2.077126316 | -0.095384622 | 0.377049919 |
| Cl | 1.199099749 | 3.832966525 | -0.300231486 |
| Al | 0.393125357 | -2.012199506 | -0.513492720 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.161089776 | 0.697826502 | -1.558914058 |

Molecular coordinates Figure S14

1 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | -1.047366793 | -1.713598000 | -0.604697500 |
| Br | -1.127109500 | 3.286326000 | 1.952210920 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.881938154 | 0.554728000 | 1.086537500 |
| Hf | 0.000000000 | 2.181505000 | 0.000000000 |
| Br | 1.127109500 | 3.286326000 | -1.952210920 |
| Al | 1.047366793 | -1.713598000 | 0.604697500 |
| Al | -1.881938154 | 0.554728000 | -1.086537500 |

2 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | -1.233384000 | -1.150560930 | -2.102328012 |
| Al | -1.780916000 | -2.467183930 | 0.178129919 |
| C | 0.000000000 | -1.664603970 | 0.042960651 |
| Br | 2.380025000 | 1.104484324 | 0.597157035 |
| Br | -2.380025000 | 1.104484324 | 0.597157035 |
| Al | 1.233384000 | -1.150560930 | -2.102328012 |
| Al | 1.780916000 | -2.467183930 | 0.178129919 |
| Hf | 0.000000000 | 0.371320893 | 0.110699347 |

3 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | 1.496584862 | -2.764145952 | -0.216789733 |
| Br | 2.445619272 | 1.654128807 | -0.093659449 |
| Al | -1.005046687 | -0.836738434 | -2.056970048 |
| Br | -1.941589671 | 0.532463982 | 1.539362961 |
| Al | -1.712704771 | -1.841980673 | 0.401027838 |
| Al | -0.915991041 | -3.436396179 | -1.436305749 |
| C | 0.110753943 | -1.330347324 | -0.328414989 |
| Hf | 0.131631821 | 0.651134688 | -0.077939491 |

4 HfAl4CBr2

| | | | |
|---|---|---|---|
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Hf | -0.127989281 | 1.962131577 | -0.594159077 |
| Al | -1.652671164 | -1.058687288 | -0.320207752 |
| Al | 0.534023628 | -2.715042450 | -1.191542039 |
| Al | 1.272313878 | -1.284907907 | 0.767082891 |
| Al | 1.288422748 | -0.095867307 | -1.668481054 |
| Br | -2.335186324 | 2.342991212 | -1.747640486 |
| Br | 1.370499982 | 3.552171069 | 0.661863813 |

5 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | 4.184091392 | -1.718176261 | 2.231329643 |
| Al | 2.672266659 | -0.323138498 | 0.400369163 |
| Br | -1.841521251 | 1.396937022 | 1.564536364 |
| Br | -0.066673084 | 1.167145050 | -2.494312964 |
| Hf | -0.628102483 | 0.164154605 | -0.255444765 |
| C | 0.888769092 | -1.059455652 | 0.427049237 |
| Al | 1.838894661 | -2.771609303 | 1.005546326 |
| Al | -0.489286814 | -2.510558220 | 0.083675169 |

6 HfAl4CBr2

| | | | |
|---|---|---|---|
| Br | -2.358571581 | 0.002924014 | 0.947302913 |
| Hf | 0.028821646 | 0.392053260 | 0.010203997 |
| Al | 3.040813410 | -1.183952180 | -0.229734017 |
| Br | 1.646143765 | 2.281944448 | -0.385635281 |
| C | 1.123252720 | -1.317573015 | 0.241983455 |
| Al | 0.339732261 | -1.590087394 | -1.771120726 |
| Al | -2.095471417 | -2.307567241 | -0.735341925 |
| Al | -0.045051893 | -2.633227131 | 1.055817383 |

7 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | -2.059597613 | -0.962488044 | 0.364605484 |
| Al | 0.195311888 | -2.173961149 | 0.556139106 |
| Br | -4.147895318 | -0.883808432 | 1.248644580 |
| Br | 2.720689226 | 1.879462967 | -0.185078616 |
| C | 1.034326246 | -1.112468180 | -0.961441524 |
| Al | -0.784260480 | -0.994149665 | -1.862832913 |
| Al | 2.871406525 | -1.078926303 | -1.689015045 |
| Hf | 0.567347877 | 0.549315667 | 0.038169366 |

8 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | -1.343065207 | -1.411945969 | -0.389763514 |
| Hf | 1.565472019 | 1.280756207 | 0.579819444 |
| Br | 1.460160330 | 2.081061729 | 2.960227257 |
| Br | 3.184825513 | 1.879943729 | -1.326031169 |
| Al | -1.222550823 | 1.535211592 | -0.127632551 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 3.695732239 | -0.662913624 | 0.163482607 |
| Al | 1.249859600 | -1.433146452 | -0.643645982 |

9 HfAl4CBr2

| | | | |
|---|---|---|---|
| Hf | 0.037289054 | 1.043800639 | -0.071519947 |
| Al | 1.996832903 | -0.429059542 | -1.618347183 |
| Al | -1.060601420 | -1.440305170 | -0.459804106 |
| Br | 0.584151433 | 3.082351750 | 1.353995492 |
| Br | -1.642368282 | -3.578271650 | 0.065162985 |
| Al | 1.638871763 | -2.115996866 | 1.297669951 |
| Al | -0.315653597 | -0.075743685 | -2.646091681 |
| C | 0.829985175 | -0.833688561 | 0.004057199 |

10 HfAl4CBr2

| | | | |
|---|---|---|---|
| Al | 0.684012747 | -2.411645142 | -0.130042567 |
| Br | 0.856113411 | 1.251885959 | -2.129078122 |
| Al | 2.295409761 | -1.334575530 | 2.701809695 |
| Hf | 0.141193216 | 0.310222878 | 0.245405482 |
| Br | -1.771103586 | 1.004763443 | 1.736363824 |
| Al | -0.112035354 | -1.240806526 | -2.442316810 |
| C | 1.312276413 | -1.100134536 | 1.050600471 |
| Al | -1.791613214 | -2.298973737 | -0.916199357 |

11 HfAl4CBr2
Al 0.907595098 -1.899999000 -0.488714822
Br 0.424330348 3.828915000 -1.354203723
C 0.000000000 0.000000000 0.000000000
Al -1.763140140 0.278764000 -1.064773696
Hf -0.177939477 2.090980000 0.369674215
Br -1.238036926 2.529155000 2.605182858
Al -1.278998351 -1.554297000 0.749592127
Al 2.001671612 0.385544000 -0.184032932

12 HfAl4CBr2
Br 1.911912480 3.606820672 -0.703827057
Hf 0.427521210 1.971533049 0.530584160
Al 0.094227386 -2.087955597 -0.363945545
C 0.000000000 0.000000000 0.000000000
Br -1.367091230 1.916588376 2.399533156
Al 2.029623331 -0.388976746 0.433139895
Al -1.013219320 0.709713516 -1.652799942
Al -1.496455715 -0.575097293 1.274340104

13 HfAl4CBr2
Al -2.347314846 -1.802012462 -0.665441854
C -0.990631019 -1.534297660 0.654790412
Hf -0.048133528 0.246614753 0.344015896
Al -0.014953390 -1.515310987 -2.155734618
Br 1.592220284 1.143993578 2.047060657
Al 0.521505229 -2.580306816 0.163332132
Br -1.565986358 1.362265244 -1.372925466
Al 2.493933327 -1.507719096 -1.364664336

14 HfAl4CBr2
Al -1.463258054 -2.435756557 0.560563977
Br -1.403684458 0.169298608 2.114940786
Hf 0.264431421 0.325858272 0.202125630
C -0.049560938 -1.538823259 -0.594759519
Al -0.529455766 -1.262766982 -2.552128964
Br -0.199683958 1.681695882 -1.898418258
Al 3.083737162 -0.230910113 0.838099263
Al 1.784065115 -2.148540768 -0.274441409

15 HfAl4CBr2
Br -2.920905871 1.710175758 1.589546614
C 0.000000000 0.000000000 0.000000000
Br -0.170398664 3.494008017 -1.389580227
Al -1.079986520 -1.158125240 -1.197110916
Hf -1.380830665 1.421747600 -0.363377715
Al 2.284029027 3.529395445 0.163138978
Al 1.251709519 -1.623594374 -0.256866602
Al 1.736627729 0.781756021 0.435471130

Molecular coordinates Figure S15

1 HfAl4CI2

| | | | |
|---|---|---|---|
| Hf | 0.000000000 | 2.162691000 | 0.000000000 |
| Al | -1.890238142 | 0.556636000 | -1.091329500 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| I | 1.235889500 | 3.312334000 | -2.140623407 |
| Al | -1.048733381 | -1.714420000 | -0.605486500 |
| Al | 1.890238142 | 0.556636000 | 1.091329500 |
| Al | 1.048733381 | -1.714420000 | 0.605486500 |
| I | -1.235889500 | 3.312334000 | 2.140623407 |

2 HfAl4CI2

| | | | |
|---|---|---|---|
| I | -2.654054000 | 0.886451308 | 0.449015297 |
| Al | -1.247837000 | -1.278454722 | -2.124209466 |
| Hf | 0.000000000 | 0.244488941 | 0.048182733 |
| Al | 1.247837000 | -1.278454722 | -2.124209466 |
| C | 0.000000000 | -1.772917825 | -0.045802250 |
| I | 2.654054000 | 0.886451308 | 0.449015297 |
| Al | -1.777720000 | -2.603448722 | 0.170747461 |
| Al | 1.777720000 | -2.603448722 | 0.170747461 |

3 HfAl4CI2

| | | | |
|---|---|---|---|
| Al | 1.666949155 | 0.073908259 | -1.063082629 |
| Al | -1.967621131 | -0.236897538 | -0.509612231 |
| I | 1.338028481 | 2.859448622 | -1.696141311 |
| Al | -0.115986581 | -1.959559302 | -0.625445349 |
| Al | 2.393571715 | -2.046784356 | 0.271744178 |
| Hf | -0.514138084 | 1.929200432 | 0.220483284 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| I | -0.762367645 | 2.728811008 | 2.814563496 |

4 HfAl4CI2

| | | | |
|---|---|---|---|
| Al | -1.084667496 | -1.541672730 | 0.554922863 |
| I | 2.163052597 | 2.868284423 | -1.451595331 |
| Al | -1.271295083 | -0.021263921 | -1.688849046 |
| Al | -0.156314426 | -2.551520128 | -1.584608716 |
| I | -2.092444078 | 3.177703463 | 1.250380227 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.810636371 | -0.729046491 | -0.417122810 |
| Hf | -0.160707570 | 2.014801752 | -0.290235595 |

5 HfAl4CI2

| | | | |
|---|---|---|---|
| C | 0.533579326 | -1.579095591 | 0.098783674 |
| I | -2.547304840 | 0.392371312 | 0.413654911 |
| Al | 2.414806530 | -1.870159340 | 0.708351693 |
| Hf | 0.183421746 | 0.385627972 | -0.155222585 |
| I | 2.725026912 | 1.386776973 | 0.188469570 |
| Al | -0.376340377 | -1.655862160 | -1.799332348 |
| Al | -3.034107770 | -2.478836291 | -1.226251927 |

| | | | |
|---|---|---|---|
| Al | -0.991056725 | -2.655562795 | 0.676518191 |

| | | | |
|---|---|---|---|
| 6 | HfAl4CI2 | | |
| Al | 2.497353523 | -1.999127819 | -1.024765566 |
| I | 2.590298168 | 0.402254573 | 0.762962267 |
| Hf | -0.091956689 | 0.209603881 | -0.071788422 |
| Al | -0.116008061 | -1.819313363 | -1.820708578 |
| Al | 0.752752078 | -2.701298490 | 0.947417924 |
| C | -0.743485226 | -1.686644315 | 0.250632474 |
| Al | -2.730311203 | -1.811957217 | 0.129600433 |
| I | -2.480249969 | 1.547565444 | -0.260039768 |

| | | | |
|---|---|---|---|
| 7 | HfAl4CI2 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.091655486 | -1.673730272 | 0.191304573 |
| Al | -1.567030432 | 1.142145349 | -0.387351920 |
| Hf | 1.610266822 | 1.091943506 | -0.591531117 |
| I | 0.319582045 | 3.015218148 | -2.110613973 |
| Al | -1.459897125 | -1.423808667 | 0.346179295 |
| I | 3.714527389 | 1.136705702 | 1.217272613 |
| Al | 3.389297732 | -1.067884731 | -1.155962093 |

