# Supporting Information

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## Detailed Experimental Materials and Methods

All reagents used for synthesis were reagent-grade or higher. Necessary reference materials for calorimetric experiments were purchased at a minimum of 99% purity.

**Synthesis and Characterization.** The selenate salts of $[(AlO_4)Al_{12}(OH)_{24}(H_2O)_{12}]^{7+}$, $[(GaO_4)Al_{12}(OH)_{24}(H_2O)_{12}]^{7+}$, and $[(GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}]^{8+}$ were synthesized according to the methods of Furrer et. al. (Furrer et al., 1992) and Casey et. al. (Casey and Phillips, 2001; Lee et al., 2002; Lee et al., 2001). Briefly, an $AlCl_3$ solution (0.25 *M*) was heated in a jacketed water reactor at 80 °C using a circulating water bath. This solution was slowly titrated with NaOH (0.25 *M*) to a final $r_{OH}$=2.4 under vigorous stirring. For $GaAl_{12}$ and $GeAl_{12}$, the appropriate metal, e.g.$GaCl_3$ for $GaAl_{12}$ and $GeO_2$ for $GeAl_{12}$, was added to the NaOH in slight excess prior to the addition to the $AlCl_3$ solution (0.25 *M*) held at 85 °C. The hydrolyzed solutions were allowed to cool to room temperature then filtered through 0.2 μm filters and diluted with millipore water (resistance of 18 MΩ). Crystallization was induced by the addition of $Na_2SeO_4$ (0.1 *M*). After several days, the tetrahedral-shaped crystals that grew along the sides of the beaker were removed from the mother liquor, filtered, and rinsed with millipore water.

**X-Ray Diffraction.** A Bruker AXS D8 Advance diffractometer (Bruker AXS, Inc.) equipped with a Cu $K_\alpha$ radiation source was used to collect Powder X-Ray Diffraction (PXRD) patterns of the $AlA1_{12}$, $GaAl_{12}$, and $GeAl_{12}$ salts. Data were collected from 5–65° 2θ at 0.02° 2θ per step and at a collection time of 0.5 second per step using a zero-background sample holder (Fig. S1). The collected diffraction patterns for the $AlA1_{12}$ and $GaAl_{12}$ were compared with the results of Parker et al., 1997 and our single crystal refinements. The collected powder diffraction of the $GeAl_{12}$ salt was compared to the structure refined by Lee et al., 2001. A Bruker SMART single crystal X-ray diffractometer equipped with monochromated Mo Kα radiation (λ = 0.71073Å) and an area detector was used for single crystal X-ray data collection for the $AlAl_{12}$ and $GaAl_{12}$ selenate salts. Pyramid-shaped single crystals were coated with Paratone oil and mounted on a glass fiber-ended copper rod, which was attached to a goniometer. The crystal was kept at 92K with a cold nitrogen stream during the data collection. Data reduction was performed using SAINT software (Bruker, 2007) and Multi-scan absorption correction was applied with SADABS software (Bruker, 2001). The crystal structure was solved with SHELXTL software package (Sheldrick, 2008).

**Thermal Analysis.** Thermogravimetric analysis (TGA) was used to characterize the water content of the synthesis products and their purity. A Netzsch STA 449 system (NETZSCH- Feinmahltechnik GmbH) was operated with a dry argon atmosphere at a flow rate of 40.5 mL/min. The sample was placed in a platinum crucible and heated from 25 °C up to 1200 °C. Buoyancy effects were corrected using a blank run. The samples were weighed before and after each run to check for any mass loss during the instrument equilibration period.

**NMR.** Solid-state $^{27}Al$ MAS NMR spectroscopy was performed using the Bruker Avance 500 system to determine the amount of $AlAl_{12}$ impurities present in the $GaAl_{12}$ and $GeAl_{12}$ solid samples (Casey and Phillips, 2001). Data were acquired at 33 kHz, with pulse lengths of 0.3 μs and a 15° tip angle.

**High Temperature Oxide Melt Solution Calorimetry.** A custom built Tian-Calvet microcalorimeter was used to measure the enthalpy of solution, $\Delta H_{soln}$, for the gallium sulfate reference material according to the method and instrument details as described previously (Navrotsky, 1977; Navrotsky, 1997). Sample was pelletized (~2-3 mg) and dropped from room temperature into molten $3Na_2O{\cdot}4MoO_3$ at 700 °C. The calorimeter was calibrated using the heat content of alumina pellets (5 mg). These procedures are standard in our laboratory and have been described previously (Navrotsky, 1977; Navrotsky, 1997). We note that in both acid and oxide melt solution calorimetry, the chemicals, thermodynamic cycles, and calorimeters used were dictated by the availability of pure and stoichiometric reference compounds and knowledge of their enthalpies of formation, as well as by finding conditions for their rapid dissolution in the chosen calorimetric solvent. A number of test runs were performed to optimize the calorimetric conditions and thermodynamic cycles used, with the goal of minimizing uncertainties in the results.

The $\Delta H^\circ_{f,el}$ for two corresponding aluminum and gallium sulfate hydrates had to be measured. The thermodynamic cycles used to calculate the $\Delta H^\circ_{f,el}$ at 25 ° C for $Al_2(SO_4)_3{\cdot}16H_2O_{(cr)}$ and $Ga_2(SO_4)_3{\cdot}\ 18H_2O_{(cr)}$ are given in Tables S5 and S7 respectively. The measured enthalpy of solution values used to calculate the $\Delta H^\circ_{f,el}$ for these two sulfate hydrates can be found in Tables S6 and S8.

## Results of Synthesis and Characterization

Thermogravimetric analysis (TGA) of the $AlAl_{12}$ produced total measured mass losses of 62.78 and 62.79% (duplicate runs) upon heating to 1200° C with initial mass loss steps of 11.64 and 11.62 % from room temperature to the first inflection point in the weight loss curve around 116 °C. (Figure S2a). The heated end product was identified as γ-$Al_2O_3$ by PXRD. The mass loss from the sample weighed before and after heating was calculated as 62.96 and 62.98% respectively, in good agreement with TGA.. TGA of the $GaAl_{12}$ produced measured mass losses of 59.95 and 60.87% (duplicate runs) upon heating to 1200 °C (Fig. S2b). The mass loss from the gallium sample weighed before and after heating was 61.60% and 61.55% (duplicate runs). In the case of the $GeAl_{12}$, thermogravimetric analysis produced mass losses of 61.60 and 62.04% (duplicate runs) upon heating to 1200 °C (Fig. S3c). The mass loss from the germanium sample weighed before and after heating was 62.00 and 62.20% (duplicate runs).

Solid state $^{27}Al$ MAS NMR spectra revealed tetrahedral aluminum impurities to be less than ~0.4% in the $Na[GaO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12\ H_2O$ crystals and less than ~1.3% in the $[GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12\ H_2O$ crystals.

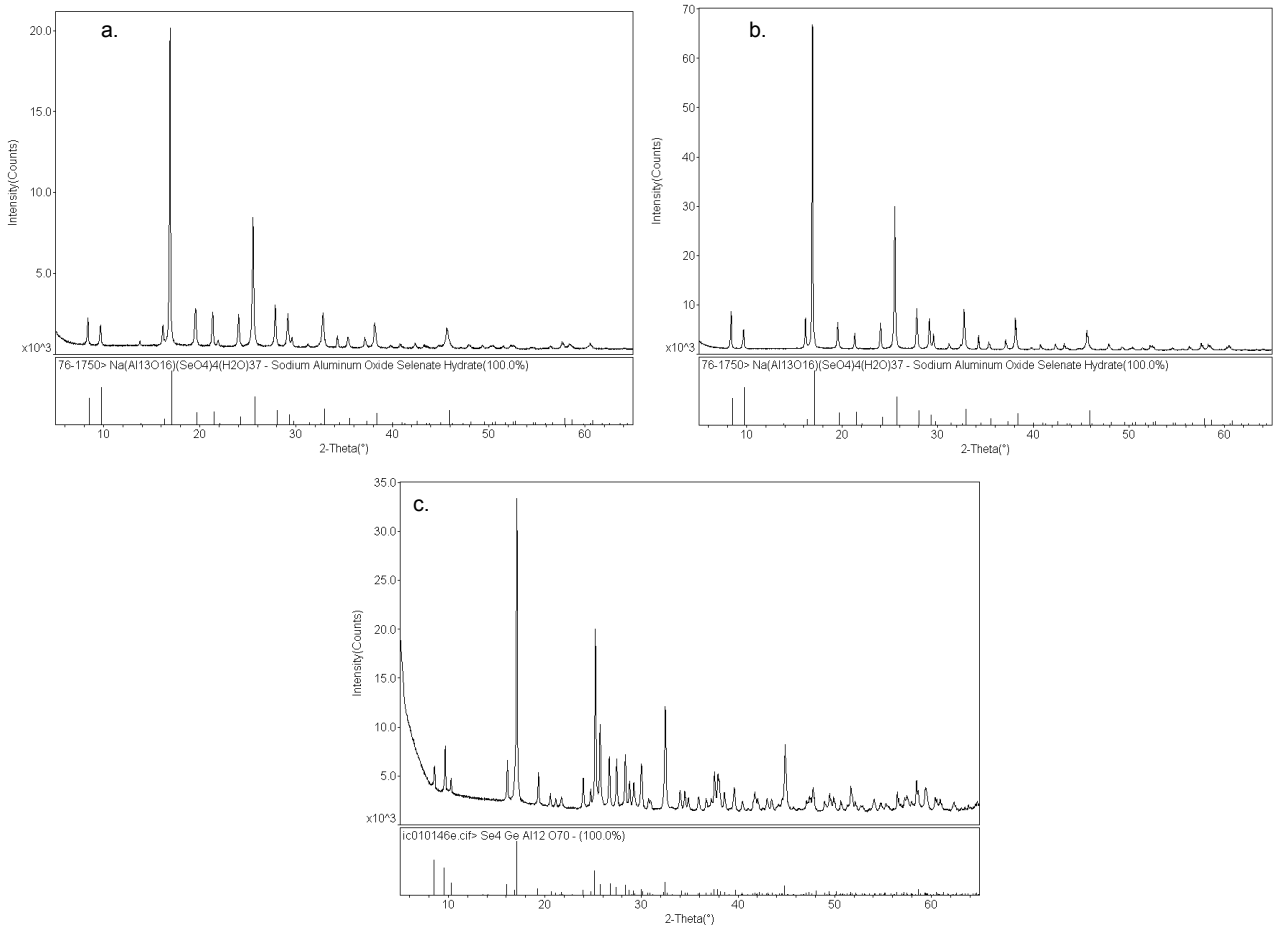


Figure S1. PXRD of **a.** $Na[AlO_4Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$ and **b.** $Na[GaO_4Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$ products compared to PDF#76-1750 (Jr and Millini, 1997); **c.** $[GeO_4Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$ compared to ic010146e.cif (Lee et al., 2001).