| | | | |
|---|---|---|---|
| 8 | HfAl4CI2 | | |
| C | -1.029546281 | -1.450976557 | -0.822608156 |
| Al | 0.015319853 | -2.209506199 | 0.742932801 |
| Hf | -0.720679378 | 0.361978994 | -0.056708256 |
| Al | 2.080679618 | -0.765020677 | 0.269249201 |
| I | 4.383044785 | -0.269148640 | 1.073015489 |
| Al | 0.709106553 | -1.233852697 | -1.846314411 |
| I | -3.263692280 | 1.396207512 | -0.348399158 |
| Al | -2.901992102 | -1.721679448 | -1.426331980 |

| | | | |
|---|---|---|---|
| 9 | HfAl4CI2 | | |
| Hf | -0.254285320 | 0.214421765 | -0.084883362 |
| I | 2.042120835 | 0.192689473 | -1.814610888 |
| Al | -3.735264038 | 0.318771022 | -1.159053996 |
| C | -1.976048135 | -0.433713939 | -0.858307696 |
| Al | 0.051540765 | -2.957349915 | 1.250899107 |
| I | -0.512801479 | 1.353235142 | 2.397378261 |
| Al | -1.465423816 | -2.232908603 | -0.724922101 |
| Al | 1.234601311 | -2.418521605 | -0.876555699 |

| | | | |
|---|---|---|---|
| 10 | HfAl4CI2 | | |
| C | 0.718969153 | -0.952162735 | 0.025886632 |
| Al | 2.050681905 | -1.018763361 | -1.491605867 |
| I | 1.142274788 | 3.345729433 | 0.934074595 |
| Al | 0.949155931 | -2.278732603 | 1.518268528 |
| Al | -1.196119727 | -1.260713194 | -0.595427506 |
| I | -2.110768387 | -3.418995488 | 0.330153183 |
| Hf | 0.334255351 | 1.013648758 | -0.324644057 |

| | | | |
|---|---|---|---|
| Al | -0.038334555 | -0.317682627 | -2.799312108 |

| | | | |
|---|---|---|---|
| 11 | HfAl4CI2 | | |
| Hf | -0.105577490 | 2.079752131 | 0.327639011 |
| Al | 2.032861592 | 0.273521916 | -0.033168602 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| I | -1.637852339 | 2.538511519 | 2.540454942 |
| Al | 0.813157804 | -1.963286347 | -0.332574466 |
| Al | -1.636241003 | 0.343324758 | -1.248684207 |
| Al | -1.442729461 | -1.401208225 | 0.727996760 |
| I | 0.830601862 | 3.849663593 | -1.541758268 |

| | | | |
|---|---|---|---|
| 12 | HfAl4CI2 | | |
| Hf | 1.086293575 | 1.633218032 | -0.399416297 |
| Al | 3.329570982 | -0.059077398 | -0.211974120 |
| I | 2.288133609 | 2.374869255 | 1.945879342 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.584600248 | 0.887682165 | -0.816534169 |
| Al | 1.252370617 | -1.444775928 | 0.517895512 |
| I | 5.808243021 | -0.307830709 | -0.234676287 |
| Al | -1.286291029 | -1.587971621 | 0.011382543 |

| | | | |
|---|---|---|---|
| 13 | HfAl4CI2 | | |
| C | 0.184867063 | -1.909492809 | 0.299829483 |
| Al | 1.632224892 | -2.637705381 | -0.917562883 |
| I | -1.383349145 | 1.311302408 | 2.058252171 |
| I | 1.848488008 | 0.456399304 | -2.022255065 |
| Al | -1.716267656 | -1.978442229 | -0.339486008 |
| Hf | 0.096468042 | 0.138205608 | 0.073975876 |
| Al | 0.228432120 | -2.704178486 | 2.118171642 |
| Al | -2.660332849 | 0.229397445 | -1.555971600 |

| | | | |
|---|---|---|---|
| 14 | HfAl4CI2 | | |
| Al | -1.486678416 | 1.168514754 | 0.541106691 |
| Al | -1.031622829 | 3.931760153 | 0.375480003 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.334144103 | -1.452903032 | 0.485588742 |
| I | 1.734516625 | 2.991139340 | 1.582441261 |
| Al | 1.131141762 | -1.553388736 | -0.411701932 |
| I | 0.311543187 | 2.991139340 | -2.327146129 |
| Hf | 1.478618517 | 1.201416130 | -0.538173128 |

| | | | |
|---|---|---|---|
| 15 | HfAl4CI2 | | |
| I | 2.400154733 | 0.443811597 | 0.469849421 |
| Al | -1.525002305 | -2.570199474 | -0.513939598 |
| Al | 1.123682199 | -2.476629584 | 0.958654361 |
| Al | 3.119053823 | -2.529547706 | -0.951013608 |
| I | -2.627911814 | 1.747770048 | -0.077992115 |
| Hf | -0.369975485 | 0.202872195 | 0.053355474 |
| C | -0.584795463 | -1.626050550 | 0.863926279 |

| | | | |
|---|---|---|---|
| Al | 0.529814289 | -1.731650912 | -1.785515875 |

Molecular coordinates Figure S16

| | | | |
|---|---|---|---|
| 1 | TiAl4C11H10 | | |
| C | 1.367133153 | -0.487352080 | -0.751630627 |
| Al | 1.243380284 | -2.125762283 | 0.297232650 |
| Al | -1.457433812 | -2.562995315 | -0.102852888 |
| C | 0.334934976 | 3.296323304 | 0.817711734 |
| C | 1.407327993 | 2.620124540 | 1.439120633 |
| C | 2.254395880 | 2.138187653 | 0.421722800 |
| C | 1.700884229 | 2.502829006 | -0.821484722 |
| C | 0.507894839 | 3.212651403 | -0.581039307 |
| H | -0.480252498 | 3.787889719 | 1.324836405 |
| H | 1.557881918 | 2.502546173 | 2.502036556 |
| H | 3.150866356 | 1.556309593 | 0.570319029 |
| H | 2.099242701 | 2.249096225 | -1.791666372 |
| H | -0.148926923 | 3.626954457 | -1.331518866 |
| Al | 0.221139146 | -1.452332210 | -1.998758538 |
| Ti | 0.156529730 | 1.019844772 | 0.229435989 |
| Al | 0.135111291 | -4.155270914 | -1.278925081 |
| C | -1.578496528 | -0.680079397 | 0.503319950 |
| C | -1.231087894 | -0.161100893 | 1.790328604 |
| C | -1.588349966 | 1.192840979 | 1.858433747 |
| C | -2.144002012 | 1.558892378 | 0.610418817 |
| C | -2.125155914 | 0.427891538 | -0.217781047 |
| H | 2.332621375 | -0.088727049 | -1.064574204 |
| H | -0.787324912 | -0.728241457 | 2.598528854 |
| H | -1.450391127 | 1.846155548 | 2.707820387 |
| H | -2.504702063 | 2.540712503 | 0.339799253 |
| H | -2.494099965 | 0.396144567 | -1.234950681 |

| | | | |
|---|---|---|---|
| 2 | TiAl4C11H10 | | |
| C | -2.484469560 | 3.864159000 | -0.521209643 |
| C | -3.132047550 | 2.616381000 | -0.544854343 |
| C | -2.605948134 | 1.827538000 | 0.507844128 |
| C | -1.660598723 | 2.616381000 | 1.208750082 |
| C | -1.571433470 | 3.864159000 | 0.566904398 |
| H | -2.671863727 | 4.688825000 | -1.191152955 |
| H | -3.891021627 | 2.307923000 | -1.246722064 |
| H | -2.930941723 | 0.834345000 | 0.780546128 |
| H | -1.101188416 | 2.307923000 | 2.078071689 |
| H | -0.944208757 | 4.688825000 | 0.867786062 |
| Al | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -0.826650578 | -1.459928000 | -0.985163796 |
| Al | 0.120745724 | -2.774067000 | 0.143899151 |
| C | 0.007297568 | 2.616381000 | -3.179077674 |
| C | -0.081867685 | 3.864159000 | -2.537231989 |
| C | 0.831168405 | 3.864159000 | -1.449117949 |
| C | 1.478746395 | 2.616381000 | -1.425473248 |

| | | | |
|---|---|---|---|
| C | 0.952646979 | 1.827538000 | -2.478171719 |
| H | -0.552112740 | 2.307923000 | -4.048399280 |
| H | -0.709092398 | 4.688825000 | -2.838113653 |
| H | 1.018562571 | 4.688825000 | -0.779174637 |
| H | 2.237720472 | 2.307923000 | -0.723605527 |
| H | 1.277640568 | 0.834345000 | -2.750873720 |
| Al | -1.653301155 | 0.000000000 | -1.970327591 |
| Ti | -0.826650578 | 2.314334000 | -0.985163796 |
| Al | -1.774046879 | -2.774067000 | -2.114226742 |

| | | | |
|---|---|---|---|
| 3 | TiAl4C11H10 | | |
| Ti | 0.000000000 | 2.332930000 | 0.000000000 |
| C | -1.939847063 | 2.041737000 | 1.358295536 |
| C | -0.930333377 | 2.565266000 | 2.190518007 |
| C | -0.596704219 | 3.850510000 | 1.707494341 |
| C | -1.421299573 | 4.125412000 | 0.597556885 |
| C | -2.246432473 | 3.006838000 | 0.365486157 |
| H | -2.397030696 | 1.070571000 | 1.462763028 |
| H | -0.546180377 | 2.112524000 | 3.091617987 |
| H | 0.144132514 | 4.509363000 | 2.133186383 |
| H | -1.411076313 | 5.031949000 | 0.012746258 |
| H | -3.025599617 | 2.938034000 | -0.375657188 |
| C | 1.939847063 | 2.041737000 | -1.358295536 |
| C | 2.246432473 | 3.006838000 | -0.365486157 |
| C | 1.421299573 | 4.125412000 | -0.597556885 |
| C | 0.596704219 | 3.850510000 | -1.707494341 |
| C | 0.930333377 | 2.565266000 | -2.190518007 |
| H | 2.397030696 | 1.070571000 | -1.462763028 |
| H | 3.025599617 | 2.938034000 | 0.375657188 |
| H | 1.411076313 | 5.031949000 | -0.012746258 |
| H | -0.144132514 | 4.509363000 | -2.133186383 |
| H | 0.546180377 | 2.112524000 | -3.091617987 |
| Al | -1.284306670 | 0.664713000 | -1.481505132 |
| Al | -0.824214499 | -1.659412000 | -0.878808751 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 0.824214499 | -1.659412000 | 0.878808751 |
| Al | 1.284306670 | 0.664713000 | 1.481505132 |

| | | | |
|---|---|---|---|
| 4 | TiAl4C11H10 | | |
| Al | -1.861365200 | -2.633813000 | -2.218287108 |
| C | -0.839348204 | -1.506919000 | -1.000296238 |
| Al | -1.678696408 | 0.000000000 | -2.000592475 |
| Al | 0.000000000 | 0.000000000 | 0.000000000 |
| C | 0.969729508 | 2.005102000 | -2.518919274 |
| C | 1.482965684 | 2.779851000 | -1.457562909 |
| C | 0.829038366 | 4.028626000 | -1.471908843 |
| C | -0.084697057 | 4.029232000 | -2.560661850 |
| C | 0.013919997 | 2.780811000 | -3.207959569 |
| H | 1.276861240 | 1.002355000 | -2.777274352 |
| H | 2.228696476 | 2.458659000 | -0.745914268 |

| | | | |
|---|---|---|---|
| H | 1.018902609 | 4.853559000 | -0.802727542 |
| H | -0.710408360 | 4.854681000 | -2.863126713 |
| H | -0.557796601 | 2.460500000 | -4.066024216 |
| C | -2.507734774 | 4.028626000 | -0.528683633 |
| C | -3.161662092 | 2.779851000 | -0.543029566 |
| C | -2.648425916 | 2.005102000 | 0.518326799 |
| C | -1.692616405 | 2.780811000 | 1.207367094 |
| C | -1.593999351 | 4.029232000 | 0.560069375 |
| H | -2.697599017 | 4.853559000 | -1.197864933 |
| H | -3.907392884 | 2.458659000 | -1.254678207 |
| H | -2.955557648 | 1.002355000 | 0.776681877 |
| H | -1.120899807 | 2.460500000 | 2.065431741 |
| H | -0.968288048 | 4.854681000 | 0.862534238 |
| Ti | -0.839348204 | 2.508470000 | -1.000296238 |
| Al | 0.182668792 | -2.633813000 | 0.217694633 |