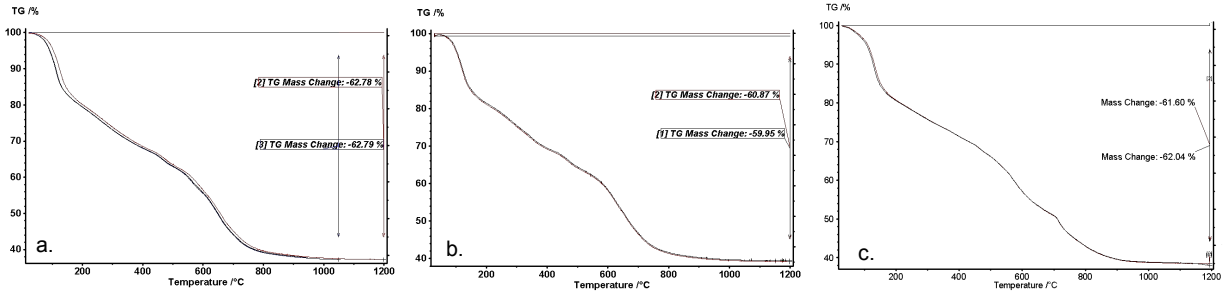


Figure S2. TGA of **a.**$Na[AlO_4Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$ **b.** $Na[GaO_4Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$; **c.** $[GeO_4Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$

Table S1. Thermodynamic cycle used to calculate $\Delta H^{\circ}_{f,el}$ at 25°C for $Na[(MO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12\ H_2O_{(cr)}$, where $M=Al^{3+}$ or $Ga^{3+}$, $x$ = mol of $H_2O$.

| | |
|---|---|
| 1 | $Na[(MO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)} + 32H^+ = Na^+ + M^{3+} + 12Al^{3+} + 4SeO_4^{2-} + 52H_2O$ |
| 2 | $M_2(SO_4)_3 \cdot xH_2O_{(cr)} = 2M^{3+} + 3SO_4^{2-} + xH_2O$ |
| 3 | $Al_2(SO_4)_{3(cr)} = 2Al^{3+} + 3SO_4^{2-}$ |
| 4 | $Na_2SeO_4 \cdot 10H_2O_{(cr)} = 2Na^+ + SeO_4^{2-} + 10H_2O$ |
| 5 | $Na_2SO_{4(cr)} = 2Na^+ + SO_4^{2-}$ |
| 6 | $NaOH_{(cr)} + H^+ = Na^+ + H_2O$ |
| 7 | $H_2O_{(l)} = H_2O$ |
| 8 | $0.5M_2(SO_4)_3 \cdot xH_2O_{(cr)} + 6Al_2(SO_4)_{3(cr)} + 4Na_2SeO_4 \cdot 10H_2O_{(cr)} + 32NaOH_{(cr)} = Na[(MO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)} + 19.5Na_2SO_{4(cr)} + (20+0.5x)H_2O_{(l)}$ |
| 9 | $2M_{(cr)} + 3S_{(cr)} + (6+0.5x)O_{2(g)} + xH_{2(g)} = M_2(SO_4)_3 \cdot xH_2O_{(cr)}$ |
| 10 | $2Al_{(cr)} + 3S_{(cr)} + 6O_{2(g)} = Al_2(SO_4)_{3(cr)}$ |
| 11 | $2Na_{(cr)} + Se_{(cr)} + 7O_{2(g)} + 10H_{2(g)} = Na_2SeO_4 \cdot 10H_2O_{(cr)}$ |
| 12 | $2Na_{(cr)} + S_{(cr)} + 2O_{2(g)} = Na_2SO_{4(cr)}$ |
| 13 | $Na_{(cr)} + 0.5O_{2(g)} + 0.5H_{2(g)} = NaOH_{(cr)}$ |
| 14 | $H_{2(g)} + 0.5O_{2(g)} = H_2O_{(l)}$ |
| 15 | $M_{(cr)} + 12Al_{(cr)} + Na_{(cr)} + 4Se_{(cr)} + 34O_{2(g)} + 36H_{2(g)} = Na[(MO_4)Al_{12}(OH)_{24}(H2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$ |

Abbreviations: cr = crystalline; l = liquid; g= gas; all other species aqueous

Table S2. Measured and calculated enthalpies (kJ/mol) for reactions in Table S1.

$\Delta H_{1,M} = -\Delta H_{soln}(Na[(MO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)})$; $\Delta H_{1,Al} = 958.04 \pm 2.79$ ; $\Delta H_{1,Ga} = 869.71 \pm 5.18$

$\Delta H_{2,M} = 0.5\Delta H_{soln}(M_2(SO_4)_3 \cdot xH_2O_{(cr)})$; $\Delta H_{2,Al}$ (x=16) = 29.33±0.74 ; ; $\Delta H_{2,Ga}$ (x=18)= 20.57 ± 0.96

$\Delta H_3 = 6\Delta H_{soln}(Al_2(SO_4)_{3(cr)}) = -1394.04 \pm 4.8$[a]

$\Delta H_4 = 4\Delta H_{soln}(Na_2SeO_4 \cdot 10H_2O_{(cr)}) = 400.48 \pm 6.68$

$\Delta H_5 = -19.5\Delta H_{soln}(Na_2SO_{4(cr)}) = -361.73 \pm 6.25$[b]

$\Delta H_6 = 32\Delta H_{soln}(NaOH_{(cr)}) = -3584 \pm 33.28$

$\Delta H_{7,M} = -(20+0.5x)\Delta H_{dilution}$[c]; $\Delta H_{7,Al}$ ($x$=16) = 11.2 ; $\Delta H_7$,Ga ($x$=18)= 11.6

$\Delta H_{8,M} = \Delta H_{1,M} + \Delta H_{2,M} + \Delta H_3 + \Delta H_4 + \Delta H_5 + \Delta H_6 + \Delta H_{7,M}$; $\Delta H_{8,Al}$= -3,940.72±34.97 ; $\Delta H_{8,Ga}$ = -4,037.41 ± 35.24

$\Delta H_{9,M} = 0.5\Delta H^{\circ}_{f,el}(M_2(SO_4)_3 \cdot xH_2O_{(cr)})$ ; $\Delta H_{9,Al}$ = -4,156.00 ± 2.14 ; $\Delta H_{2,Ga}$ = -4,085.95 ± 12.62

$\Delta H_{10} = 6\Delta H^{\circ}_{f,el}(Al_2(SO_4)_{3(cr)}) = -20,650.8 \pm 7.8$[d]

$\Delta H_{11} = 4\Delta H^{\circ}_{f,el}(Na_2SeO_4 \cdot 10H_2O_{(cr)}) = -16,025.56 \pm 47.64$[b]

$\Delta H_{12} = -19.5\Delta H^{\circ}_{f,el}(Na_2SO_{4(cr)}) = 27,062.1 \pm 7.8$[d]

$\Delta H_{13} = 32\Delta H^{\circ}_{f,el}(NaOH_{(cr)}) = -13,625.6 \pm 3.2$[d]

$\Delta H_{14,M} = -(20+0.5x)\Delta H^{\circ}_{f,el}(H_2O_{(l)})$; $\Delta H_{14,Al}$ (x=16)= 8,002.4 ± 1.12[§]; $\Delta H_{14,Ga}$ (x=18)= 8,288.2 ± 1.16[d]

$\Delta H_{15,M} = \Delta H^{\circ}_{f,el}(Na[(MO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}) = \Delta H_{8,M} + \Delta H_{9,M} + \Delta H_{10} + \Delta H_{11} + \Delta H_{12} + \Delta H_{13} + \Delta H_{14}$ ;

**$\Delta H_{15,Al}$ = -23,334.18 ± 60.38 ; $\Delta H_{15,Ga}$ = -23,075.02 ± 61.68**

[a](Majzlan et al., 2006)

[b](Armstrong et al., 2011)

[c]calculated (Parker et al., 1965)

[d](Robie, 1995)

Table S3. $[(GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}$ thermodynamic cycle used to calculate $\Delta H_{soln}$ to compare to $MAl_{12}^{7+}$ with sodium counterions;

| | |
|---|---|
| 1 | $[(GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)} + 28H^+ = Ge(OH)_4^0 + 12Al^{3+} + 4SeO_4^{2-} + 48H_2O$ |
| 2 | $NaOH_{(cr)} + H^+ = Na^+ + H_2O$ |
| 3 | $H_2O_{(l)} = H_2O$ |
| 4 | $[(GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)} + NaOH_{(cr)} + 29H^+ + 3H_2O_{(l)} = Na^+ + Ge(OH)_4^0 + 12Al^{3+} + 4SeO_4^{2-} + 52H_2O$ |

Abbreviations: cr = crystalline; l = liquid; g= gas; all other species aqueous

Table S4. Measured and calculated enthalpies (kJ/mol) for reactions in Table S3.

| |
|---|
| $\Delta H_1 = \Delta H_{soln}([(GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}) = -859.53 \pm 11.52$ |
| $\Delta H_2 = \Delta H_{soln}(NaOH_{(cr)}) = -114.46 \pm 0.25$ |
| $\Delta H_3 = 3\Delta H_{dilution}$[a]$= -1.2$ |
| $\Delta H_4 = \boldsymbol{\Delta H_{soln}}$[b]$([(GeO_4)Al_{12}(OH)_{24}(H_2O)_{12}](SeO_4)_4 \cdot 12H_2O_{(cr)}) = \Delta H_1 + \Delta H_2 + \Delta H_3 =$ **$-975.19 \pm 11.52$** |

[a]calculated (Parker et al., 1965)

[b]enthalpy of solution calculated with sodium

Table S5. Thermodynamic cycle used to calculate $\Delta H^\circ_{f,el}$ at 25 °C for $Al_2(SO_4)_3 \cdot 16H_2O_{(cr)}$

| | |
|---|---|
| 1 | $Al_2(SO_4)_3 \cdot 16H_2O_{(cr)} = 2M^{3+} + 3SO_4^{2-} + 16H_2O$ |
| 2 | $Al_2(SO_4)_{3(cr)} = 2Al^{3+} + 3SO_4^{2-}$ |
| 3 | $H_2O_{(l)} = H_2O$ |
| 4 | $Al_2(SO_4)_{3(cr)} + 16H_2O_{(l)} = Al_2(SO_4)_3 \cdot 16H_2O_{(cr)}$ |
| 5 | $2Al_{(cr)} + 3S_{(cr)} + 6O_{2(g)} = Al_2(SO_4)_{3(cr)}$ |
| 6 | $H_{2(g)} + 0.5O_{2(g)} = H_2O_{(l)}$ |
| 7 | $2Al_{(cr)} + 3S_{(cr)} + 14O_{2(g)} + 16H_{2(g)} = Al_2(SO_4)_3 \cdot 16H_2O_{(cr)}$ |

Abbreviations: cr = crystalline; l = liquid; g= gas; all other species aqueous.