| | | | |
|---|---|---|---|
| 5 | TiAl4C11H10 | | |
| C | 0.984919839 | -0.416008867 | -1.731805223 |
| Al | 1.641395359 | -1.562788192 | -0.293747536 |
| Al | -0.890721049 | -2.302940599 | 0.270673994 |
| C | 0.511789658 | 2.892665059 | 0.319603129 |
| C | 0.549216281 | 2.177098762 | 1.538893736 |
| C | 1.614846949 | 1.252463272 | 1.476934932 |
| C | 2.240599624 | 1.412598165 | 0.221035123 |
| C | 1.561104231 | 2.412898939 | -0.492126507 |
| H | -0.178691109 | 3.681123870 | 0.062839543 |
| H | -0.113027058 | 2.312489855 | 2.379052670 |
| H | 1.931375038 | 0.585784766 | 2.263375961 |
| H | 3.099742906 | 0.862559882 | -0.133326830 |
| H | 1.784327524 | 2.736481985 | -1.497866536 |
| Al | -0.199696765 | -1.778199694 | -2.415054497 |
| Ti | -0.055239328 | 0.680940129 | -0.153975634 |
| Al | 1.003102774 | -2.363879002 | 2.009999721 |
| C | -1.981851320 | -0.692464110 | 0.106910722 |
| C | -1.998487223 | 0.273263584 | 1.164138741 |
| C | -2.195944585 | 1.554216893 | 0.634602793 |
| C | -2.225484508 | 1.447577502 | -0.768846687 |
| C | -2.144716312 | 0.070457560 | -1.083369350 |
| H | 1.700928990 | 0.189097279 | -2.294861542 |
| H | -1.862414064 | 0.043429056 | 2.213204925 |
| H | -2.260530544 | 2.474755725 | 1.195938197 |
| H | -2.358481009 | 2.261694166 | -1.466989759 |
| H | -2.226963185 | -0.335206937 | -2.084075673 |

| | | | |
|---|---|---|---|
| 6 | TiAl4C11H10 | | |
| Al | -0.053530273 | -0.500484507 | -2.283810660 |
| C | 3.408070558 | -1.035782466 | -0.509911397 |
| C | 3.637310913 | 0.023216520 | 0.391366819 |
| C | 3.229007664 | -0.403610800 | 1.683763243 |
| C | 2.753447159 | -1.726463437 | 1.577475934 |

| | | | |
|---|---|---|---|
| C | 2.842627942 | -2.115919196 | 0.217109525 |
| H | 3.578094968 | -1.012622441 | -1.575897768 |
| H | 4.027976827 | 0.997710089 | 0.138608355 |
| H | 3.261913555 | 0.188036754 | 2.586747431 |
| H | 2.332899946 | -2.319028405 | 2.375992628 |
| H | 2.543438254 | -3.070223068 | -0.191349603 |
| C | -0.628201028 | 2.300058319 | 1.716437468 |
| C | -0.145147035 | 2.873057535 | 0.516958928 |
| C | -1.222749599 | 2.972026098 | -0.387372603 |
| C | -2.378197005 | 2.461171126 | 0.254705343 |
| C | -2.004941259 | 2.043087361 | 1.556143429 |
| H | -0.044127473 | 2.086544630 | 2.599311819 |
| H | 0.872616745 | 3.177672094 | 0.323054631 |
| H | -1.174278634 | 3.369722698 | -1.390387943 |
| H | -3.369495651 | 2.404123708 | -0.171521490 |
| H | -2.658161239 | 1.604102679 | 2.295988219 |
| Al | -2.991012055 | -1.835713220 | -1.977148437 |
| Al | -1.149274565 | -1.918121331 | 0.687285060 |
| C | -1.538881732 | -0.955844030 | -1.023495975 |
| Ti | -0.953239463 | 0.666495232 | -0.032725384 |
| Al | 1.415840534 | -0.414828896 | 0.325237424 |

| | | | |
|---|---|---|---|
| 7 | TiAl4C11H10 | | |
| C | -2.550596385 | 4.118156000 | -0.331007998 |
| C | -3.192359429 | 2.870408000 | -0.308092081 |
| C | -2.579430785 | 2.084877000 | 0.699834895 |
| C | -1.571503809 | 2.870408000 | 1.312763538 |
| C | -1.548587892 | 4.118156000 | 0.671000495 |
| H | -2.784533471 | 4.937719000 | -0.992900250 |
| H | -4.000740871 | 2.558801000 | -0.951447529 |
| H | -2.877139004 | 1.090447000 | 0.997543113 |
| H | -0.928148361 | 2.558801000 | 2.121144981 |
| H | -0.886695640 | 4.937719000 | 0.904937581 |
| Al | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -0.939797945 | -1.425814000 | -0.939797945 |
| Al | -0.013266030 | -2.829969000 | -0.013266030 |
| C | -0.308092081 | 2.870408000 | -3.192359429 |
| C | -0.331007998 | 4.118156000 | -2.550596385 |
| C | 0.671000495 | 4.118156000 | -1.548587892 |
| C | 1.312763538 | 2.870408000 | -1.571503809 |
| C | 0.699834895 | 2.084877000 | -2.579430785 |
| H | -0.951447529 | 2.558801000 | -4.000740871 |
| H | -0.992900250 | 4.937719000 | -2.784533471 |
| H | 0.904937581 | 4.937719000 | -0.886695640 |
| H | 2.121144981 | 2.558801000 | -0.928148361 |
| H | 0.997543113 | 1.090447000 | -2.877139004 |
| Al | -1.879595890 | 0.000000000 | -1.879595890 |
| Ti | -0.939797945 | 2.498085000 | -0.939797945 |
| Al | -1.866329860 | -2.829969000 | -1.866329860 |

| | | | |
|---|---|---|---|
| 8 | TiAl4C11H10 | | |
| Al | -0.099980016 | -2.960240325 | -0.997544742 |
| Al | 1.745167550 | -0.903497138 | 0.021070672 |
| Al | -1.340014369 | -0.454768292 | -1.428967149 |
| Ti | 0.088428889 | 1.689201309 | -1.291462140 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.872023511 | -1.423667494 | 0.958020798 |
| C | 1.551468021 | 0.349712426 | -2.764398218 |
| C | 0.541295578 | 0.977167521 | -3.527211206 |
| C | 0.728193400 | 2.375636310 | -3.400115733 |
| C | 1.834462931 | 2.602587745 | -2.543802232 |
| C | 2.339000107 | 1.345854985 | -2.158541893 |
| H | 1.707472895 | -0.719619809 | -2.680962818 |
| H | -0.164344667 | 0.482420613 | -4.174419682 |
| H | 0.140561347 | 3.134940210 | -3.891869539 |
| H | 2.247787527 | 3.561154519 | -2.270859242 |
| H | 3.186811988 | 1.170337971 | -1.510398038 |
| C | -2.031201842 | 2.400589792 | -0.502032015 |
| C | -1.075533808 | 2.601381632 | 0.519180791 |
| C | -0.153749264 | 3.574393989 | 0.072788863 |
| C | -0.563390600 | 4.001194112 | -1.207872256 |
| C | -1.701915988 | 3.266405670 | -1.571395766 |
| H | -2.903654877 | 1.767096016 | -0.445177515 |
| H | -1.037605862 | 2.082908625 | 1.462010525 |
| H | 0.701391422 | 3.940656874 | 0.622193784 |
| H | -0.054199681 | 4.724518059 | -1.825907196 |
| H | -2.228772442 | 3.332436188 | -2.511879222 |

| | | | |
|---|---|---|---|
| 9 | TiAl4C11H10 | | |
| C | -2.142005176 | 1.179005489 | 1.069611975 |
| C | -1.448726453 | 2.381423067 | 0.837619907 |
| C | -1.199868824 | 2.492090187 | -0.545687241 |
| C | -1.782403427 | 1.378370255 | -1.180030570 |
| C | -2.379458530 | 0.577910289 | -0.186294248 |
| H | -2.486002669 | 0.813557215 | 2.025876831 |
| H | -1.149503145 | 3.088432891 | 1.594954162 |
| H | -0.673587700 | 3.295331378 | -1.039203147 |
| H | -1.784798695 | 1.188887593 | -2.244704550 |
| H | -2.960609373 | -0.319471719 | -0.352580338 |
| Al | 1.222529840 | -1.143023897 | -2.143592678 |
| Ti | 0.034814927 | 0.591085494 | 0.257549150 |
| Al | -1.380667643 | -1.693033338 | -2.066572649 |
| Al | -1.352874059 | -2.643067983 | 0.368057720 |
| C | 2.438921598 | 0.340070670 | 0.629489165 |
| C | 2.193476215 | 1.605689371 | 0.053900870 |
| C | 1.466376100 | 2.361341536 | 0.994665460 |
| C | 1.216061098 | 1.551458618 | 2.120183993 |
| C | 1.824753470 | 0.301396466 | 1.897680896 |
| H | 3.030381775 | -0.447833783 | 0.183225973 |
| H | 2.548410949 | 1.947752830 | -0.906833837 |

| | | | |
|---|---|---|---|
| H | 1.147279876 | 3.383406511 | 0.865145521 |
| H | 0.669700510 | 1.838371129 | 3.005987948 |
| H | 1.844071474 | -0.526508845 | 2.593038831 |
| C | 0.061922940 | -1.392027340 | -0.523320998 |
| Al | 1.322891530 | -2.515197370 | 0.580730230 |

10 TiAl4C11H10

| | | | |
|---|---|---|---|
| C | 2.892811565 | -2.181519105 | -0.345439540 |
| C | 3.451152553 | -1.042206128 | 0.273683931 |
| C | 2.903147358 | -0.933247768 | 1.567061812 |
| C | 2.023114277 | -2.026969667 | 1.769185565 |
| C | 2.017725000 | -2.803390257 | 0.586607417 |
| H | 3.093768698 | -2.526366922 | -1.348851061 |
| H | 4.112868216 | -0.330309092 | -0.195981489 |
| H | 3.099359586 | -0.143082308 | 2.276598762 |
| H | 1.440262608 | -2.224662122 | 2.657044917 |
| H | 1.441039672 | -3.701385718 | 0.418829319 |
| Al | -1.753870209 | -2.505729842 | 0.883979787 |
| Al | 0.197900978 | 0.061328931 | -2.304409064 |
| Al | -2.179583475 | -0.984931448 | -1.595912587 |
| Ti | -0.803516146 | 0.968175079 | -0.030690207 |
| C | -0.890506834 | -1.032244618 | -0.051503454 |
| C | 0.077812131 | 3.205638605 | -0.059572594 |
| C | -0.260970205 | 2.855214441 | 1.265661771 |
| C | -1.660552970 | 2.647626777 | 1.316433904 |
| C | -2.180940091 | 2.864092888 | 0.017069578 |
| C | -1.104170762 | 3.212153745 | -0.828484051 |
| H | 1.072043792 | 3.414212546 | -0.425456108 |
| H | 0.425925379 | 2.770344481 | 2.095140613 |
| H | -2.233387189 | 2.380182563 | 2.193278692 |
| H | -3.217979385 | 2.787006782 | -0.275263213 |
| H | -1.174556139 | 3.435653213 | -1.882533252 |
| Al | 1.120651489 | -0.859309996 | 0.100815519 |

11 TiAl4C11H10

| | | | |
|---|---|---|---|
| Al | -2.246237343 | -2.227473914 | 0.838439310 |
| C | -2.469518949 | -0.760086385 | 1.948301797 |
| Al | -0.293101526 | -2.001084381 | -0.930261149 |
| Al | -1.028578812 | 0.084565694 | 1.055320507 |
| C | 1.930767753 | 0.367446370 | 1.473024874 |
| C | 2.636562392 | 1.194364137 | 0.576075341 |
| C | 3.156452312 | 0.384512828 | -0.465265798 |
| C | 2.774843608 | -0.943744365 | -0.220172924 |
| C | 1.994647954 | -0.962839862 | 0.965940231 |
| H | 1.523616352 | 0.668754532 | 2.424831406 |
| H | 2.775561677 | 2.259861427 | 0.677322436 |
| H | 3.756178627 | 0.726643339 | -1.294140120 |
| H | 3.030198771 | -1.798103902 | -0.826480931 |
| H | 1.619804894 | -1.843608295 | 1.468076720 |
| C | 1.154219617 | 1.631441863 | -2.516681963 |

| | | | |
|---|---|---|---|
| C | 0.200974847 | 0.659182058 | -2.857267002 |
| C | -0.945934362 | 0.868464501 | -2.046875468 |
| C | -0.703935979 | 2.008258944 | -1.226398542 |
| C | 0.599310838 | 2.463101841 | -1.511219896 |
| H | 2.133484917 | 1.737207149 | -2.956694184 |
| H | 0.319946436 | -0.110241979 | -3.603308750 |
| H | -1.885391015 | 0.339320074 | -2.123221916 |
| H | -1.423192934 | 2.503936860 | -0.594364224 |
| H | 1.083592450 | 3.313567902 | -1.056208851 |
| Ti | 0.832779440 | 0.336120631 | -0.608506295 |
| Al | -3.603258643 | -0.213900754 | 3.386852130 |