Table S6 Measured and calculated enthalpies (kJ/mol) for reactions in Table S5.

| |
|---|
| $\Delta H_1 = -\Delta H_{soln}(Al_2(SO_4)_3 \cdot 16H_2O_{(cr)}) = -58.66 \pm 1.48$ |
| $\Delta H_2 = \Delta H_{soln}(Al_2(SO_4)_{3(cr)}) = -232.34 \pm 0.8$[a] |
| $\Delta H_3 = 16\Delta H_{dilution}$[c]$;= -6.4$ |
| $\Delta H_4 = \Delta H_1 + \Delta H_2 + \Delta H_3 = -297.4 \pm 1.68$ |
| $\Delta H_5 = \Delta H^\circ_{f,el}(Al_2(SO_4)_{3(cr)}) = -3{,}441.8 \pm 1.3$[b] |
| $\Delta H_6 = 16\Delta H^\circ_{f,el}(H_2O_{(l)}) = -4{,}572.8 \pm 0.64$[b] |
| $\Delta H_7 = \boldsymbol{\Delta H^\circ_{f,el}}(Al_2(SO_4)_3 \cdot 16H_2O_{(cr)}) = \Delta H_4 + \Delta H_5 + \Delta H_6 + \Delta H_7 =$ **$-8{,}312.0 \pm 2.22$** |

[a](Majzlan et al., 2006)

[b](Robie, 1995)

[c]calculated (Parker et al., 1965)

Table S7. Thermodynamic cycle used to calculate $\Delta H^{\circ}_{f,el}$ at 25 °C for $Ga_2(SO_4)_3 \cdot 18H_2O_{(cr)}$

| | |
|---|---|
| 1 | $Ga_2(SO_4)_3 \cdot 18H_2O_{(cr,\ 25\ °C)} = Ga_2O_{3(soln,\ 700\ °C)} + 3SO_{3(soln,\ 700\ °C)} + 18H_2O_{(g,\ 700\ °C)}$ |
| 2 | $\beta\text{-}Ga_2O_{3\ (cr,\ 25\ °C)} = Ga_2O_{3(soln,\ 700\ °C)}$ |
| 3 | $H_2O_{(l,\ 25\ °C)} = H_2O_{(g,\ 700\ °C)}$ |
| 4 | $SO_{3(g,\ 25\ °C)} = SO_{3(soln,\ 700\ °C)}$ |
| 5 | $\beta\text{-}Ga_2O_{3(cr,\ 25\ °C)} + 18H_2O_{(l,\ 25\ °C)} + 3SO_{3(g,\ 25\ °C)} = Ga_2(SO_4)_3 \cdot 18H_2O_{(cr,\ 25\ °C)}$ |
| 6 | $2Ga_{(cr)} + 1.5O_{2(g)} = \beta\text{-}Ga_2O_{3(cr,\ 25\ °C)}$ |
| 7 | $H_{2(g)} + 0.5O_{2(g)} = H_2O_{(l,\ 25\ °C)}$ |
| 8 | $S_{(cr)} + O_{2(g)} = SO_{3(g,\ 25\ °C)}$ |
| 9 | $2Ga_{(cr)} + 3S_{(cr)} + 15O_{2(g)} + 18H_{2(g)} = Ga_2(SO_4)_3 \cdot 18H_2O_{(cr,\ 25\ °C)}$ |

Abbreviations: cr = crystalline; l = liquid; g= gas; all other species aqueous.

Table S8. Measured and calculated enthalpies (kJ/mol) for reactions in Table S7.

| |
|---|
| $\Delta H_1 = -\Delta H_{ds}(Ga_2(SO_4)_3 \cdot 18H_2O_{(cr,\ 25\ °C)}) = -1{,}445.61 \pm 22.60$ |
| $\Delta H_2 = \Delta H_{ds}(\beta\text{-}Ga_2O_{3(cr,\ 25\ °C)}) = 104.3 \pm 0.6$ |
| $\Delta H_3 = 18\Delta H_{ds}\,(H_2O_{(l,\ 25\ °C)}) = 1{,}242$[b] |
| $\Delta H_4 = 3\Delta H_{ds}\,(SO_{3(g,\ 25\ °C)}) = -651$[a] |
| $\boldsymbol{\Delta H_5 = \Delta H_{f,ox}} = \Delta H_1 + \Delta H_2 + \Delta H_3 + \Delta H_4 = -750.31 \pm 25.19$ |
| $\Delta H_6 = \Delta H^{\circ}_{f,el}(\beta\text{-}Ga_2O_{3(cr,\ 25\ °C)}) = -1{,}089.1 \pm 1.5$[§] |
| $\Delta H_7 = 18\Delta H^{\circ}_{f,el}\,(H_2O_{(l,\ 25\ °C)}) = -5{,}144.4 \pm 0.72$[§] |
| $\Delta H_8 = 3\Delta H^{\circ}_{f,el}\,(SO_{3(g,\ 25\ °C)}) = -1{,}187.55 \pm 1.14$[§] |
| $\Delta H_9 = \boldsymbol{\Delta H^{\circ}_{f,el}}(Ga_2(SO_4)_3 \cdot 18H_2O_{(cr,\ 25\ °C)}) = \Delta H_5 + \Delta H_6 + \Delta H_7 + \Delta H_8 =$ **-8,171.90 ± 25.23** |

Majzlan et al., 2006)

[b](Robie, 1995)

**Computational Results**

The converged geometries for all optimized structures are given in the following tables as Cartesian coordinates. These coordinates can be read into a molecular viewing software of your choice giving the optimized spatial arrangement. All of the clusters contain 101 atoms.

CONVERGED GEOMETRY – b3lyp/6-31G*/PCM
Coordinates (Angstroms)

Table S9. $AlAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Al | 0 | 0 | 0 |
| Al | -1.0324501 | 3.1025362 | 1.0324501 |
| Al | -3.1025362 | 1.0324501 | 1.0324501 |
| Al | 3.1025362 | 1.0324501 | -1.0324501 |
| Al | 1.0324501 | 1.0324501 | -3.1025362 |
| Al | 1.0324501 | 3.1025362 | -1.0324501 |
| Al | -1.0324501 | -3.1025362 | -1.0324501 |
| Al | -3.1025362 | -1.0324501 | -1.0324501 |
| Al | -1.0324501 | -1.0324501 | -3.1025362 |
| Al | 1.0324501 | -1.0324501 | 3.1025362 |
| Al | 3.1025362 | -1.0324501 | 1.0324501 |
| Al | 1.0324501 | -3.1025362 | 1.0324501 |
| Al | -1.0324501 | 1.0324501 | 3.1025362 |
| O | 1.0749711 | -1.0749711 | 1.0749711 |
| O | -1.0749711 | 1.0749711 | 1.0749711 |
| O | 1.0749711 | 1.0749711 | -1.0749711 |
| O | -1.0749711 | -1.0749711 | -1.0749711 |
| O | -2.8906472 | 2.8906472 | 0.8992851 |
| O | -2.8906472 | 0.8992851 | 2.8906472 |
| O | -0.8992851 | 2.8906472 | 2.8906472 |
| O | 0.8992851 | 2.8906472 | -2.8906472 |
| O | 2.8906472 | 2.8906472 | -0.8992851 |
| O | 2.8906472 | 0.8992851 | -2.8906472 |
| O | -2.8906472 | -0.8992851 | -2.8906472 |
| O | -0.8992851 | -2.8906472 | -2.8906472 |
| O | -2.8906472 | -2.8906472 | -0.8992851 |
| O | 2.8906472 | -2.8906472 | 0.8992851 |
| O | 0.8992851 | -2.8906472 | 2.8906472 |
| O | 2.8906472 | -0.8992851 | 2.8906472 |
| O | -3.2613542 | 0.8139001 | -0.8139001 |
| O | -3.2613542 | -0.8139001 | 0.8139001 |
| O | -0.8139001 | 0.8139001 | -3.2613542 |
| O | 0.8139001 | -0.8139001 | -3.2613542 |
| O | -0.8139001 | 3.2613542 | -0.8139001 |
| O | 0.8139001 | 3.2613542 | 0.8139001 |
| O | 0.8139001 | 0.8139001 | 3.2613542 |

| | | | |
|---|---|---|---|
| O | -0.8139001 | -0.8139001 | 3.2613542 |
| O | -0.8139001 | -3.2613542 | 0.8139001 |
| O | 0.8139001 | -3.2613542 | -0.8139001 |
| O | 3.2613542 | -0.8139001 | -0.8139001 |
| O | 3.2613542 | 0.8139001 | 0.8139001 |
| O | -1.3235411 | 1.3235411 | 5.0703654 |
| O | -1.3235411 | 5.0703654 | 1.3235411 |
| O | -5.0703654 | 1.3235411 | 1.3235411 |
| O | 5.0703654 | 1.3235411 | -1.3235411 |
| O | 1.3235411 | 1.3235411 | -5.0703654 |
| O | 1.3235411 | 5.0703654 | -1.3235411 |
| O | -1.3235411 | -5.0703654 | -1.3235411 |
| O | -5.0703654 | -1.3235411 | -1.3235411 |
| O | -1.3235411 | -1.3235411 | -5.0703654 |
| O | 1.3235411 | -1.3235411 | 5.0703654 |
| O | 5.0703654 | -1.3235411 | 1.3235411 |
| O | 1.3235411 | -5.0703654 | 1.3235411 |
| H | -3.4757993 | 3.4757993 | 1.4035041 |
| H | -3.4757993 | 1.4035041 | 3.4757993 |
| H | -1.4035041 | 3.4757993 | 3.4757993 |
| H | 1.4035041 | 3.4757993 | -3.4757993 |
| H | 3.4757993 | 3.4757993 | -1.4035041 |
| H | 3.4757993 | 1.4035041 | -3.4757993 |
| H | -3.4757993 | -1.4035041 | -3.4757993 |
| H | -1.4035041 | -3.4757993 | -3.4757993 |
| H | -3.4757993 | -3.4757993 | -1.4035041 |
| H | 3.4757993 | -3.4757993 | 1.4035041 |
| H | 1.4035041 | -3.4757993 | 3.4757993 |
| H | 3.4757993 | -1.4035041 | 3.4757993 |
| H | -3.3700753 | 1.4905121 | -1.4905121 |
| H | -3.3700753 | -1.4905121 | 1.4905121 |
| H | 1.4905121 | -1.4905121 | -3.3700753 |
| H | -1.4905121 | 1.4905121 | -3.3700753 |
| H | -1.4905121 | 3.3700753 | -1.4905121 |
| H | 1.4905121 | 3.3700753 | 1.4905121 |
| H | 1.4905121 | 1.4905121 | 3.3700753 |
| H | -1.4905121 | -1.4905121 | 3.3700753 |
| H | -1.4905121 | -3.3700753 | 1.4905121 |
| H | 1.4905121 | -3.3700753 | -1.4905121 |
| H | 3.3700753 | -1.4905121 | -1.4905121 |
| H | 3.3700753 | 1.4905121 | 1.4905121 |
| H | -1.6511372 | 0.549115 | 5.5633424 |
| H | -0.549115 | 1.6511372 | 5.5633424 |
| H | -0.549115 | 5.5633424 | 1.6511372 |
| H | -1.6511372 | 5.5633424 | 0.549115 |
| H | -5.5633424 | 1.6511372 | 0.549115 |
| H | -5.5633424 | 0.549115 | 1.6511372 |

| | | | |
|---|---|---|---|
| H | 5.5633424 | 1.6511372 | -0.549115 |
| H | 5.5633424 | 0.549115 | -1.6511372 |
| H | 1.6511372 | 0.549115 | -5.5633424 |
| H | 0.549115 | 1.6511372 | -5.5633424 |
| H | 0.549115 | 5.5633424 | -1.6511372 |
| H | 1.6511372 | 5.5633424 | -0.549115 |
| H | -0.549115 | -5.5633424 | -1.6511372 |
| H | -1.6511372 | -5.5633424 | -0.549115 |
| H | -5.5633424 | -1.6511372 | -0.549115 |
| H | -5.5633424 | -0.549115 | -1.6511372 |
| H | -1.6511372 | -0.549115 | -5.5633424 |
| H | -0.549115 | -1.6511372 | -5.5633424 |
| H | 1.6511372 | -0.549115 | 5.5633424 |
| H | 0.549115 | -1.6511372 | 5.5633424 |
| H | 5.5633424 | -1.6511372 | 0.549115 |
| H | 5.5633424 | -0.549115 | 1.6511372 |
| H | 0.549115 | -5.5633424 | 1.6511372 |
| H | 1.6511372 | -5.5633424 | 0.549115 |

Table S10. $GaAl_{12}$

| Symbol | X | Y | Z |
|---|---|---|---|
| Ga | 0 | 0 | 0 |
| Al | -1.0372542 | 1.0372542 | 3.1090047 |
| Al | -1.0372542 | 3.1090047 | 1.0372542 |
| Al | -3.1090047 | 1.0372542 | 1.0372542 |
| Al | 3.1090047 | 1.0372542 | -1.0372542 |
| Al | 1.0372542 | 1.0372542 | -3.1090047 |
| Al | 1.0372542 | 3.1090047 | -1.0372542 |
| Al | -1.0372542 | -3.1090047 | -1.0372542 |
| Al | -3.1090047 | -1.0372542 | -1.0372542 |
| Al | -1.0372542 | -1.0372542 | -3.1090047 |
| Al | 1.0372542 | -1.0372542 | 3.1090047 |
| Al | 3.1090047 | -1.0372542 | 1.0372542 |
| Al | 1.0372542 | -3.1090047 | 1.0372542 |
| O | 1.1076388 | -1.1076388 | 1.1076388 |
| O | -1.1076388 | 1.1076388 | 1.1076388 |
| O | 1.1076388 | 1.1076388 | -1.1076388 |
| O | -1.1076388 | -1.1076388 | -1.1076388 |
| O | -2.8999907 | 2.8999907 | 0.9006672 |
| O | -2.8999907 | 0.9006672 | 2.8999907 |
| O | -0.9006672 | 2.8999907 | 2.8999907 |
| O | 0.9006672 | 2.8999907 | -2.8999907 |
| O | 2.8999907 | 2.8999907 | -0.9006672 |
| O | 2.8999907 | 0.9006672 | -2.8999907 |
| O | -2.8999907 | -0.9006672 | -2.8999907 |
| O | -0.9006672 | -2.8999907 | -2.8999907 |

| | | | |
|---|---|---|---|
| O | -2.8999907 | -2.8999907 | -0.9006672 |
| O | 2.8999907 | -2.8999907 | 0.9006672 |
| O | 0.9006672 | -2.8999907 | 2.8999907 |
| O | 2.8999907 | -0.9006672 | 2.8999907 |
| O | -3.2485602 | 0.8136597 | -0.8136597 |
| O | -3.2485602 | -0.8136597 | 0.8136597 |
| O | -0.8136597 | 0.8136597 | -3.2485602 |
| O | 0.8136597 | -0.8136597 | -3.2485602 |
| O | -0.8136597 | 3.2485602 | -0.8136597 |
| O | 0.8136597 | 3.2485602 | 0.8136597 |
| O | 0.8136597 | 0.8136597 | 3.2485602 |
| O | -0.8136597 | -0.8136597 | 3.2485602 |
| O | -0.8136597 | -3.2485602 | 0.8136597 |
| O | 0.8136597 | -3.2485602 | -0.8136597 |
| O | 3.2485602 | -0.8136597 | -0.8136597 |
| O | 3.2485602 | 0.8136597 | 0.8136597 |
| O | -1.3204491 | 1.3204491 | 5.0757062 |
| O | -1.3204491 | 5.0757062 | 1.3204491 |
| O | -5.0757062 | 1.3204491 | 1.3204491 |
| O | 5.0757062 | 1.3204491 | -1.3204491 |
| O | 1.3204491 | 1.3204491 | -5.0757062 |
| O | 1.3204491 | 5.0757062 | -1.3204491 |
| O | -1.3204491 | -5.0757062 | -1.3204491 |
| O | -5.0757062 | -1.3204491 | -1.3204491 |
| O | -1.3204491 | -1.3204491 | -5.0757062 |
| O | 1.3204491 | -1.3204491 | 5.0757062 |
| O | 5.0757062 | -1.3204491 | 1.3204491 |
| O | 1.3204491 | -5.0757062 | 1.3204491 |
| H | -3.4885853 | 3.4885853 | 1.3966398 |
| H | -3.4885853 | 1.3966398 | 3.4885853 |
| H | -1.3966398 | 3.4885853 | 3.4885853 |
| H | 1.3966398 | 3.4885853 | -3.4885853 |
| H | 3.4885853 | 3.4885853 | -1.3966398 |
| H | 3.4885853 | 1.3966398 | -3.4885853 |
| H | -3.4885853 | -1.3966398 | -3.4885853 |
| H | -1.3966398 | -3.4885853 | -3.4885853 |
| H | -3.4885853 | -3.4885853 | -1.3966398 |
| H | 3.4885853 | -3.4885853 | 1.3966398 |
| H | 1.3966398 | -3.4885853 | 3.4885853 |
| H | 3.4885853 | -1.3966398 | 3.4885853 |
| H | -3.3666744 | 1.4893449 | -1.4893449 |
| H | -3.3666744 | -1.4893449 | 1.4893449 |
| H | 1.4893449 | -1.4893449 | -3.3666744 |
| H | -1.4893449 | 1.4893449 | -3.3666744 |
| H | -1.4893449 | 3.3666744 | -1.4893449 |
| H | 1.4893449 | 3.3666744 | 1.4893449 |
| H | 1.4893449 | 1.4893449 | 3.3666744 |

| | | | |
|---|---|---|---|
| H | -1.4893449 | -1.4893449 | 3.3666744 |
| H | -1.4893449 | -3.3666744 | 1.4893449 |
| H | 1.4893449 | -3.3666744 | -1.4893449 |
| H | 3.3666744 | -1.4893449 | -1.4893449 |
| H | 3.3666744 | 1.4893449 | 1.4893449 |
| H | -1.6501667 | 0.5478274 | 5.5700977 |
| H | -0.5478274 | 1.6501667 | 5.5700977 |
| H | -0.5478274 | 5.5700977 | 1.6501667 |
| H | -1.6501667 | 5.5700977 | 0.5478274 |
| H | -5.5700977 | 1.6501667 | 0.5478274 |
| H | -5.5700977 | 0.5478274 | 1.6501667 |
| H | 5.5700977 | 1.6501667 | -0.5478274 |
| H | 5.5700977 | 0.5478274 | -1.6501667 |
| H | 1.6501667 | 0.5478274 | -5.5700977 |
| H | 0.5478274 | 1.6501667 | -5.5700977 |
| H | 0.5478274 | 5.5700977 | -1.6501667 |
| H | 1.6501667 | 5.5700977 | -0.5478274 |
| H | -0.5478274 | -5.5700977 | -1.6501667 |
| H | -1.6501667 | -5.5700977 | -0.5478274 |
| H | -5.5700977 | -1.6501667 | -0.5478274 |
| H | -5.5700977 | -0.5478274 | -1.6501667 |
| H | -1.6501667 | -0.5478274 | -5.5700977 |
| H | -0.5478274 | -1.6501667 | -5.5700977 |
| H | 1.6501667 | -0.5478274 | 5.5700977 |
| H | 0.5478274 | -1.6501667 | 5.5700977 |
| H | 5.5700977 | -1.6501667 | 0.5478274 |
| H | 5.5700977 | -0.5478274 | 1.6501667 |
| H | 0.5478274 | -5.5700977 | 1.6501667 |
| H | 1.6501667 | -5.5700977 | 0.5478274 |

Table S11. $GeAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Ge | 0 | 0 | 0 |
| Al | -1.0285634 | 1.0285634 | 3.1451547 |
| Al | -1.0285634 | 3.1451547 | 1.0285634 |
| Al | -3.1451547 | 1.0285634 | 1.0285634 |
| Al | 3.1451547 | 1.0285634 | -1.0285634 |
| Al | 1.0285634 | 1.0285634 | -3.1451547 |
| Al | 1.0285634 | 3.1451547 | -1.0285634 |
| Al | -1.0285634 | -3.1451547 | -1.0285634 |
| Al | -3.1451547 | -1.0285634 | -1.0285634 |
| Al | -1.0285634 | -1.0285634 | -3.1451547 |
| Al | 1.0285634 | -1.0285634 | 3.1451547 |
| Al | 3.1451547 | -1.0285634 | 1.0285634 |
| Al | 1.0285634 | -3.1451547 | 1.0285634 |
| O | 1.0506763 | -1.0506763 | 1.0506763 |
| O | -1.0506763 | 1.0506763 | 1.0506763 |