12 TiAl4C11H10

| | | | |
|---|---|---|---|
| C | 2.077518000 | 1.435460719 | -0.614939935 |
| C | 1.484718000 | 2.376720751 | 0.259642745 |
| C | 1.504324000 | 1.844805533 | 1.562340302 |
| C | 2.087720000 | 0.565317031 | 1.505925215 |
| C | 2.492800000 | 0.334195493 | 0.175369676 |
| H | 2.302294000 | 1.596763974 | -1.658701497 |
| H | 1.125227000 | 3.351929355 | -0.024780062 |
| H | 1.144589000 | 2.330630683 | 2.455289729 |
| H | 2.242839000 | -0.105233226 | 2.338759578 |
| H | 3.098862000 | -0.499227286 | -0.158990062 |
| Al | -1.470480000 | -2.631281666 | 0.272650505 |
| Ti | 0.000000000 | 0.515194457 | 0.243908356 |
| Al | 1.470480000 | -2.631281666 | 0.272650505 |
| Al | 1.295680000 | -1.017766923 | -1.970711217 |
| C | -2.492800000 | 0.334195493 | 0.175369676 |
| C | -2.087720000 | 0.565317031 | 1.505925215 |
| C | -1.504324000 | 1.844805533 | 1.562340302 |
| C | -1.484718000 | 2.376720751 | 0.259642745 |
| C | -2.077518000 | 1.435460719 | -0.614939935 |
| H | -3.098862000 | -0.499227286 | -0.158990062 |
| H | -2.242839000 | -0.105233226 | 2.338759578 |
| H | -1.144589000 | 2.330630683 | 2.455289729 |
| H | -1.125227000 | 3.351929355 | -0.024780062 |
| H | -2.302294000 | 1.596763974 | -1.658701497 |
| C | 0.000000000 | -1.414452163 | -0.296604576 |
| Al | -1.295680000 | -1.017766923 | -1.970711217 |

13 TiAl4C11H10

| | | | |
|---|---|---|---|
| Al | -0.785869973 | -1.440176082 | 1.534572929 |
| C | -2.191969170 | -1.657379320 | -1.972920900 |
| C | -2.752889136 | -0.390074310 | -2.242201960 |
| C | -1.883086336 | 0.293374737 | -3.129651806 |
| C | -0.792937130 | -0.557864165 | -3.417452506 |
| C | -0.972919436 | -1.759688965 | -2.692832712 |
| H | -2.597491317 | -2.407852876 | -1.310595293 |
| H | -3.663920960 | 0.002941053 | -1.816155891 |
| H | -2.024353932 | 1.294250221 | -3.510407615 |

| | | | |
|---|---|---|---|
| H | 0.060149089 | -0.312920324 | -4.032201074 |
| H | -0.298866410 | -2.604025714 | -2.679450949 |
| C | 1.089845210 | 3.061752777 | 0.703813774 |
| C | -0.311988568 | 2.959522784 | 0.852681749 |
| C | -0.576557535 | 2.367400964 | 2.110697401 |
| C | 0.662743783 | 2.099678503 | 2.734523506 |
| C | 1.691887981 | 2.524337523 | 1.862885889 |
| H | 1.609632072 | 3.463236554 | -0.153873715 |
| H | -1.051457020 | 3.290619585 | 0.139472065 |
| H | -1.553606192 | 2.160119645 | 2.519824289 |
| H | 0.802868097 | 1.636047595 | 3.699551919 |
| H | 2.752863117 | 2.442977829 | 2.050050204 |
| Al | 1.176782478 | -3.005281772 | 0.910675797 |
| Al | 2.087813138 | -1.019158240 | -0.486602472 |
| C | 1.162841244 | -1.012800646 | 1.304364443 |
| Ti | 0.587906197 | 0.724930562 | 0.841608237 |
| Al | -0.764846404 | -0.111031783 | -1.197495714 |

14 TiAl4C11H10

| | | | |
|---|---|---|---|
| Ti | 0.009470005 | 0.368769332 | -0.285972148 |
| C | 0.604232031 | 1.576035072 | 1.711977384 |
| C | 1.788693468 | 1.387824717 | 0.972871942 |
| C | 1.661201116 | 2.107627445 | -0.245894742 |
| C | 0.398336658 | 2.723503259 | -0.247354396 |
| C | -0.263044135 | 2.388690797 | 0.957063198 |
| H | 0.384605661 | 1.134201095 | 2.668961706 |
| H | 2.678515380 | 0.880700252 | 1.325607022 |
| H | 2.416947568 | 2.198776283 | -1.011500526 |
| H | 0.008500278 | 3.363259813 | -1.021675916 |
| H | -1.244427467 | 2.725490158 | 1.256826971 |
| Al | -2.469603725 | -0.085524100 | 1.444072008 |
| C | -0.778142227 | -1.029198085 | 1.217860359 |
| C | -0.811083239 | 1.074920085 | -2.413300040 |
| C | 0.311323424 | 0.267583590 | -2.663385734 |
| C | 0.000592492 | -1.049569599 | -2.229431517 |
| C | -1.314364112 | -1.039239678 | -1.724029388 |
| C | -1.815134437 | 0.273007101 | -1.822569615 |
| H | -0.902670128 | 2.121226171 | -2.653487644 |
| H | 1.229013750 | 0.579481191 | -3.138966829 |
| H | 0.616644329 | -1.929875240 | -2.366990258 |
| H | -1.828104849 | -1.881986520 | -1.293773404 |
| H | -2.801318802 | 0.603262085 | -1.531403992 |
| Al | 0.913669617 | -1.963544612 | 0.984353601 |
| Al | -1.053573663 | -2.460543418 | 2.461106743 |
| Al | 2.650914504 | -0.874584505 | -0.814537268 |

15 TiAl4C11H10

| | | | |
|---|---|---|---|
| Ti | 0.852816344 | 0.543703778 | -0.600089581 |
| C | -1.563875583 | -2.314422388 | 0.451572529 |
| Al | -1.248960809 | -0.491186600 | 1.075433341 |

| | | | |
|---|---|---|---|
| C | -0.140416893 | 2.591118917 | -1.189115456 |
| C | 0.932107545 | 2.342175484 | -2.076292498 |
| C | 0.625811424 | 1.195864986 | -2.836673655 |
| C | -0.654369684 | 0.746381008 | -2.436273553 |
| C | -1.127857504 | 1.612273303 | -1.424097180 |
| H | -0.201241031 | 3.392195186 | -0.467907396 |
| H | 1.838141329 | 2.923914868 | -2.150194159 |
| H | 1.248539093 | 0.745128545 | -3.594491034 |
| H | -1.199211638 | -0.079304607 | -2.866973900 |
| H | -2.093499056 | 1.559918955 | -0.945837450 |
| C | 2.621263466 | 1.705375486 | 0.410735340 |
| C | 1.992871681 | 0.962767579 | 1.424129829 |
| C | 2.166223942 | -0.410398767 | 1.122010319 |
| C | 2.922275100 | -0.506345187 | -0.070627764 |
| C | 3.190810805 | 0.797341845 | -0.518202916 |
| H | 2.659129964 | 2.782340463 | 0.348130283 |
| H | 1.464304037 | 1.363879494 | 2.275017172 |
| H | 1.826049283 | -1.240244479 | 1.722921806 |
| H | 3.221886694 | -1.420309438 | -0.559165337 |
| H | 3.736691013 | 1.059923303 | -1.411880411 |
| Al | -3.099404768 | -0.512244131 | 3.014629768 |
| Al | -0.174156942 | -2.008939575 | -0.783796803 |
| Al | -2.943000615 | -2.786223023 | 1.594454617 |

Molecular coordinates Figure S17

| | | | |
|---|---|---|---|
| 1 | ZrAl4C11H10 | | |
| Zr | 0.000000000 | 2.456529000 | 0.000000000 |
| C | 2.357060552 | 2.985278000 | -0.736920524 |
| C | 1.782213145 | 2.226970000 | -1.782213145 |
| C | 0.736920524 | 2.985278000 | -2.357060552 |
| C | 0.656648348 | 4.208576000 | -1.655364552 |
| C | 1.655364552 | 4.208576000 | -0.656648348 |
| H | 3.214451566 | 2.709800000 | -0.143833297 |
| H | 2.089115165 | 1.239099000 | -2.089115165 |
| H | 0.143833297 | 2.709800000 | -3.214451566 |
| H | -0.033791926 | 5.011780000 | -1.864221268 |
| H | 1.864221268 | 5.011780000 | 0.033791926 |
| Al | -0.851509300 | -1.677770000 | -0.851509300 |
| Al | -1.410488524 | 0.627473000 | -1.410488524 |
| Al | 0.851509300 | -1.677770000 | 0.851509300 |
| C | -0.736920524 | 2.985278000 | 2.357060552 |
| C | -0.656648348 | 4.208576000 | 1.655364552 |
| C | -1.655364552 | 4.208576000 | 0.656648348 |
| C | -2.357060552 | 2.985278000 | 0.736920524 |
| C | -1.782213145 | 2.226970000 | 1.782213145 |
| H | -0.143833297 | 2.709800000 | 3.214451566 |

| | | | |
|---|---|---|---|
| H | 0.033791926 | 5.011780000 | 1.864221268 |
| H | -1.864221268 | 5.011780000 | -0.033791926 |
| H | -3.214451566 | 2.709800000 | 0.143833297 |
| H | -2.089115165 | 1.239099000 | 2.089115165 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.410488524 | 0.627473000 | 1.410488524 |

| | | | |
|---|---|---|---|
| 2 | ZrAl4C11H10 | | |
| Al | -0.998867565 | 1.566637446 | -0.574838760 |
| Zr | 0.000000000 | 3.856984793 | 0.680090483 |
| Al | 0.998867565 | 1.275551213 | 1.075993305 |
| Al | -1.127786716 | -1.130750645 | -1.160305860 |
| C | -1.651029554 | 5.298795730 | 1.810263070 |
| C | -2.292702431 | 4.051309873 | 1.680314940 |
| C | -1.594833194 | 3.112267698 | 2.478745517 |
| C | -0.538708854 | 3.795738763 | 3.129730728 |
| C | -0.562831249 | 5.140236399 | 2.709497723 |
| H | -1.953827060 | 6.222227654 | 1.338568412 |
| H | -3.162751909 | 3.842883075 | 1.076244833 |
| H | -1.860318618 | 2.074880410 | 2.617100232 |
| H | 0.162585735 | 3.358354372 | 3.824143655 |
| H | 0.105136470 | 5.922219945 | 3.039996677 |
| C | 0.538708854 | 4.637258659 | -1.642765755 |
| C | 0.562831249 | 5.756945013 | -0.788030626 |
| C | 1.651029554 | 5.598385681 | 0.111204026 |
| C | 2.292702431 | 4.381687549 | -0.193349967 |
| C | 1.594833194 | 3.772355886 | -1.264800627 |
| H | -0.162585735 | 4.463754983 | -2.444894729 |
| H | -0.105136470 | 6.604806480 | -0.831143930 |
| H | 1.953827060 | 6.304798771 | 0.870284335 |
| H | 3.162751909 | 3.979226280 | 0.303004093 |
| H | 1.860318618 | 2.844850806 | -1.749618881 |
| Al | 1.127786716 | -1.459406013 | 0.703591356 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |

| | | | |
|---|---|---|---|
| 3 | ZrAl4C11H10 | | |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| C | -1.026752932 | 5.654771900 | 2.239601916 |
| C | -2.105403957 | 4.984001954 | 1.610205406 |
| C | -2.098512657 | 3.646732544 | 2.067741352 |
| C | -1.017360428 | 3.489199883 | 2.961153466 |
| C | -0.343737680 | 4.727312870 | 3.065961544 |
| H | -0.789458886 | 6.702769419 | 2.137233539 |
| H | -2.829975207 | 5.422908269 | 0.940982481 |
| H | -2.814464453 | 2.883550699 | 1.801838173 |
| H | -0.765663269 | 2.585023727 | 3.494868765 |
| H | 0.506183581 | 4.936802838 | 3.697823375 |
| Al | -0.990598115 | 1.601002791 | -0.561733287 |
| Al | 1.181061277 | -1.355846866 | 0.767243903 |
| C | 0.343737680 | 5.490841627 | -1.264225214 |

| | | | |
|---|---|---|---|
| C | 1.026752932 | 6.079736395 | -0.170491498 |
| C | 2.105403957 | 5.234152542 | 0.191530925 |
| C | 2.098512657 | 4.134016855 | -0.695785302 |
| C | 1.017360428 | 4.291549516 | -1.589197417 |
| H | -0.506183581 | 5.903807278 | -1.786331325 |
| H | 0.789458886 | 7.029519883 | 0.284139572 |
| H | 2.829975207 | 5.417701846 | 0.970509569 |
| H | 2.814464453 | 3.325916264 | -0.706941612 |
| H | 0.765663269 | 3.624443236 | -2.399972204 |
| Al | 0.990598115 | 1.312326410 | 1.075431828 |
| Zr | 0.000000000 | 4.049171010 | 0.713978099 |
| Al | -1.181061277 | -1.011666425 | -1.184700374 |

| | | | |
|---|---|---|---|
| 4 | ZrAl4C11H10 | | |
| Al | 2.221062144 | 0.471944808 | 1.282330827 |
| C | 0.956871032 | -0.751801034 | 0.552449748 |
| Al | 2.155387880 | -2.157785545 | 1.244413773 |
| Al | -0.043254549 | -2.361717434 | -0.024973025 |
| Al | 4.365010274 | -0.868435244 | 2.520139857 |
| C | -0.552357458 | 1.960993367 | -2.227142207 |
| C | 0.739923241 | 1.394279200 | -2.125329547 |
| C | 0.664382509 | 0.052668978 | -2.544244933 |
| C | -0.669781839 | -0.219566654 | -2.914738885 |
| C | -1.424302533 | 0.961089345 | -2.721464354 |
| H | -0.815834930 | 2.985226144 | -2.009420806 |
| H | 1.630962087 | 1.900848296 | -1.782292932 |
| H | 1.480993435 | -0.651666734 | -2.551692217 |
| H | -1.042559531 | -1.158693239 | -3.294030121 |
| H | -2.476009597 | 1.083500739 | -2.933167766 |
| C | -1.470627759 | 1.394279200 | 1.703457097 |
| C | -2.204940458 | 1.960993367 | 0.635215513 |
| C | -3.069008533 | 0.961089345 | 0.127250001 |
| C | -2.859128839 | -0.219566654 | 0.877321355 |
| C | -1.871189491 | 0.052668978 | 1.847494597 |
| H | -0.728029913 | 1.900848296 | 2.303601066 |
| H | -2.148126930 | 2.985226144 | 0.298176628 |
| H | -3.778202597 | 1.083500739 | -0.677703329 |
| H | -3.373993531 | -1.158693239 | 0.744132022 |
| H | -1.469333565 | -0.651666734 | 2.558424046 |
| Zr | -0.744889375 | 0.257668075 | -0.430062081 |

| | | | |
|---|---|---|---|
| 5 | ZrAl4C11H10 | | |
| Al | -2.147309386 | -1.772336057 | 0.613445305 |
| Zr | 0.057864803 | 0.745352211 | -0.188179997 |
| Al | 0.040994222 | -2.339487640 | 2.405201366 |
| C | 0.376157179 | 2.658780772 | 1.392859349 |
| C | 1.177026936 | 1.607707668 | 1.892069634 |
| C | 2.214651640 | 1.368296084 | 0.966256829 |
| C | 2.056048485 | 2.286119309 | -0.103510296 |
| C | 0.936768063 | 3.091836056 | 0.170572647 |

| | | | |
|---|---|---|---|
| H | -0.497026462 | 3.076490847 | 1.874597287 |
| H | 1.007379393 | 1.067014708 | 2.808943667 |
| H | 3.025533233 | 0.665873416 | 1.079841347 |
| H | 2.693824712 | 2.355171814 | -0.972934117 |
| H | 0.552402549 | 3.881702155 | -0.457554299 |
| C | 0.027347581 | 0.182392745 | -2.658099712 |
| C | -1.162202294 | -0.393516714 | -2.157859821 |
| C | -1.998874737 | 0.644884285 | -1.704699161 |
| C | -1.332747070 | 1.872729858 | -1.915261041 |
| C | -0.084005714 | 1.584708057 | -2.519979952 |
| H | 0.849434506 | -0.352938217 | -3.105963479 |
| H | -1.401291410 | -1.449091393 | -2.147651735 |
| H | -2.984490006 | 0.517320769 | -1.278202995 |
| H | -1.731404639 | 2.854463457 | -1.706301725 |
| H | 0.653527612 | 2.311187961 | -2.826935188 |
| Al | 1.215758001 | -1.710793825 | 0.114853964 |
| Al | -0.282277458 | -4.042836959 | 0.518587516 |
| C | -0.416109350 | -0.985668655 | 1.101352482 |

| | | | |
|---|---|---|---|
| 6 | ZrAl4C11H10 | | |
| C | 1.638092063 | 1.461559299 | 1.917428693 |
| C | 2.252300637 | 0.260454212 | 1.489171014 |
| C | 2.575490852 | 0.411983141 | 0.117658507 |
| C | 2.118879570 | 1.681341581 | -0.304421227 |
| C | 1.569411600 | 2.338708471 | 0.816521566 |
| H | 1.309002484 | 1.676645588 | 2.922667224 |
| H | 2.511492855 | -0.579502627 | 2.116275881 |
| H | 3.148706336 | -0.280870732 | -0.483750079 |
| H | 2.223247760 | 2.090772697 | -1.299407905 |
| H | 1.170501268 | 3.341867736 | 0.825878707 |
| Al | -1.285101022 | -2.405847474 | -0.007083740 |
| C | -0.015787360 | -1.122701583 | -1.144619292 |
| Al | 1.367007039 | -1.163070838 | -2.598024209 |
| Al | -1.503869454 | -1.237161106 | -2.485755594 |
| C | -2.139631177 | 0.147109244 | 1.660922082 |
| C | -1.556551241 | 1.379113405 | 2.042358547 |
| C | -1.619262252 | 2.256416634 | 0.941217978 |
| C | -2.219946503 | 1.569367142 | -0.134746915 |
| C | -2.576243417 | 0.279029538 | 0.319122441 |
| H | -2.305488656 | -0.703817084 | 2.304648960 |
| H | -1.161531207 | 1.612887184 | 3.019280017 |
| H | -1.273034042 | 3.278806094 | 0.921435700 |
| H | -2.422593501 | 1.970874949 | -1.117727443 |
| H | -3.158198648 | -0.443636453 | -0.237111991 |
| Zr | 0.001154722 | 0.422873501 | 0.308598046 |
| Al | 1.402824178 | -2.336478729 | -0.112197855 |

| | | | |
|---|---|---|---|
| 7 | ZrAl4C11H10 | | |
| C | -1.087126335 | 2.658927954 | 0.812860845 |
| C | -1.652991514 | 2.301811726 | -0.424821324 |

| | | | |
|---|---|---|---|
| C | -2.436789292 | 1.140909104 | -0.223111253 |
| C | -2.326257201 | 0.765238971 | 1.126880301 |
| C | -1.469062327 | 1.690817436 | 1.771485119 |
| H | -0.459288284 | 3.517740409 | 0.995006757 |
| H | -1.548576383 | 2.837788053 | -1.356300959 |
| H | -3.041377643 | 0.651775631 | -0.973724899 |
| H | -2.818809049 | -0.076296261 | 1.594245263 |
| H | -1.215262506 | 1.697321555 | 2.821696629 |
| Al | 1.374152187 | -2.413416635 | -1.462039318 |
| C | -0.295756538 | -1.587431673 | -0.400064341 |
| Al | -2.245160378 | -2.001569015 | -0.689261930 |
| Al | 0.236345921 | -3.038349410 | 0.865226360 |
| C | 2.421229971 | 0.911648835 | -0.587356134 |
| C | 1.991862282 | 2.086374318 | 0.075592900 |
| C | 1.828398889 | 1.786209736 | 1.442403184 |
| C | 2.120168090 | 0.419814986 | 1.627853604 |
| C | 2.519559953 | -0.110711817 | 0.379696528 |
| H | 2.667879272 | 0.825199810 | -1.634478480 |
| H | 1.833835073 | 3.049369999 | -0.388199057 |
| H | 1.515298911 | 2.473985514 | 2.213523198 |
| H | 2.095663441 | -0.116946966 | 2.566178472 |
| H | 2.893585426 | -1.112962897 | 0.218006751 |
| Zr | 0.038915471 | 0.499882662 | 0.194130797 |
| Al | -0.377569155 | -0.710043254 | -2.362364232 |

| | | | |
|---|---|---|---|
| 8 | ZrAl4C11H10 | | |
| Al | 1.241592776 | -3.436353000 | -0.029405263 |
| Al | 1.427326732 | -1.317953000 | -1.424139433 |
| C | 1.280469507 | 1.022103000 | 2.109760972 |
| C | 2.245238417 | 0.667800000 | 1.144988239 |
| C | 2.290617748 | 1.693202000 | 0.167759665 |
| C | 1.360291742 | 2.683174000 | 0.538029286 |
| C | 0.716160371 | 2.263683000 | 1.722739751 |
| H | 1.051804490 | 0.479616000 | 3.014085087 |
| H | 2.861346354 | -0.218618000 | 1.161089243 |
| H | 2.939822823 | 1.716972000 | -0.694296350 |
| H | 1.159134587 | 3.595716000 | -0.003146344 |
| H | -0.046107090 | 2.806321000 | 2.262207532 |
| Al | -1.018233530 | -1.338701000 | 1.657538352 |
| Zr | 0.003959908 | 0.651780000 | -0.037672048 |
| Al | -1.297979037 | -3.330721000 | 0.055907448 |
| C | 0.071814679 | -1.732394000 | -0.006474407 |
| C | -2.451758243 | 1.162457000 | -0.253752434 |
| C | -1.741457507 | 2.361824000 | -0.491274323 |
| C | -1.002969842 | 2.206730000 | -1.684689675 |
| C | -1.271370429 | 0.913648000 | -2.198778814 |
| C | -2.164451321 | 0.275445000 | -1.317441681 |
| H | -3.130568485 | 0.975188000 | 0.564314459 |
| H | -1.765240260 | 3.243769000 | 0.131276848 |
| H | -0.370084814 | 2.950986000 | -2.145118500 |

| | | | |
|---|---|---|---|
| H | -0.879672536 | 0.503736000 | -3.117207773 |
| H | -2.559525355 | -0.722426000 | -1.430258213 |

| | | | |
|---|---|---|---|
| 9 | ZrAl4C11H10 | | |
| Al | -1.649738001 | -1.990641485 | -1.338118914 |
| C | -1.834927273 | 2.021834345 | 0.731384311 |
| C | -2.639393977 | 0.946782601 | 0.318178793 |
| C | -2.362837035 | -0.154577584 | 1.171509441 |
| C | -1.394971995 | 0.253716354 | 2.109381215 |
| C | -1.053029223 | 1.594161218 | 1.834741501 |
| H | -1.821048205 | 3.010232202 | 0.297984558 |
| H | -3.350632618 | 0.952578241 | -0.494370880 |
| H | -2.874311782 | -1.108317897 | 1.162627253 |
| H | -0.960391163 | -0.364293210 | 2.878367057 |
| H | -0.361119566 | 2.204690571 | 2.395720477 |
| Al | 2.245613437 | 0.694582409 | 1.670614097 |
| C | 0.969221414 | 2.068425627 | -1.434652387 |
| C | 1.679075280 | 0.879380639 | -1.709398144 |
| C | 0.841395393 | 0.028365371 | -2.452242466 |
| C | -0.391689705 | 0.703609821 | -2.667247186 |
| C | -0.305982123 | 1.961589946 | -2.042259611 |
| H | 1.350013052 | 2.921187602 | -0.891812856 |
| H | 2.682552665 | 0.650748060 | -1.386547235 |
| H | 1.108750266 | -0.945874008 | -2.837088658 |
| H | -1.217243754 | 0.349293233 | -3.265375889 |
| H | -1.077013416 | 2.716404179 | -2.038242508 |
| Al | 0.554938960 | -2.524442224 | 0.210532236 |
| Zr | -0.249188867 | 0.290284336 | -0.165970241 |
| Al | 2.488269032 | -2.217710485 | 1.760771391 |
| C | 1.356457502 | -0.886828088 | 0.951963760 |

| | | | |
|---|---|---|---|
| 10 | ZrAl4C11H10 | | |
| Al | -1.119852974 | -2.063502876 | -0.933385037 |
| Al | -2.347531516 | -1.275164275 | 1.973437831 |
| Al | 1.409911141 | -1.990839370 | -1.781033115 |
| Al | -3.249768436 | 0.368714997 | -0.578324638 |
| C | -0.492223166 | 2.481365761 | -1.031282497 |
| C | 0.862683869 | 2.617567683 | -0.656296928 |
| C | 1.615948479 | 1.700390965 | -1.416563836 |
| C | 0.724964072 | 0.973624649 | -2.251577573 |
| C | -0.577090687 | 1.484294522 | -2.018014942 |
| H | -1.322562770 | 3.049583743 | -0.633941638 |
| H | 1.251644675 | 3.323914163 | 0.061499181 |
| H | 2.688822982 | 1.586551283 | -1.398946912 |
| H | 1.010516649 | 0.316416007 | -3.063880517 |
| H | -1.474696636 | 1.188926439 | -2.543454425 |
| C | 1.798283281 | 0.912901818 | 1.989823410 |
| C | 0.795246593 | 0.135590718 | 2.610019403 |
| C | 0.882301777 | -1.174724378 | 2.109529428 |
| C | 1.929148976 | -1.220405057 | 1.154172931 |

| | | | |
|---|---|---|---|
| C | 2.507041774 | 0.076815420 | 1.103681545 |
| H | 2.003441534 | 1.954137281 | 2.187777733 |
| H | 0.085349412 | 0.484362123 | 3.348003001 |
| H | 0.284324029 | -2.016016239 | 2.431517022 |
| H | 2.346925241 | -2.118525787 | 0.715833232 |
| H | 3.363966686 | 0.356436758 | 0.510536424 |
| C | -1.785093566 | -0.651309614 | 0.211580409 |
| Zr | 0.229729184 | 0.308695765 | 0.117639640 |