| | | | |
|---|---|---|---|
| O | 1.0506763 | 1.0506763 | -1.0506763 |
| O | -1.0506763 | -1.0506763 | -1.0506763 |
| O | -2.8743786 | 2.8743786 | 0.904454 |
| O | -2.8743786 | 0.904454 | 2.8743786 |
| O | -0.904454 | 2.8743786 | 2.8743786 |
| O | 0.904454 | 2.8743786 | -2.8743786 |
| O | 2.8743786 | 2.8743786 | -0.904454 |
| O | 2.8743786 | 0.904454 | -2.8743786 |
| O | -2.8743786 | -0.904454 | -2.8743786 |
| O | -0.904454 | -2.8743786 | -2.8743786 |
| O | -2.8743786 | -2.8743786 | -0.904454 |
| O | 2.8743786 | -2.8743786 | 0.904454 |
| O | 0.904454 | -2.8743786 | 2.8743786 |
| O | 2.8743786 | -0.904454 | 2.8743786 |
| O | -3.2152665 | 0.8177386 | -0.8177386 |
| O | -3.2152665 | -0.8177386 | 0.8177386 |
| O | -0.8177386 | 0.8177386 | -3.2152665 |
| O | 0.8177386 | -0.8177386 | -3.2152665 |
| O | -0.8177386 | 3.2152665 | -0.8177386 |
| O | 0.8177386 | 3.2152665 | 0.8177386 |
| O | 0.8177386 | 0.8177386 | 3.2152665 |
| O | -0.8177386 | -0.8177386 | 3.2152665 |
| O | -0.8177386 | -3.2152665 | 0.8177386 |
| O | 0.8177386 | -3.2152665 | -0.8177386 |
| O | 3.2152665 | -0.8177386 | -0.8177386 |
| O | 3.2152665 | 0.8177386 | 0.8177386 |
| O | -1.3198574 | 1.3198574 | 5.0753345 |
| O | -1.3198574 | 5.0753345 | 1.3198574 |
| O | -5.0753345 | 1.3198574 | 1.3198574 |
| O | 5.0753345 | 1.3198574 | -1.3198574 |
| O | 1.3198574 | 1.3198574 | -5.0753345 |
| O | 1.3198574 | 5.0753345 | -1.3198574 |
| O | -1.3198574 | -5.0753345 | -1.3198574 |
| O | -5.0753345 | -1.3198574 | -1.3198574 |
| O | -1.3198574 | -1.3198574 | -5.0753345 |
| O | 1.3198574 | -1.3198574 | 5.0753345 |
| O | 5.0753345 | -1.3198574 | 1.3198574 |
| O | 1.3198574 | -5.0753345 | 1.3198574 |
| H | -3.4620453 | 3.4620453 | 1.4053557 |
| H | -3.4620453 | 1.4053557 | 3.4620453 |
| H | -1.4053557 | 3.4620453 | 3.4620453 |
| H | 1.4053557 | 3.4620453 | -3.4620453 |
| H | 3.4620453 | 3.4620453 | -1.4053557 |
| H | 3.4620453 | 1.4053557 | -3.4620453 |
| H | -3.4620453 | -1.4053557 | -3.4620453 |
| H | -1.4053557 | -3.4620453 | -3.4620453 |
| H | -3.4620453 | -3.4620453 | -1.4053557 |

| | | | |
|---|---|---|---|
| H | 3.4620453 | -3.4620453 | 1.4053557 |
| H | 1.4053557 | -3.4620453 | 3.4620453 |
| H | 3.4620453 | -1.4053557 | 3.4620453 |
| H | -3.3779875 | 1.4897762 | -1.4897762 |
| H | -3.3779875 | -1.4897762 | 1.4897762 |
| H | 1.4897762 | -1.4897762 | -3.3779875 |
| H | -1.4897762 | 1.4897762 | -3.3779875 |
| H | -1.4897762 | 3.3779875 | -1.4897762 |
| H | 1.4897762 | 3.3779875 | 1.4897762 |
| H | 1.4897762 | 1.4897762 | 3.3779875 |
| H | -1.4897762 | -1.4897762 | 3.3779875 |
| H | -1.4897762 | -3.3779875 | 1.4897762 |
| H | 1.4897762 | -3.3779875 | -1.4897762 |
| H | 3.3779875 | -1.4897762 | -1.4897762 |
| H | 3.3779875 | 1.4897762 | 1.4897762 |
| H | -1.7002043 | 0.5924856 | 5.6012053 |
| H | -0.5924856 | 1.7002043 | 5.6012053 |
| H | -0.5924856 | 5.6012053 | 1.7002043 |
| H | -1.7002043 | 5.6012053 | 0.5924856 |
| H | -5.6012053 | 1.7002043 | 0.5924856 |
| H | -5.6012053 | 0.5924856 | 1.7002043 |
| H | 5.6012053 | 1.7002043 | -0.5924856 |
| H | 5.6012053 | 0.5924856 | -1.7002043 |
| H | 1.7002043 | 0.5924856 | -5.6012053 |
| H | 0.5924856 | 1.7002043 | -5.6012053 |
| H | 0.5924856 | 5.6012053 | -1.7002043 |
| H | 1.7002043 | 5.6012053 | -0.5924856 |
| H | -0.5924856 | -5.6012053 | -1.7002043 |
| H | -1.7002043 | -5.6012053 | -0.5924856 |
| H | -5.6012053 | -1.7002043 | -0.5924856 |
| H | -5.6012053 | -0.5924856 | -1.7002043 |
| H | -1.7002043 | -0.5924856 | -5.6012053 |
| H | -0.5924856 | -1.7002043 | -5.6012053 |
| H | 1.7002043 | -0.5924856 | 5.6012053 |
| H | 0.5924856 | -1.7002043 | 5.6012053 |
| H | 5.6012053 | -1.7002043 | 0.5924856 |
| H | 5.6012053 | -0.5924856 | 1.7002043 |
| H | 0.5924856 | -5.6012053 | 1.7002043 |
| H | 1.7002043 | -5.6012053 | 0.5924856 |

Table S12. $BeAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Be | 0 | 0 | 0 |
| Al | -1.0206141 | 1.0206141 | 3.0475395 |
| Al | -1.0206141 | 3.0475395 | 1.0206141 |
| Al | -3.0475395 | 1.0206141 | 1.0206141 |
| Al | 3.0475395 | 1.0206141 | -1.0206141 |

| | | | |
|---|---|---|---|
| Al | 1.0206141 | 1.0206141 | -3.0475395 |
| Al | 1.0206141 | 3.0475395 | -1.0206141 |
| Al | -1.0206141 | -3.0475395 | -1.0206141 |
| Al | -3.0475395 | -1.0206141 | -1.0206141 |
| Al | -1.0206141 | -1.0206141 | -3.0475395 |
| Al | 1.0206141 | -1.0206141 | 3.0475395 |
| Al | 3.0475395 | -1.0206141 | 1.0206141 |
| Al | 1.0206141 | -3.0475395 | 1.0206141 |
| O | 1.0582854 | -1.0582854 | 1.0582854 |
| O | -1.0582854 | 1.0582854 | 1.0582854 |
| O | 1.0582854 | 1.0582854 | -1.0582854 |
| O | -1.0582854 | -1.0582854 | -1.0582854 |
| O | -2.8845656 | 2.8845656 | 0.8847827 |
| O | -2.8845656 | 0.8847827 | 2.8845656 |
| O | -0.8847827 | 2.8845656 | 2.8845656 |
| O | 0.8847827 | 2.8845656 | -2.8845656 |
| O | 2.8845656 | 2.8845656 | -0.8847827 |
| O | 2.8845656 | 0.8847827 | -2.8845656 |
| O | -2.8845656 | -0.8847827 | -2.8845656 |
| O | -0.8847827 | -2.8845656 | -2.8845656 |
| O | -2.8845656 | -2.8845656 | -0.8847827 |
| O | 2.8845656 | -2.8845656 | 0.8847827 |
| O | 0.8847827 | -2.8845656 | 2.8845656 |
| O | 2.8845656 | -0.8847827 | 2.8845656 |
| O | -3.316774 | 0.8146948 | -0.8146948 |
| O | -3.316774 | -0.8146948 | 0.8146948 |
| O | -0.8146948 | 0.8146948 | -3.316774 |
| O | 0.8146948 | -0.8146948 | -3.316774 |
| O | -0.8146948 | 3.316774 | -0.8146948 |
| O | 0.8146948 | 3.316774 | 0.8146948 |
| O | 0.8146948 | 0.8146948 | 3.316774 |
| O | -0.8146948 | -0.8146948 | 3.316774 |
| O | -0.8146948 | -3.316774 | 0.8146948 |
| O | 0.8146948 | -3.316774 | -0.8146948 |
| O | 3.316774 | -0.8146948 | -0.8146948 |
| O | 3.316774 | 0.8146948 | 0.8146948 |
| O | -1.3413498 | 1.3413498 | 5.0463233 |
| O | -1.3413498 | 5.0463233 | 1.3413498 |
| O | -5.0463233 | 1.3413498 | 1.3413498 |
| O | 5.0463233 | 1.3413498 | -1.3413498 |
| O | 1.3413498 | 1.3413498 | -5.0463233 |
| O | 1.3413498 | 5.0463233 | -1.3413498 |
| O | -1.3413498 | -5.0463233 | -1.3413498 |
| O | -5.0463233 | -1.3413498 | -1.3413498 |
| O | -1.3413498 | -1.3413498 | -5.0463233 |
| O | 1.3413498 | -1.3413498 | 5.0463233 |
| O | 5.0463233 | -1.3413498 | 1.3413498 |

| | | | |
|---|---|---|---|
| O | 1.3413498 | -5.0463233 | 1.3413498 |
| H | -3.4591202 | 3.4591202 | 1.4113379 |
| H | -3.4591202 | 1.4113379 | 3.4591202 |
| H | -1.4113379 | 3.4591202 | 3.4591202 |
| H | 1.4113379 | 3.4591202 | -3.4591202 |
| H | 3.4591202 | 3.4591202 | -1.4113379 |
| H | 3.4591202 | 1.4113379 | -3.4591202 |
| H | -3.4591202 | -1.4113379 | -3.4591202 |
| H | -1.4113379 | -3.4591202 | -3.4591202 |
| H | -3.4591202 | -3.4591202 | -1.4113379 |
| H | 3.4591202 | -3.4591202 | 1.4113379 |
| H | 1.4113379 | -3.4591202 | 3.4591202 |
| H | 3.4591202 | -1.4113379 | 3.4591202 |
| H | -3.3286971 | 1.494625 | -1.494625 |
| H | -3.3286971 | -1.494625 | 1.494625 |
| H | 1.494625 | -1.494625 | -3.3286971 |
| H | -1.494625 | 1.494625 | -3.3286971 |
| H | -1.494625 | 3.3286971 | -1.494625 |
| H | 1.494625 | 3.3286971 | 1.494625 |
| H | 1.494625 | 1.494625 | 3.3286971 |
| H | -1.494625 | -1.494625 | 3.3286971 |
| H | -1.494625 | -3.3286971 | 1.494625 |
| H | 1.494625 | -3.3286971 | -1.494625 |
| H | 3.3286971 | -1.494625 | -1.494625 |
| H | 3.3286971 | 1.494625 | 1.494625 |
| H | -1.6438886 | 0.5450177 | 5.518588 |
| H | -0.5450177 | 1.6438886 | 5.518588 |
| H | -0.5450177 | 5.518588 | 1.6438886 |
| H | -1.6438886 | 5.518588 | 0.5450177 |
| H | -5.518588 | 1.6438886 | 0.5450177 |
| H | -5.518588 | 0.5450177 | 1.6438886 |
| H | 5.518588 | 1.6438886 | -0.5450177 |
| H | 5.518588 | 0.5450177 | -1.6438886 |
| H | 1.6438886 | 0.5450177 | -5.518588 |
| H | 0.5450177 | 1.6438886 | -5.518588 |
| H | 0.5450177 | 5.518588 | -1.6438886 |
| H | 1.6438886 | 5.518588 | -0.5450177 |
| H | -0.5450177 | -5.518588 | -1.6438886 |
| H | -1.6438886 | -5.518588 | -0.5450177 |
| H | -5.518588 | -1.6438886 | -0.5450177 |
| H | -5.518588 | -0.5450177 | -1.6438886 |
| H | -1.6438886 | -0.5450177 | -5.518588 |
| H | -0.5450177 | -1.6438886 | -5.518588 |
| H | 1.6438886 | -0.5450177 | 5.518588 |
| H | 0.5450177 | -1.6438886 | 5.518588 |
| H | 5.518588 | -1.6438886 | 0.5450177 |
| H | 5.518588 | -0.5450177 | 1.6438886 |

| | | | |
|---|---|---|---|
| H | 0.5450177 | -5.518588 | 1.6438886 |
| H | 1.6438886 | -5.518588 | 0.5450177 |

Table S13. $MgAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Mg | 0 | 0 | 0 |
| Al | -1.0537803 | 1.0537803 | 3.0921344 |
| Al | -1.0537803 | 3.0921344 | 1.0537803 |
| Al | -3.0921344 | 1.0537803 | 1.0537803 |
| Al | 3.0921344 | 1.0537803 | -1.0537803 |
| Al | 1.0537803 | 1.0537803 | -3.0921344 |
| Al | 1.0537803 | 3.0921344 | -1.0537803 |
| Al | -1.0537803 | -3.0921344 | -1.0537803 |
| Al | -3.0921344 | -1.0537803 | -1.0537803 |
| Al | -1.0537803 | -1.0537803 | -3.0921344 |
| Al | 1.0537803 | -1.0537803 | 3.0921344 |
| Al | 3.0921344 | -1.0537803 | 1.0537803 |
| Al | 1.0537803 | -3.0921344 | 1.0537803 |
| O | 1.1714806 | -1.1714806 | 1.1714806 |
| O | -1.1714806 | 1.1714806 | 1.1714806 |
| O | 1.1714806 | 1.1714806 | -1.1714806 |
| O | -1.1714806 | -1.1714806 | -1.1714806 |
| O | -2.9376467 | 2.9376467 | 0.8986858 |
| O | -2.9376467 | 0.8986858 | 2.9376467 |
| O | -0.8986858 | 2.9376467 | 2.9376467 |
| O | 0.8986858 | 2.9376467 | -2.9376467 |
| O | 2.9376467 | 2.9376467 | -0.8986858 |
| O | 2.9376467 | 0.8986858 | -2.9376467 |
| O | -2.9376467 | -0.8986858 | -2.9376467 |
| O | -0.8986858 | -2.9376467 | -2.9376467 |
| O | -2.9376467 | -2.9376467 | -0.8986858 |
| O | 2.9376467 | -2.9376467 | 0.8986858 |
| O | 0.8986858 | -2.9376467 | 2.9376467 |
| O | 2.9376467 | -0.8986858 | 2.9376467 |
| O | -3.3069157 | 0.8072054 | -0.8072054 |
| O | -3.3069157 | -0.8072054 | 0.8072054 |
| O | -0.8072054 | 0.8072054 | -3.3069157 |
| O | 0.8072054 | -0.8072054 | -3.3069157 |
| O | -0.8072054 | 3.3069157 | -0.8072054 |
| O | 0.8072054 | 3.3069157 | 0.8072054 |
| O | 0.8072054 | 0.8072054 | 3.3069157 |
| O | -0.8072054 | -0.8072054 | 3.3069157 |
| O | -0.8072054 | -3.3069157 | 0.8072054 |
| O | 0.8072054 | -3.3069157 | -0.8072054 |

| | | | |
|---|---|---|---|
| O | 3.3069157 | -0.8072054 | -0.8072054 |
| O | 3.3069157 | 0.8072054 | 0.8072054 |
| O | -1.3424269 | 1.3424269 | 5.0849814 |
| O | -1.3424269 | 5.0849814 | 1.3424269 |
| O | -5.0849814 | 1.3424269 | 1.3424269 |
| O | 5.0849814 | 1.3424269 | -1.3424269 |
| O | 1.3424269 | 1.3424269 | -5.0849814 |
| O | 1.3424269 | 5.0849814 | -1.3424269 |
| O | -1.3424269 | -5.0849814 | -1.3424269 |
| O | -5.0849814 | -1.3424269 | -1.3424269 |
| O | -1.3424269 | -1.3424269 | -5.0849814 |
| O | 1.3424269 | -1.3424269 | 5.0849814 |
| O | 5.0849814 | -1.3424269 | 1.3424269 |
| O | 1.3424269 | -5.0849814 | 1.3424269 |
| H | -3.5254471 | 3.5254471 | 1.3945709 |
| H | -3.5254471 | 1.3945709 | 3.5254471 |
| H | -1.3945709 | 3.5254471 | 3.5254471 |
| H | 1.3945709 | 3.5254471 | -3.5254471 |
| H | 3.5254471 | 3.5254471 | -1.3945709 |
| H | 3.5254471 | 1.3945709 | -3.5254471 |
| H | -3.5254471 | -1.3945709 | -3.5254471 |
| H | -1.3945709 | -3.5254471 | -3.5254471 |
| H | -3.5254471 | -3.5254471 | -1.3945709 |
| H | 3.5254471 | -3.5254471 | 1.3945709 |
| H | 1.3945709 | -3.5254471 | 3.5254471 |
| H | 3.5254471 | -1.3945709 | 3.5254471 |
| H | -3.3468817 | 1.4873626 | -1.4873626 |
| H | -3.3468817 | -1.4873626 | 1.4873626 |
| H | 1.4873626 | -1.4873626 | -3.3468817 |
| H | -1.4873626 | 1.4873626 | -3.3468817 |
| H | -1.4873626 | 3.3468817 | -1.4873626 |
| H | 1.4873626 | 3.3468817 | 1.4873626 |
| H | 1.4873626 | 1.4873626 | 3.3468817 |
| H | -1.4873626 | -1.4873626 | 3.3468817 |
| H | -1.4873626 | -3.3468817 | 1.4873626 |
| H | 1.4873626 | -3.3468817 | -1.4873626 |
| H | 3.3468817 | -1.4873626 | -1.4873626 |
| H | 3.3468817 | 1.4873626 | 1.4873626 |
| H | -1.6424915 | 0.5426649 | 5.5530987 |
| H | -0.5426649 | 1.6424915 | 5.5530987 |
| H | -0.5426649 | 5.5530987 | 1.6424915 |
| H | -1.6424915 | 5.5530987 | 0.5426649 |
| H | -5.5530987 | 1.6424915 | 0.5426649 |
| H | -5.5530987 | 0.5426649 | 1.6424915 |
| H | 5.5530987 | 1.6424915 | -0.5426649 |
| H | 5.5530987 | 0.5426649 | -1.6424915 |
| H | 1.6424915 | 0.5426649 | -5.5530987 |

| | | | |
|---|---|---|---|
| H | 0.5426649 | 1.6424915 | -5.5530987 |
| H | 0.5426649 | 5.5530987 | -1.6424915 |
| H | 1.6424915 | 5.5530987 | -0.5426649 |
| H | -0.5426649 | -5.5530987 | -1.6424915 |
| H | -1.6424915 | -5.5530987 | -0.5426649 |
| H | -5.5530987 | -1.6424915 | -0.5426649 |
| H | -5.5530987 | -0.5426649 | -1.6424915 |
| H | -1.6424915 | -0.5426649 | -5.5530987 |
| H | -0.5426649 | -1.6424915 | -5.5530987 |
| H | 1.6424915 | -0.5426649 | 5.5530987 |
| H | 0.5426649 | -1.6424915 | 5.5530987 |
| H | 5.5530987 | -1.6424915 | 0.5426649 |
| H | 5.5530987 | -0.5426649 | 1.6424915 |
| H | 0.5426649 | -5.5530987 | 1.6424915 |
| H | 1.6424915 | -5.5530987 | 0.5426649 |

Table S14. $ZnAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Zn | 0 | 0 | 0 |
| Al | -1.0562965 | 1.0562965 | 3.0983099 |
| Al | -1.0562965 | 3.0983099 | 1.0562965 |
| Al | -3.0983099 | 1.0562965 | 1.0562965 |
| Al | 3.0983099 | 1.0562965 | -1.0562965 |
| Al | 1.0562965 | 1.0562965 | -3.0983099 |
| Al | 1.0562965 | 3.0983099 | -1.0562965 |
| Al | -1.0562965 | -3.0983099 | -1.0562965 |
| Al | -3.0983099 | -1.0562965 | -1.0562965 |
| Al | -1.0562965 | -1.0562965 | -3.0983099 |
| Al | 1.0562965 | -1.0562965 | 3.0983099 |
| Al | 3.0983099 | -1.0562965 | 1.0562965 |
| Al | 1.0562965 | -3.0983099 | 1.0562965 |
| O | 1.1861481 | -1.1861481 | 1.1861481 |
| O | -1.1861481 | 1.1861481 | 1.1861481 |
| O | 1.1861481 | 1.1861481 | -1.1861481 |
| O | -1.1861481 | -1.1861481 | -1.1861481 |
| O | -2.9433119 | 2.9433119 | 0.8994477 |
| O | -2.9433119 | 0.8994477 | 2.9433119 |
| O | -0.8994477 | 2.9433119 | 2.9433119 |
| O | 0.8994477 | 2.9433119 | -2.9433119 |
| O | 2.9433119 | 2.9433119 | -0.8994477 |
| O | 2.9433119 | 0.8994477 | -2.9433119 |
| O | -2.9433119 | -0.8994477 | -2.9433119 |
| O | -0.8994477 | -2.9433119 | -2.9433119 |
| O | -2.9433119 | -2.9433119 | -0.8994477 |
| O | 2.9433119 | -2.9433119 | 0.8994477 |
| O | 0.8994477 | -2.9433119 | 2.9433119 |
| O | 2.9433119 | -0.8994477 | 2.9433119 |
| O | -3.3045424 | 0.8069305 | -0.8069305 |