11 ZrAl4C11H10

| | | | |
|---|---|---|---|
| C | -2.462580683 | -0.981409969 | 2.276925930 |
| C | 3.177496751 | 0.411555823 | -0.629947595 |
| C | 2.759032372 | 1.299259200 | 0.396071053 |
| C | 2.165353297 | 0.538431449 | 1.422827374 |
| C | 2.193458670 | -0.824430629 | 1.022095737 |
| C | 2.841698812 | -0.897868203 | -0.238728654 |
| H | 3.688184825 | 0.690250551 | -1.540009024 |
| H | 2.898808291 | 2.370549961 | 0.401971026 |
| H | 1.802295684 | 0.918398008 | 2.364015989 |
| H | 1.865925395 | -1.662932314 | 1.619405258 |
| H | 3.049192226 | -1.798173909 | -0.795811428 |
| Al | -1.147103976 | 0.013417514 | 1.332308184 |
| Al | -2.188045061 | -2.413556859 | 1.133069107 |
| C | 0.306622006 | 2.525464383 | -1.727778624 |
| C | 0.751328532 | 1.624639932 | -2.731070907 |
| C | -0.242189022 | 0.644075714 | -2.909453861 |
| C | -1.297376188 | 0.920986800 | -2.001055931 |
| C | -0.962988926 | 2.102602561 | -1.286396463 |
| H | 0.837157860 | 3.401375176 | -1.383470621 |
| H | 1.678812213 | 1.694936857 | -3.280176752 |
| H | -0.209894041 | -0.168630776 | -3.618262929 |
| H | -2.233912249 | 0.386986508 | -1.931158294 |
| H | -1.588098898 | 2.613595299 | -0.572151848 |
| Al | -0.419315028 | -2.124282065 | -0.742271533 |
| Zr | 0.708221181 | 0.361113272 | -0.609294535 |
| Al | -3.591416555 | -0.634865310 | 3.780470972 |

12 ZrAl4C11H10

| | | | |
|---|---|---|---|
| Al | -2.754274474 | -1.357150000 | 0.204507025 |
| Zr | 0.086664574 | 0.730763000 | 0.045874075 |
| Al | -0.486813631 | -3.030386000 | 0.965440970 |
| C | 1.379491500 | 0.234923000 | 2.152290125 |
| C | 2.252468256 | -0.093770000 | 1.102192029 |
| C | 2.574419041 | 1.098503000 | 0.409759803 |
| C | 1.913638303 | 2.164171000 | 1.046778486 |
| C | 1.144381806 | 1.630875000 | 2.107880653 |
| H | 0.939766875 | -0.458360000 | 2.852744598 |
| H | 2.617680264 | -1.082083000 | 0.864752013 |
| H | 3.225953859 | 1.171714000 | -0.448996459 |
| H | 1.963376886 | 3.204279000 | 0.763001197 |

| | | | |
|---|---|---|---|
| H | 0.535411915 | 2.196123000 | 2.799005911 |
| C | -0.607877081 | 1.808423000 | -2.143322592 |
| C | -1.810461295 | 1.300499000 | -1.603411144 |
| C | -2.085331988 | 1.992593000 | -0.410186678 |
| C | -1.058847551 | 2.943816000 | -0.207329468 |
| C | -0.153602626 | 2.837067000 | -1.286886521 |
| H | -0.145245703 | 1.494468000 | -3.066042824 |
| H | -2.416659422 | 0.517373000 | -2.035947865 |
| H | -2.940896384 | 1.829647000 | 0.231727549 |
| H | -1.000208806 | 3.650372000 | 0.607510496 |
| H | 0.730240435 | 3.438802000 | -1.438252077 |
| Al | 0.470644907 | -1.668827000 | -1.245734489 |
| Al | 0.970164425 | -4.191611000 | -0.812192952 |
| C | -0.810340458 | -1.245296000 | 0.262113299 |

13 ZrAl4C11H10

| | | | |
|---|---|---|---|
| Al | -1.627151338 | -1.961198654 | -1.139343632 |
| C | -1.894353737 | 2.088229095 | 0.657120175 |
| C | -2.614520360 | 0.930099537 | 0.308936211 |
| C | -2.254181906 | -0.101624124 | 1.220141465 |
| C | -1.320719410 | 0.439749748 | 2.131249601 |
| C | -1.094451671 | 1.786754137 | 1.784752075 |
| H | -1.958294376 | 3.047404600 | 0.166790148 |
| H | -3.334386393 | 0.843319331 | -0.490595693 |
| H | -2.709770874 | -1.081513115 | 1.289055293 |
| H | -0.844115191 | -0.097013632 | 2.936199004 |
| H | -0.444371041 | 2.476302020 | 2.301166499 |
| Al | 2.133596290 | 0.598210194 | 1.493960206 |
| C | 1.302793838 | 1.786754137 | -1.638869319 |
| C | 1.551006881 | 0.439749748 | -1.970000578 |
| C | 0.375582312 | -0.101624124 | -2.535551062 |
| C | -0.603913551 | 0.930099537 | -2.562507897 |
| C | -0.030416158 | 2.088229095 | -2.004858564 |
| H | 2.010405331 | 2.476302020 | -1.204617484 |
| H | 2.470420139 | -0.097013632 | -1.797448021 |
| H | 0.284519524 | -1.081513115 | -2.987234571 |
| H | -1.601436464 | 0.843319331 | -2.965504679 |
| H | -0.513044652 | 3.047404600 | -1.897240365 |
| Al | 0.418068355 | -2.533463620 | 0.292734613 |
| Zr | -0.214415309 | 0.414035287 | -0.150135215 |
| Al | 2.616351048 | -2.419210128 | 1.831988727 |
| C | 1.447413841 | -1.092218450 | 1.013490082 |

14 ZrAl4C11H10

| | | | |
|---|---|---|---|
| C | -1.849041806 | -2.296713041 | 0.809081677 |
| Zr | 0.744008563 | 0.302268452 | -0.684592316 |
| Al | -0.597411892 | -2.164305665 | -0.559730625 |
| C | 2.127026695 | 0.518306207 | 1.411745315 |
| C | 2.216866733 | -0.840409770 | 1.036976421 |
| C | 2.884833033 | -0.907209253 | -0.207543481 |

| | | | |
|---|---|---|---|
| C | 3.184532464 | 0.410022688 | -0.618626128 |
| C | 2.711921383 | 1.295632355 | 0.388900934 |
| H | 1.683751354 | 0.893362078 | 2.321943492 |
| H | 1.865433956 | -1.680765368 | 1.616359013 |
| H | 3.114141398 | -1.812784876 | -0.749912492 |
| H | 3.721814823 | 0.693558476 | -1.511734519 |
| H | 2.822113368 | 2.369982942 | 0.391283132 |
| Al | -2.825998213 | 0.373071768 | 3.478574743 |
| Al | -1.262598555 | -0.417380610 | 1.216948423 |
| Al | -3.009563133 | -2.116265650 | 2.253317628 |
| C | 0.740757286 | 1.631910277 | -2.734997513 |
| C | -0.273866699 | 0.672140613 | -2.943057692 |
| C | -1.318252808 | 0.927150001 | -2.024526908 |
| C | -0.963454203 | 2.063546656 | -1.264689653 |
| C | 0.311018089 | 2.496084002 | -1.690342311 |
| H | 1.655979735 | 1.726476020 | -3.300800185 |
| H | -0.256949169 | -0.127239592 | -3.669362562 |
| H | -2.240190650 | 0.372046935 | -1.939216195 |
| H | -1.564181011 | 2.517328260 | -0.490848446 |
| H | 0.846130338 | 3.357974457 | -1.319968369 |

| | | | |
|---|---|---|---|
| 15 | ZrAl4C11H10 | | |
| Al | -1.034990859 | -3.924304694 | 1.698544265 |
| Al | 1.164306264 | -2.261324584 | 1.701756163 |
| C | -2.245186948 | 1.227936432 | 0.942989765 |
| C | -1.240579793 | 1.524787986 | 1.883051338 |
| C | -0.581406232 | 2.700065854 | 1.457649265 |
| C | -1.209852197 | 3.152222591 | 0.274654891 |
| C | -2.219823827 | 2.232488986 | -0.057494732 |
| H | -2.927767891 | 0.393211803 | 0.980889503 |
| H | -0.984372122 | 0.934512189 | 2.747592473 |
| H | 0.239433861 | 3.185722035 | 1.966655715 |
| H | -0.936288689 | 4.028683275 | -0.293349303 |
| H | -2.871196129 | 2.286067727 | -0.918635649 |
| Al | -0.612477086 | -1.799216620 | -0.147749390 |
| Zr | -0.030634837 | 0.953829873 | -0.258706240 |
| Al | 0.668033685 | -4.351881615 | -0.050702168 |
| C | 0.669050946 | -0.691003502 | 0.849504157 |
| C | 0.633937792 | 0.871016423 | -2.713706259 |
| C | 0.546185450 | 2.234550366 | -2.356191624 |
| C | 1.562485103 | 2.501892286 | -1.411291094 |
| C | 2.292340354 | 1.305770944 | -1.206571651 |
| C | 1.720102332 | 0.305854326 | -2.010425622 |
| H | -0.007693075 | 0.352834648 | -3.411315675 |
| H | -0.178822236 | 2.943143440 | -2.728988335 |
| H | 1.768527937 | 3.457846157 | -0.951983771 |
| H | 3.126194420 | 1.174588636 | -0.533414089 |
| H | 2.030531214 | -0.725833638 | -2.046238892 |

Molecular coordinates Figure S18

1 HfAl4C11H10

| | | | |
|---|---|---|---|
| Al | -0.922025647 | -1.679268000 | -0.773671380 |
| Hf | 0.000000000 | 2.426043000 | 0.000000000 |
| C | -1.625178554 | 2.213905000 | 1.936812381 |
| C | -0.529003679 | 2.969085000 | 2.411612024 |
| C | -0.506368781 | 4.190876000 | 1.701848285 |
| C | -1.588063369 | 4.190876000 | 0.794198755 |
| C | -2.283113694 | 2.969085000 | 0.939738957 |
| H | -1.906794734 | 1.227847000 | 2.272429474 |
| H | 0.137431186 | 2.693925000 | 3.213480740 |
| H | 0.202039562 | 4.992316000 | 1.847709412 |
| H | -1.854722356 | 4.992316000 | 0.121881245 |
| H | -3.188525422 | 2.693925000 | 0.422671777 |
| Al | 0.922025647 | -1.679268000 | 0.773671380 |
| Al | -1.548352776 | 0.618788000 | -1.299222243 |
| C | 1.588063369 | 4.190876000 | -0.794198755 |
| C | 2.283113694 | 2.969085000 | -0.939738957 |
| C | 1.625178554 | 2.213905000 | -1.936812381 |
| C | 0.529003679 | 2.969085000 | -2.411612024 |
| C | 0.506368781 | 4.190876000 | -1.701848285 |
| H | 1.854722356 | 4.992316000 | -0.121881245 |
| H | 3.188525422 | 2.693925000 | -0.422671777 |
| H | 1.906794734 | 1.227847000 | -2.272429474 |
| H | -0.137431186 | 2.693925000 | -3.213480740 |
| H | -0.202039562 | 4.992316000 | -1.847709412 |
| Al | 1.548352776 | 0.618788000 | 1.299222243 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |

2 HfAl4C11H10

| | | | |
|---|---|---|---|
| Al | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | 1.966623058 | -2.747070000 | 1.966623058 |
| C | -0.823193209 | 2.077227000 | 2.697658332 |
| C | -1.428114575 | 2.858214000 | 1.683767617 |
| C | -0.769491277 | 4.103488000 | 1.638898863 |
| C | 0.235566260 | 4.103488000 | 2.643956401 |
| C | 0.190697506 | 2.858214000 | 3.302579698 |
| H | -1.115783388 | 1.079762000 | 2.990248512 |
| H | -2.247737601 | 2.548377000 | 1.053125949 |
| H | -1.011991426 | 4.928430000 | 0.985111469 |
| H | 0.889353655 | 4.928430000 | 2.886456550 |
| H | 0.821339175 | 2.548377000 | 4.122202725 |
| Al | 1.874465124 | 0.000000000 | 1.874465124 |
| Al | -0.092157934 | -2.747070000 | -0.092157934 |
| C | 1.683767617 | 2.858214000 | -1.428114575 |
| C | 1.638898863 | 4.103488000 | -0.769491277 |
| C | 2.643956401 | 4.103488000 | 0.235566260 |
| C | 3.302579698 | 2.858214000 | 0.190697506 |
| C | 2.697658332 | 2.077227000 | -0.823193209 |
| H | 1.053125949 | 2.548377000 | -2.247737601 |

| | | | |
|---|---|---|---|
| H | 0.985111469 | 4.928430000 | -1.011991426 |
| H | 2.886456550 | 4.928430000 | 0.889353655 |
| H | 4.122202725 | 2.548377000 | 0.821339175 |
| H | 2.990248512 | 1.079762000 | -1.115783388 |
| Hf | 0.937232562 | 2.469048000 | 0.937232562 |
| C | 0.937232562 | -1.410058000 | 0.937232562 |

3 HfAl4C11H10

| | | | |
|---|---|---|---|
| C | -0.999114477 | -0.861395733 | 0.637120316 |
| Al | -2.147674314 | -2.359915505 | 1.233346925 |
| Al | -2.042171644 | 0.197984616 | 1.827084042 |
| C | 2.988498810 | 0.798743739 | -0.172694008 |
| C | 2.281191962 | 1.680488528 | 0.680784753 |
| C | 1.717302640 | 0.910529730 | 1.725453950 |
| C | 2.064802227 | -0.437115304 | 1.513138936 |
| C | 2.849105772 | -0.511467471 | 0.341721388 |
| H | 3.551623900 | 1.079238637 | -1.050184245 |
| H | 2.223358787 | 2.753994595 | 0.580894722 |
| H | 1.121329469 | 1.289110675 | 2.543815587 |
| H | 1.756315964 | -1.270808782 | 2.123835809 |
| H | 3.279389129 | -1.408993222 | -0.075682144 |
| Al | -0.231170900 | -2.360871919 | -0.431775596 |
| C | 0.886812159 | 1.447005890 | -2.592041293 |
| C | 0.039312720 | 0.355209057 | -2.892759447 |
| C | -1.192241159 | 0.567514930 | -2.236192140 |
| C | -1.111051547 | 1.782931412 | -1.530393453 |
| C | 0.176862168 | 2.329565953 | -1.741605175 |
| H | 1.890805986 | 1.591515475 | -2.962027434 |
| H | 0.282318621 | -0.484551239 | -3.525746593 |
| H | -2.039233026 | -0.100077287 | -2.245393611 |
| H | -1.896513363 | 2.219959851 | -0.930160832 |
| H | 0.535462802 | 3.274623625 | -1.362119270 |
| Hf | 0.566067872 | 0.260054878 | -0.422061588 |
| Al | -4.015186680 | -1.326432137 | 3.132575692 |

4 HfAl4C11H10

| | | | |
|---|---|---|---|
| C | -2.385169092 | 2.422014265 | 0.448987272 |
| C | -1.099726880 | 2.830317033 | 0.853287997 |
| C | -0.618597827 | 3.766415259 | -0.094403642 |
| C | -1.635215377 | 3.967266289 | -1.057887008 |
| C | -2.710929399 | 3.121852841 | -0.739723815 |
| H | -3.028187259 | 1.728772943 | 0.969636629 |
| H | -0.560338722 | 2.468226485 | 1.714027622 |
| H | 0.330731187 | 4.281965400 | -0.054646664 |
| H | -1.576251376 | 4.627785698 | -1.909808273 |
| H | -3.630622125 | 3.020545522 | -1.298038189 |
| Hf | -0.753262556 | 1.599065210 | -1.302102163 |
| C | -1.216564529 | 0.816152905 | -3.664057235 |
| C | 0.063143286 | 0.295112567 | -3.368444809 |
| C | 0.949869333 | 1.375783587 | -3.189470123 |

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|---|---|---|---|
| C | 0.226285767 | 2.574299244 | -3.374233950 |
| C | -1.113053086 | 2.226423661 | -3.680081331 |
| H | -2.099822953 | 0.237834487 | -3.883732982 |
| H | 0.324780594 | -0.753460112 | -3.310412509 |
| H | 2.003437489 | 1.292933680 | -2.959559195 |
| H | 0.634033997 | 3.573754367 | -3.335150908 |
| H | -1.915542186 | 2.916640368 | -3.894280346 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -0.162266198 | -1.203951596 | 1.503920690 |
| Al | 1.592484572 | -0.876416893 | -0.753152112 |
| Al | -0.277745711 | -3.091884646 | -0.210063995 |
| Al | -1.831925864 | -0.787500565 | -0.512927087 |

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|---|---|---|---|
| 5 | HfAl4C11H10 | | |
| C | -2.399694000 | 1.158389886 | -2.029092346 |
| C | -2.266324000 | 2.144096105 | -1.038733907 |
| C | -1.601285000 | 3.256076106 | -1.611894323 |
| C | -1.367907000 | 2.962844109 | -2.975174856 |
| C | -1.829038000 | 1.656908076 | -3.226733606 |
| H | -2.857293000 | 0.187811763 | -1.903640982 |
| H | -2.593727000 | 2.060523902 | -0.012726522 |
| H | -1.378616000 | 4.188721308 | -1.113426802 |
| H | -0.896410000 | 3.619342311 | -3.690012722 |
| H | -1.786335000 | 1.134152036 | -4.171179096 |
| Hf | 0.099837000 | 1.419908129 | -1.592672390 |
| C | 2.263636000 | 1.207592734 | -2.911249204 |
| C | 2.658173000 | 1.181377180 | -1.555181510 |
| C | 2.347469000 | 2.428208311 | -0.980846078 |
| C | 1.780485000 | 3.244199108 | -1.987907098 |
| C | 1.738604000 | 2.491339854 | -3.182144088 |
| H | 2.388987000 | 0.407081644 | -3.624192187 |
| H | 3.128623000 | 0.347882701 | -1.052030970 |
| H | 2.522128000 | 2.711697065 | 0.047481369 |
| H | 1.461322000 | 4.269269285 | -1.869081904 |
| H | 1.375316000 | 2.833130169 | -4.139491234 |
| C | 0.000000000 | 0.000000000 | 0.000000000 |
| Al | -1.523048000 | -0.793047157 | 0.957535500 |
| Al | 1.536632000 | -0.556693409 | 1.083502419 |
| Al | 0.192887000 | -2.837454941 | 0.575738408 |
| Al | 0.094027000 | -1.380747684 | -1.520087355 |

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|---|---|---|---|
| 6 | HfAl4C11H10 | | |
| Al | -1.251492788 | -1.774062429 | -1.417469934 |
| Al | -2.532183212 | -1.512999923 | 1.579152852 |
| C | 0.682509525 | -1.695266781 | 1.809157647 |
| C | 1.768442235 | -1.611486540 | 0.901879182 |
| C | 2.421872818 | -0.372236201 | 1.140497137 |
| C | 1.717387945 | 0.310805784 | 2.152409697 |
| C | 0.642298008 | -0.509232448 | 2.562854005 |
| H | 0.021385969 | -2.542786625 | 1.926809858 |

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|---|---|---|---|
| H | 2.149384104 | -2.422863073 | 0.294163559 |
| H | 3.319436998 | -0.032928282 | 0.646820009 |
| H | 1.971067835 | 1.273768055 | 2.569095658 |
| H | -0.079646569 | -0.273732879 | 3.333285598 |
| Al | 1.304474530 | -1.707311863 | -2.173395460 |
| Hf | 0.208639528 | 0.201999676 | 0.140062726 |
| Al | -3.224446884 | 0.690130814 | -0.567015049 |
| C | 1.733115011 | 1.819737111 | -0.994801819 |
| C | 0.833709535 | 1.363302439 | -1.995995424 |
| C | -0.444459474 | 1.891314663 | -1.684691284 |
| C | -0.342128125 | 2.623705994 | -0.489081047 |
| C | 1.003665286 | 2.582229796 | -0.060285729 |
| H | 2.795849666 | 1.633389612 | -0.976414563 |
| H | 1.110590052 | 0.883101398 | -2.926323863 |
| H | -1.337106275 | 1.780618082 | -2.284811473 |
| H | -1.152510269 | 3.140658330 | 0.007174855 |
| H | 1.403840540 | 3.078970232 | 0.810567713 |
| C | -1.862562935 | -0.587372322 | -0.002177536 |

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|---|---|---|---|
| 7 | HfAl4C11H10 | | |
| Al | 2.272699339 | -2.120064575 | 0.289612778 |
| C | -1.895353397 | 0.815845691 | 1.416299001 |
| C | -0.740661661 | 1.096044356 | 2.166000117 |
| C | -0.156388939 | 2.277982590 | 1.648048190 |
| C | -0.988101964 | 2.748013342 | 0.602802678 |
| C | -2.042788547 | 1.832357015 | 0.440750964 |
| H | -2.556964869 | -0.025962504 | 1.559070258 |
| H | -0.347773818 | 0.497435542 | 2.973220424 |
| H | 0.727973368 | 2.769776590 | 2.027608749 |
| H | -0.823978421 | 3.639589889 | 0.017089468 |
| H | -2.838296844 | 1.895080880 | -0.287715847 |
| C | 0.470590271 | -1.432895062 | 0.562168645 |
| Al | -0.126668658 | -2.832147533 | 1.773690846 |
| C | 0.561794852 | 0.788703829 | -2.635747662 |
| C | 0.576622167 | 2.094946177 | -2.093708123 |
| C | 1.685103799 | 2.197598806 | -1.223737179 |
| C | 2.365556559 | 0.958174695 | -1.242532634 |
| C | 1.678985066 | 0.096446976 | -2.119056771 |
| H | -0.148911068 | 0.400961198 | -3.348931535 |
| H | -0.134422779 | 2.877383987 | -2.314004299 |
| H | 1.982013955 | 3.075628211 | -0.669252486 |
| H | 3.267311496 | 0.715659866 | -0.695996204 |
| H | 1.958699885 | -0.920060386 | -2.356713892 |
| Hf | 0.089365043 | 0.586007144 | -0.154225074 |
| Al | -2.221139195 | -3.854844440 | 0.708264712 |
| Al | -1.202742333 | -1.805044808 | -0.535251832 |

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|---|---|---|---|
| 8 | HfAl4C11H10 | | |
| C | -2.994368521 | -0.800165403 | 1.959061133 |
| C | 3.123169446 | 0.069187032 | -0.093747454 |

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|---|---|---|---|
| C | 2.655936198 | 1.010164047 | 0.862104547 |
| C | 1.860844159 | 0.324257101 | 1.802716226 |
| C | 1.817146398 | -1.042376540 | 1.418407128 |
| C | 2.616868215 | -1.197367441 | 0.256269243 |
| H | 3.777796098 | 0.282294500 | -0.925986417 |
| H | 2.895564302 | 2.063409114 | 0.883182578 |
| H | 1.404456447 | 0.753914989 | 2.679782934 |
| H | 1.328913262 | -1.835534105 | 1.965802328 |
| H | 2.812378094 | -2.122641597 | -0.262868908 |
| Al | -4.308407996 | -0.357869933 | 3.276860907 |
| Al | -0.620394631 | -2.132842031 | -0.729789237 |
| Al | -1.471839287 | 0.079914984 | 1.236165187 |
| Al | -2.659948061 | -2.249535568 | 0.851877897 |
| C | 0.681426848 | 2.420109843 | -1.579993208 |
| C | 1.176985594 | 1.458906326 | -2.500811880 |
| C | 0.123891652 | 0.582802314 | -2.827075218 |
| C | -1.022552532 | 0.985378643 | -2.093767875 |
| C | -0.678249097 | 2.137357587 | -1.337665934 |
| H | 1.241094543 | 3.244822958 | -1.163086226 |
| H | 2.178282991 | 1.424465227 | -2.904284148 |
| H | 0.178496744 | -0.241855397 | -3.520486165 |
| H | -2.007669199 | 0.547032691 | -2.160924414 |
| H | -1.346224567 | 2.718104793 | -0.722293602 |
| Hf | 0.682750122 | 0.250844246 | -0.407198978 |