| | | | |
|---|---|---|---|
| O | -3.3045424 | -0.8069305 | 0.8069305 |
| O | -0.8069305 | 0.8069305 | -3.3045424 |
| O | 0.8069305 | -0.8069305 | -3.3045424 |
| O | -0.8069305 | 3.3045424 | -0.8069305 |
| O | 0.8069305 | 3.3045424 | 0.8069305 |
| O | 0.8069305 | 0.8069305 | 3.3045424 |
| O | -0.8069305 | -0.8069305 | 3.3045424 |
| O | -0.8069305 | -3.3045424 | 0.8069305 |
| O | 0.8069305 | -3.3045424 | -0.8069305 |
| O | 3.3045424 | -0.8069305 | -0.8069305 |
| O | 3.3045424 | 0.8069305 | 0.8069305 |
| O | -1.3427138 | 1.3427138 | 5.0896084 |
| O | -1.3427138 | 5.0896084 | 1.3427138 |
| O | -5.0896084 | 1.3427138 | 1.3427138 |
| O | 5.0896084 | 1.3427138 | -1.3427138 |
| O | 1.3427138 | 1.3427138 | -5.0896084 |
| O | 1.3427138 | 5.0896084 | -1.3427138 |
| O | -1.3427138 | -5.0896084 | -1.3427138 |
| O | -5.0896084 | -1.3427138 | -1.3427138 |
| O | -1.3427138 | -1.3427138 | -5.0896084 |
| O | 1.3427138 | -1.3427138 | 5.0896084 |
| O | 5.0896084 | -1.3427138 | 1.3427138 |
| O | 1.3427138 | -5.0896084 | 1.3427138 |
| H | -3.5309134 | 3.5309134 | 1.3961479 |
| H | -3.5309134 | 1.3961479 | 3.5309134 |
| H | -1.3961479 | 3.5309134 | 3.5309134 |
| H | 1.3961479 | 3.5309134 | -3.5309134 |
| H | 3.5309134 | 3.5309134 | -1.3961479 |
| H | 3.5309134 | 1.3961479 | -3.5309134 |
| H | -3.5309134 | -1.3961479 | -3.5309134 |
| H | -1.3961479 | -3.5309134 | -3.5309134 |
| H | -3.5309134 | -3.5309134 | -1.3961479 |
| H | 3.5309134 | -3.5309134 | 1.3961479 |
| H | 1.3961479 | -3.5309134 | 3.5309134 |
| H | 3.5309134 | -1.3961479 | 3.5309134 |
| H | -3.3512364 | 1.4870398 | -1.4870398 |
| H | -3.3512364 | -1.4870398 | 1.4870398 |
| H | 1.4870398 | -1.4870398 | -3.3512364 |
| H | -1.4870398 | 1.4870398 | -3.3512364 |
| H | -1.4870398 | 3.3512364 | -1.4870398 |
| H | 1.4870398 | 3.3512364 | 1.4870398 |
| H | 1.4870398 | 1.4870398 | 3.3512364 |
| H | -1.4870398 | -1.4870398 | 3.3512364 |
| H | -1.4870398 | -3.3512364 | 1.4870398 |
| H | 1.4870398 | -3.3512364 | -1.4870398 |
| H | 3.3512364 | -1.4870398 | -1.4870398 |
| H | 3.3512364 | 1.4870398 | 1.4870398 |

| | | | |
|---|---|---|---|
| H | -1.6422181 | 0.5415933 | 5.5566736 |
| H | -0.5415933 | 1.6422181 | 5.5566736 |
| H | -0.5415933 | 5.5566736 | 1.6422181 |
| H | -1.6422181 | 5.5566736 | 0.5415933 |
| H | -5.5566736 | 1.6422181 | 0.5415933 |
| H | -5.5566736 | 0.5415933 | 1.6422181 |
| H | 5.5566736 | 1.6422181 | -0.5415933 |
| H | 5.5566736 | 0.5415933 | -1.6422181 |
| H | 1.6422181 | 0.5415933 | -5.5566736 |
| H | 0.5415933 | 1.6422181 | -5.5566736 |
| H | 0.5415933 | 5.5566736 | -1.6422181 |
| H | 1.6422181 | 5.5566736 | -0.5415933 |
| H | -0.5415933 | -5.5566736 | -1.6422181 |
| H | -1.6422181 | -5.5566736 | -0.5415933 |
| H | -5.5566736 | -1.6422181 | -0.5415933 |
| H | -5.5566736 | -0.5415933 | -1.6422181 |
| H | -1.6422181 | -0.5415933 | -5.5566736 |
| H | -0.5415933 | -1.6422181 | -5.5566736 |
| H | 1.6422181 | -0.5415933 | 5.5566736 |
| H | 0.5415933 | -1.6422181 | 5.5566736 |
| H | 5.5566736 | -1.6422181 | 0.5415933 |
| H | 5.5566736 | -0.5415933 | 1.6422181 |
| H | 0.5415933 | -5.5566736 | 1.6422181 |
| H | 1.6422181 | -5.5566736 | 0.5415933 |

Table S15. $SiAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Si | 0 | 0 | 0 |
| Al | 1.0232723 | 1.0232723 | 3.1682953 |
| Al | 3.1682953 | 1.0232723 | 1.0232723 |
| Al | 1.0232723 | 3.1682953 | 1.0232723 |
| Al | 1.0232723 | -3.1682953 | -1.0232723 |
| Al | 1.0232723 | -1.0232723 | -3.1682953 |
| Al | 3.1682953 | -1.0232723 | -1.0232723 |
| Al | -3.1682953 | 1.0232723 | -1.0232723 |
| Al | -1.0232723 | 3.1682953 | -1.0232723 |
| Al | -1.0232723 | 1.0232723 | -3.1682953 |
| Al | -1.0232723 | -1.0232723 | 3.1682953 |
| Al | -1.0232723 | -3.1682953 | 1.0232723 |
| Al | -3.1682953 | -1.0232723 | 1.0232723 |
| O | -0.9971774 | -0.9971774 | 0.9971774 |
| O | 0.9971774 | 0.9971774 | 0.9971774 |
| O | 0.9971774 | -0.9971774 | -0.9971774 |
| O | -0.9971774 | 0.9971774 | -0.9971774 |
| O | 2.8504589 | 2.8504589 | 0.9054759 |
| O | 0.9054759 | 2.8504589 | 2.8504589 |
| O | 2.8504589 | 0.9054759 | 2.8504589 |
| O | 2.8504589 | -0.9054759 | -2.8504589 |

| | | | |
|---|---|---|---|
| O | 2.8504589 | -2.8504589 | -0.9054759 |
| O | 0.9054759 | -2.8504589 | -2.8504589 |
| O | -0.9054759 | 2.8504589 | -2.8504589 |
| O | -2.8504589 | 0.9054759 | -2.8504589 |
| O | -2.8504589 | 2.8504589 | -0.9054759 |
| O | -2.8504589 | -2.8504589 | 0.9054759 |
| O | -2.8504589 | -0.9054759 | 2.8504589 |
| O | -0.9054759 | -2.8504589 | 2.8504589 |
| O | 0.812099 | 3.2715882 | -0.812099 |
| O | -0.812099 | 3.2715882 | 0.812099 |
| O | 0.812099 | 0.812099 | -3.2715882 |
| O | -0.812099 | -0.812099 | -3.2715882 |
| O | 3.2715882 | 0.812099 | -0.812099 |
| O | 3.2715882 | -0.812099 | 0.812099 |
| O | 0.812099 | -0.812099 | 3.2715882 |
| O | -0.812099 | 0.812099 | 3.2715882 |
| O | -3.2715882 | 0.812099 | 0.812099 |
| O | -3.2715882 | -0.812099 | -0.812099 |
| O | -0.812099 | -3.2715882 | -0.812099 |
| O | 0.812099 | -3.2715882 | 0.812099 |
| O | 1.3510155 | 1.3510155 | 5.0803907 |
| O | 5.0803907 | 1.3510155 | 1.3510155 |
| O | 1.3510155 | 5.0803907 | 1.3510155 |
| O | 1.3510155 | -5.0803907 | -1.3510155 |
| O | 1.3510155 | -1.3510155 | -5.0803907 |
| O | 5.0803907 | -1.3510155 | -1.3510155 |
| O | -5.0803907 | 1.3510155 | -1.3510155 |
| O | -1.3510155 | 5.0803907 | -1.3510155 |
| O | -1.3510155 | 1.3510155 | -5.0803907 |
| O | -1.3510155 | -1.3510155 | 5.0803907 |
| O | -1.3510155 | -5.0803907 | 1.3510155 |
| O | -5.0803907 | -1.3510155 | 1.3510155 |
| H | 3.495781 | 3.495781 | 1.2886629 |
| H | 1.2886629 | 3.495781 | 3.495781 |
| H | 3.495781 | 1.2886629 | 3.495781 |
| H | 3.495781 | -1.2886629 | -3.495781 |
| H | 3.495781 | -3.495781 | -1.2886629 |
| H | 1.2886629 | -3.495781 | -3.495781 |
| H | -1.2886629 | 3.495781 | -3.495781 |
| H | -3.495781 | 1.2886629 | -3.495781 |
| H | -3.495781 | 3.495781 | -1.2886629 |
| H | -3.495781 | -3.495781 | 1.2886629 |
| H | -3.495781 | -1.2886629 | 3.495781 |
| H | -1.2886629 | -3.495781 | 3.495781 |
| H | 1.4981624 | 3.4100776 | -1.4981624 |
| H | -1.4981624 | 3.4100776 | 1.4981624 |
| H | -1.4981624 | -1.4981624 | -3.4100776 |

| | | | |
|---|---|---|---|
| H | 1.4981624 | 1.4981624 | -3.4100776 |
| H | 3.4100776 | 1.4981624 | -1.4981624 |
| H | 3.4100776 | -1.4981624 | 1.4981624 |
| H | 1.4981624 | -1.4981624 | 3.4100776 |
| H | -1.4981624 | 1.4981624 | 3.4100776 |
| H | -3.4100776 | 1.4981624 | 1.4981624 |
| H | -3.4100776 | -1.4981624 | -1.4981624 |
| H | -1.4981624 | -3.4100776 | -1.4981624 |
| H | 1.4981624 | -3.4100776 | 1.4981624 |
| H | 0.8221299 | 1.9645996 | 5.6619968 |
| H | 1.9645996 | 0.8221299 | 5.6619968 |
| H | 5.6619968 | 0.8221299 | 1.9645996 |
| H | 5.6619968 | 1.9645996 | 0.8221299 |
| H | 1.9645996 | 5.6619968 | 0.8221299 |
| H | 0.8221299 | 5.6619968 | 1.9645996 |
| H | 1.9645996 | -5.6619968 | -0.8221299 |
| H | 0.8221299 | -5.6619968 | -1.9645996 |
| H | 0.8221299 | -1.9645996 | -5.6619968 |
| H | 1.9645996 | -0.8221299 | -5.6619968 |
| H | 5.6619968 | -0.8221299 | -1.9645996 |
| H | 5.6619968 | -1.9645996 | -0.8221299 |
| H | -5.6619968 | 0.8221299 | -1.9645996 |
| H | -5.6619968 | 1.9645996 | -0.8221299 |
| H | -1.9645996 | 5.6619968 | -0.8221299 |
| H | -0.8221299 | 5.6619968 | -1.9645996 |
| H | -0.8221299 | 1.9645996 | -5.6619968 |
| H | -1.9645996 | 0.8221299 | -5.6619968 |
| H | -0.8221299 | -1.9645996 | 5.6619968 |
| H | -1.9645996 | -0.8221299 | 5.6619968 |
| H | -1.9645996 | -5.6619968 | 0.8221299 |
| H | -0.8221299 | -5.6619968 | 1.9645996 |
| H | -5.6619968 | -0.8221299 | 1.9645996 |
| H | -5.6619968 | -1.9645996 | 0.8221299 |