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|---|---|---|---|
| 9 | HfAl4C11H10 | | |
| Al | -0.152701986 | -3.853914266 | 1.177342122 |
| C | -1.481680507 | 0.745084133 | 1.920817077 |
| C | -0.257830089 | 1.422921176 | 2.108011754 |
| C | -0.200901707 | 2.482177566 | 1.159182685 |
| C | -1.376458918 | 2.437915708 | 0.388844700 |
| C | -2.168000613 | 1.359572746 | 0.852356099 |
| H | -1.815357381 | -0.115985917 | 2.478118847 |
| H | 0.451558223 | 1.241729208 | 2.905505754 |
| H | 0.595695034 | 3.204797424 | 1.066738979 |
| H | -1.641851116 | 3.119586610 | -0.404274940 |
| H | -3.140482957 | 1.081114771 | 0.475676907 |
| C | 0.623385281 | -0.649919984 | -2.372564127 |
| C | -0.450739485 | 0.221562544 | -2.650079166 |
| C | -0.024372087 | 1.541902526 | -2.368800320 |
| C | 1.302970163 | 1.485578096 | -1.908035099 |
| C | 1.706900233 | 0.120915840 | -1.899148634 |
| H | 0.611091845 | -1.723967330 | -2.470739074 |
| H | -1.416186080 | -0.061557945 | -3.041108100 |
| H | -0.611425805 | 2.436735006 | -2.505876079 |
| H | 1.918721788 | 2.328042037 | -1.631636640 |
| H | 2.701009850 | -0.248957827 | -1.682357195 |
| C | -0.292661285 | -2.027123568 | 0.515159115 |
| Al | 1.461059690 | -1.779897640 | 1.294688507 |
| Al | -1.971990705 | -1.885952990 | -0.354093408 |

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|---|---|---|---|
| Al | 2.558642829 | 0.525630373 | 1.083727423 |
| Hf | -0.091271538 | 0.344703983 | -0.156751995 |

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|---|---|---|---|
| 10 | HfAl4C11H10 | | |
| C | -3.315185912 | -0.504691563 | 1.436585430 |
| C | 3.210642191 | -0.052240963 | -0.065715997 |
| C | 2.854084219 | 1.056325593 | 0.746666404 |
| C | 2.103585736 | 0.573280729 | 1.837208651 |
| C | 1.988915550 | -0.831241014 | 1.700485670 |
| C | 2.684658691 | -1.219255414 | 0.531026325 |
| H | 3.811833603 | -0.014734377 | -0.962257310 |
| H | 3.129207235 | 2.086353929 | 0.571196993 |
| H | 1.690442415 | 1.166264586 | 2.638832482 |
| H | 1.487477076 | -1.494608341 | 2.389647584 |
| H | 2.808934900 | -2.230025493 | 0.173193456 |
| Al | -4.759441170 | 0.327969192 | 2.364448696 |
| Al | -0.520212743 | -2.364305155 | -0.125973346 |
| Al | -1.565963483 | 0.098707323 | 1.244165902 |
| Al | -3.137863168 | -1.949291554 | 0.262070010 |
| C | 0.437480971 | 2.265825892 | -1.542441565 |
| C | 1.284663407 | 1.435764100 | -2.316534368 |
| C | 0.541958930 | 0.308225717 | -2.728840602 |
| C | -0.775579763 | 0.449698498 | -2.229374647 |
| C | -0.843547901 | 1.662689064 | -1.505843936 |
| H | 0.705395455 | 3.214637985 | -1.101214317 |
| H | 2.319931806 | 1.633704386 | -2.552431001 |
| H | 0.903624581 | -0.508324536 | -3.335876077 |
| H | -1.596567407 | -0.230157590 | -2.401591361 |
| H | -1.730480800 | 2.080619077 | -1.054419952 |
| Hf | 0.767019090 | 0.193888353 | -0.253134479 |

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|---|---|---|---|
| 11 | HfAl4C11H10 | | |
| Al | -3.383416070 | -2.044955135 | 2.097566192 |
| C | 2.704057272 | -1.087217242 | 0.117299503 |
| C | 3.101908906 | 0.198145222 | -0.312499592 |
| C | 2.629599456 | 1.140019732 | 0.644381902 |
| C | 1.942476800 | 0.428588463 | 1.650963006 |
| C | 1.972201394 | -0.943559133 | 1.317966358 |
| H | 2.910520307 | -2.020213341 | -0.386007851 |
| H | 3.707209493 | 0.422643354 | -1.178391763 |
| H | 2.805743678 | 2.205325298 | 0.625846537 |
| H | 1.465928053 | 0.855415114 | 2.520793560 |
| H | 1.530942435 | -1.743675794 | 1.893119068 |
| Al | -3.226676482 | 0.419255358 | 3.368412419 |
| C | 0.902729372 | 1.508585277 | -2.582248347 |
| C | -0.165836422 | 0.622885818 | -2.844685883 |
| C | -1.246195030 | 0.974208617 | -2.003704822 |
| C | -0.859708218 | 2.098345495 | -1.241141008 |
| C | 0.468402243 | 2.427827004 | -1.586165724 |
| H | 1.856874651 | 1.525214951 | -3.088101788 |

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|---|---|---|---|
| H | -0.160140384 | -0.190477886 | -3.555202623 |
| H | -2.207329037 | 0.483873434 | -1.965109372 |
| H | -1.474140050 | 2.607333476 | -0.513618053 |
| H | 1.039358185 | 3.257873427 | -1.197220299 |
| Hf | 0.665974525 | 0.231326027 | -0.511712432 |
| C | -2.114859494 | -2.250643259 | 0.749696475 |
| Al | -0.763013971 | -2.187714814 | -0.523786789 |
| Al | -1.506416439 | -0.399039451 | 1.229194603 |

12 HfAl4C11H10

| | | | |
|---|---|---|---|
| Al | -2.799665367 | -2.511581334 | 1.020505932 |
| Hf | -0.570475903 | 0.761418435 | 0.220423979 |
| C | 0.609095072 | 1.693494621 | -1.803498389 |
| C | -0.393721807 | 0.811578368 | -2.279880961 |
| C | -1.648314621 | 1.354638867 | -1.948125647 |
| C | -1.431080587 | 2.576847855 | -1.269628770 |
| C | -0.037451395 | 2.790373211 | -1.189608866 |
| H | 1.673283217 | 1.578807594 | -1.942613782 |
| H | -0.226523518 | -0.120732678 | -2.799517205 |
| H | -2.606818313 | 0.905736541 | -2.157107982 |
| H | -2.200513740 | 3.233111951 | -0.889988288 |
| H | 0.450606861 | 3.637359082 | -0.727408720 |
| Al | -0.439695588 | -2.444342238 | -0.069879273 |
| Al | -2.972418191 | 0.059070238 | 1.414459316 |
| C | -1.701022785 | -0.968737982 | 0.292424792 |
| Al | 1.767339935 | -0.907957577 | 0.203199140 |
| C | 3.532575506 | -2.220138340 | -0.145095033 |
| C | 3.692559406 | -1.074833981 | -0.961148969 |
| C | 3.890970766 | 0.043637255 | -0.109372700 |
| C | 3.810085060 | -0.399145434 | 1.218435850 |
| C | 3.571415691 | -1.800205032 | 1.204028657 |
| H | 3.341904400 | -3.224666991 | -0.490461710 |
| H | 3.697881656 | -1.063811228 | -2.041459494 |
| H | 4.021521544 | 1.066330031 | -0.430550953 |
| H | 3.870280082 | 0.220545928 | 2.100681019 |
| H | 3.459648847 | -2.437347024 | 2.069029505 |

13 HfAl4C11H10

| | | | |
|---|---|---|---|
| Al | -0.705707720 | -2.190348720 | 0.347589056 |
| Al | 0.254102161 | -1.029863426 | -2.071541086 |
| Hf | -0.538481559 | 0.597148327 | 0.072812094 |
| C | -0.813164158 | 3.086678161 | -0.189334627 |
| C | -0.507389032 | 2.865631391 | 1.173366422 |
| C | -1.583736835 | 2.154995463 | 1.752837074 |
| C | -2.574033650 | 1.977257704 | 0.755186333 |
| C | -2.100544535 | 2.549743116 | -0.438208123 |
| H | -0.196907415 | 3.609488017 | -0.906406587 |
| H | 0.394871004 | 3.178779368 | 1.681566333 |
| H | -1.660821701 | 1.839501030 | 2.783281591 |
| H | -3.524443850 | 1.479872162 | 0.885823706 |

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|---|---|---|---|
| H | -2.624142701 | 2.568406739 | -1.383319056 |
| C | -1.480394470 | -0.866248701 | -1.002908474 |
| Al | -3.282620762 | -0.692140217 | -1.634434758 |
| Al | 1.789008304 | -1.428014590 | 0.024768372 |
| C | 3.988063210 | -0.822689091 | -0.160128637 |
| C | 3.601210322 | -0.541098915 | 1.169238426 |
| C | 3.217289786 | -1.754614508 | 1.782549032 |
| C | 3.369973568 | -2.791770876 | 0.832741478 |
| C | 3.847454723 | -2.214458776 | -0.370714618 |
| H | 4.299335708 | -0.100238088 | -0.899858072 |
| H | 3.569412685 | 0.437074697 | 1.625863883 |
| H | 2.836694617 | -1.868685683 | 2.786621112 |
| H | 3.135642665 | -3.834358707 | 0.986951682 |
| H | 4.040509128 | -2.740304308 | -1.293697618 |

14 HfAl4C11H10

| | | | |
|---|---|---|---|
| Al | -3.460096248 | -1.053137488 | -1.878024278 |
| Hf | -0.650208626 | 0.671739668 | 0.064265803 |
| C | 0.962337663 | 2.542983509 | 0.768906979 |
| C | -0.131823544 | 3.132372273 | 0.100090557 |
| C | -1.288315151 | 2.926573263 | 0.892762065 |
| C | -0.904010282 | 2.198738049 | 2.046330381 |
| C | 0.486065707 | 1.967133424 | 1.969315380 |
| H | 1.985385652 | 2.537990418 | 0.422201555 |
| H | -0.089231125 | 3.668007896 | -0.837274524 |
| H | -2.283984317 | 3.285542379 | 0.669923817 |
| H | -1.554095928 | 1.896871659 | 2.854809364 |
| H | 1.080076602 | 1.443400897 | 2.703966362 |
| Al | -0.182825768 | -0.622329098 | -2.348989145 |
| Al | -1.313968633 | -1.989969383 | 0.501973166 |
| C | -1.735140940 | -0.744884560 | -1.045761431 |
| Al | 1.434560526 | -1.172146775 | 0.006881099 |
| C | 3.387785780 | -1.840858904 | -0.890269704 |
| C | 3.689896232 | -0.959571170 | 0.167277659 |
| C | 3.211568975 | -1.537906273 | 1.372866293 |
| C | 2.614983327 | -2.775237575 | 1.057521982 |
| C | 2.704458520 | -2.959093008 | -0.346495583 |
| H | 3.584289543 | -1.670138275 | -1.938043463 |
| H | 4.177784481 | -0.000772180 | 0.073674182 |
| H | 3.272186436 | -1.095711119 | 2.356167379 |
| H | 2.120856242 | -3.439543714 | 1.750432429 |
| H | 2.325232407 | -3.803830440 | -0.902187199 |

15 HfAl4C11H10

| | | | |
|---|---|---|---|
| Hf | 0.535020359 | 0.847705764 | 0.011966344 |
| Al | 1.866401519 | -2.561295963 | 1.352008730 |
| C | 0.884702835 | -1.183690380 | 0.386000819 |
| C | -2.020442132 | -2.592739110 | 1.840043107 |
| C | -3.019523705 | -1.660787211 | 1.471232658 |
| C | -3.381325484 | -1.909285611 | 0.129753645 |

| | | | |
|---|---|---|---|
| C | -2.589121515 | -2.975709621 | -0.347637867 |
| C | -1.749232798 | -3.407678184 | 0.715751886 |
| H | -1.522441344 | -2.651720702 | 2.796738220 |
| H | -3.419367877 | -0.881339309 | 2.102872666 |
| H | -4.082165430 | -1.333567698 | -0.455523592 |
| H | -2.607083481 | -3.388038479 | -1.345163818 |
| H | -1.027835312 | -4.210844806 | 0.671141740 |
| Al | -0.096878197 | -0.621645466 | -2.306740481 |
| Al | -1.125052891 | -1.362198684 | 0.188779582 |
| C | -0.485556237 | 2.963332240 | -1.045801958 |
| C | -0.859557000 | 2.966658431 | 0.315906502 |
| C | 0.313539033 | 3.115223340 | 1.088442572 |
| C | 1.412482271 | 3.198422331 | 0.201626918 |
| C | 0.914594035 | 3.107922084 | -1.119446698 |
| H | -1.158214973 | 2.870432057 | -1.885694564 |
| H | -1.867266115 | 2.886914455 | 0.696762217 |
| H | 0.360840380 | 3.182710694 | 2.166807171 |
| H | 2.446998106 | 3.339653945 | 0.481973681 |
| H | 1.502465314 | 3.146537446 | -2.024228220 |
| Al | 2.150086497 | -1.126057504 | -1.225007549 |