Table S16. $FeAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Fe | 0.0000028 | 0.0000571 | 0.013942 |
| Al | -1.4659568 | 0.8600689 | 3.0132636 |
| Al | -0.0000109 | -1.6946488 | 3.0112665 |
| Al | 1.4659868 | 0.8600208 | 3.013299 |
| Al | -1.4743444 | -2.5419823 | -1.7869338 |
| Al | 1.4743155 | -2.5419457 | -1.7869708 |
| Al | 0.0000125 | -3.3986159 | 0.5976462 |
| Al | 1.4747765 | 2.5058525 | -1.8184706 |
| Al | 2.9362148 | 1.7213074 | 0.611681 |
| Al | 2.9745923 | -0.0118188 | -1.7632762 |
| Al | -2.9361634 | 1.7213774 | 0.6116139 |

| | | | |
|---|---|---|---|
| Al | -2.9746178 | -0.0118743 | -1.7632477 |
| Al | -1.4747552 | 2.5057945 | -1.8185988 |
| O | -1.5927108 | 0.9012628 | -0.6323743 |
| O | 0.0000094 | 0.005857 | 1.9478606 |
| O | -0.0000043 | -1.8192321 | -0.6454149 |
| O | 1.5927244 | 0.9012714 | -0.6323385 |
| O | 1.4189513 | -0.8137496 | 3.8740265 |
| O | 0.0000175 | 1.641374 | 3.8992729 |
| O | -1.418974 | -0.8137096 | 3.8739866 |
| O | 1.4184854 | -3.9309276 | -0.5214259 |
| O | -1.4184629 | -3.9309662 | -0.5213988 |
| O | -0.0000216 | -3.0774076 | -2.8264923 |
| O | 4.1218176 | 0.7463343 | -0.4870448 |
| O | 2.7255403 | 1.5294136 | -2.825171 |
| O | 2.6724535 | 3.1881069 | -0.5283217 |
| O | -2.725538 | 1.5292749 | -2.8252297 |
| O | -2.6724281 | 3.1881152 | -0.5284998 |
| O | -4.121805 | 0.7463657 | -0.4870387 |
| O | 2.9213937 | 0.3808483 | 1.9269351 |
| O | 1.7241962 | 2.3471037 | 1.9001319 |
| O | 2.8863893 | -1.6748661 | -0.8940746 |
| O | 1.7989911 | -1.012177 | -2.8231873 |
| O | 1.1453949 | -2.6810317 | 1.8974302 |
| O | -1.1453916 | -2.6810338 | 1.8974277 |
| O | -2.9213573 | 0.3809378 | 1.9268891 |
| O | -1.7241155 | 2.3471605 | 1.9000602 |
| O | -0.0000355 | 3.3385165 | -1.0216058 |
| O | 0.000062 | 1.8656565 | -2.8203069 |
| O | -1.7990605 | -1.0122549 | -2.8231714 |
| O | -2.886398 | -1.6748975 | -0.8939941 |
| O | -2.6444174 | 1.5378462 | 4.48462 |
| O | -0.0000477 | -3.0616673 | 4.4772292 |
| O | 2.6444708 | 1.5377418 | 4.484665 |
| O | -2.633499 | -3.689838 | -2.9529369 |
| O | 2.6334263 | -3.6897823 | -2.9530355 |
| O | 0.0000584 | -5.2477905 | 1.379841 |
| O | 1.8961744 | 4.0945382 | -2.9676437 |
| O | 4.5277811 | 2.6541362 | 1.3989154 |
| O | 4.5805026 | -0.4578687 | -2.8813994 |
| O | -4.5276783 | 2.6542844 | 1.3988556 |
| O | -4.5805868 | -0.4579401 | -2.8812907 |
| O | -1.8961686 | 4.0940882 | -2.96833 |
| H | 1.5118045 | -0.8638781 | 4.8370065 |
| H | 0.0000036 | 1.661417 | 4.8683225 |
| H | -1.5118533 | -0.8638644 | 4.8369623 |
| H | 1.4716084 | -4.8514226 | -0.8190734 |
| H | -1.4715696 | -4.851456 | -0.8190684 |

| | | | |
|---|---|---|---|
| H | -0.000013 | -3.9457667 | -3.256143 |
| H | 4.9513044 | 1.1566828 | -0.774282 |
| H | 3.506583 | 1.9799983 | -3.1801299 |
| H | 3.4264862 | 3.7257535 | -0.8127953 |
| H | -3.5066042 | 1.9798182 | -3.1801893 |
| H | -3.4264435 | 3.7257807 | -0.8129806 |
| H | -4.9512902 | 1.1567115 | -0.7742837 |
| H | 3.230924 | -0.5189236 | 1.7735938 |
| H | 1.3803475 | 3.2393254 | 2.0249132 |
| H | 1.2237335 | -0.6211621 | -3.490435 |
| H | 3.5623829 | -2.1031647 | -0.3550163 |
| H | 2.1083875 | -2.7181522 | 1.9070526 |
| H | -2.1083856 | -2.7181287 | 1.9070292 |
| H | -3.2308924 | -0.5188275 | 1.7735214 |
| H | -1.3802892 | 3.2393861 | 2.0248755 |
| H | -0.0000944 | 3.8044245 | -0.1777981 |
| H | 0.0001401 | 1.7730267 | -3.7826876 |
| H | -1.2238453 | -0.6212577 | -3.4904674 |
| H | -3.5623817 | -2.1032 | -0.3549227 |
| H | -2.7293269 | 2.5067435 | 4.5427603 |
| H | -3.5520717 | 1.1831398 | 4.4784191 |
| H | -0.7797039 | -3.6464131 | 4.4973654 |
| H | 0.7797453 | -3.6462224 | 4.4975697 |
| H | 3.5521043 | 1.1829833 | 4.478444 |
| H | 2.7294376 | 2.5066339 | 4.5428134 |
| H | -3.5322017 | -3.8941866 | -2.6376045 |
| H | -2.7329792 | -3.3551688 | -3.8630457 |
| H | 2.7328648 | -3.3551048 | -3.8631459 |
| H | 3.5321404 | -3.8941512 | -2.63775 |
| H | 0.7801357 | -5.4789376 | 1.916106 |
| H | -0.7800963 | -5.4790546 | 1.9159434 |
| H | 1.7825605 | 4.0443352 | -3.9333504 |
| H | 1.5165723 | 4.9447434 | -2.682195 |
| H | 4.3482715 | 3.4410458 | 1.9445979 |
| H | 5.1210326 | 2.0864346 | 1.9236801 |
| H | 5.1927398 | -1.1374051 | -2.5455141 |
| H | 4.3901248 | -0.6935557 | -3.8074088 |
| H | -5.1209298 | 2.0866197 | 1.9236603 |
| H | -4.3481164 | 3.4412014 | 1.9445112 |
| H | -4.3902733 | -0.6936605 | -3.8073045 |
| H | -5.1928367 | -1.1374389 | -2.5453516 |
| H | -1.5162264 | 4.9444335 | -2.683764 |
| H | -1.7832023 | 4.0431785 | -3.9340751 |

CONVERGED GEOMETRY – SVWN5/6-31G*/PCM
Coordinates (Angstroms)

Table S17. $AlAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Al | 0 | 0 | 0 |
| Al | -1.0189755 | 1.0189755 | 3.0504585 |
| Al | -1.0189755 | 3.0504585 | 1.0189755 |
| Al | -3.0504585 | 1.0189755 | 1.0189755 |
| Al | 3.0504585 | 1.0189755 | -1.0189755 |
| Al | 1.0189755 | 1.0189755 | -3.0504585 |
| Al | 1.0189755 | 3.0504585 | -1.0189755 |
| Al | -1.0189755 | -3.0504585 | -1.0189755 |
| Al | -3.0504585 | -1.0189755 | -1.0189755 |
| Al | -1.0189755 | -1.0189755 | -3.0504585 |
| Al | 1.0189755 | -1.0189755 | 3.0504585 |
| Al | 3.0504585 | -1.0189755 | 1.0189755 |
| Al | 1.0189755 | -3.0504585 | 1.0189755 |
| O | 1.0629627 | -1.0629627 | 1.0629627 |
| O | -1.0629627 | 1.0629627 | 1.0629627 |
| O | 1.0629627 | 1.0629627 | -1.0629627 |
| O | -1.0629627 | -1.0629627 | -1.0629627 |
| O | -2.861885 | 2.861885 | 0.8772731 |
| O | -2.861885 | 0.8772731 | 2.861885 |
| O | -0.8772731 | 2.861885 | 2.861885 |
| O | 0.8772731 | 2.861885 | -2.861885 |
| O | 2.861885 | 2.861885 | -0.8772731 |
| O | 2.861885 | 0.8772731 | -2.861885 |
| O | -2.861885 | -0.8772731 | -2.861885 |
| O | -0.8772731 | -2.861885 | -2.861885 |
| O | -2.861885 | -2.861885 | -0.8772731 |
| O | 2.861885 | -2.861885 | 0.8772731 |
| O | 0.8772731 | -2.861885 | 2.861885 |
| O | 2.861885 | -0.8772731 | 2.861885 |
| O | -3.1965956 | 0.8112882 | -0.8112882 |
| O | -3.1965956 | -0.8112882 | 0.8112882 |
| O | -0.8112882 | 0.8112882 | -3.1965956 |
| O | 0.8112882 | -0.8112882 | -3.1965956 |
| O | -0.8112882 | 3.1965956 | -0.8112882 |
| O | 0.8112882 | 3.1965956 | 0.8112882 |
| O | 0.8112882 | 0.8112882 | 3.1965956 |
| O | -0.8112882 | -0.8112882 | 3.1965956 |
| O | -0.8112882 | -3.1965956 | 0.8112882 |

| | | | |
|---|---|---|---|
| O | 0.8112882 | -3.1965956 | -0.8112882 |
| O | 3.1965956 | -0.8112882 | -0.8112882 |
| O | 3.1965956 | 0.8112882 | 0.8112882 |
| O | -1.3136065 | 1.3136065 | 4.965708 |
| O | -1.3136065 | 4.965708 | 1.3136065 |
| O | -4.965708 | 1.3136065 | 1.3136065 |
| O | 4.965708 | 1.3136065 | -1.3136065 |
| O | 1.3136065 | 1.3136065 | -4.965708 |
| O | 1.3136065 | 4.965708 | -1.3136065 |
| O | -1.3136065 | -4.965708 | -1.3136065 |
| O | -4.965708 | -1.3136065 | -1.3136065 |
| O | -1.3136065 | -1.3136065 | -4.965708 |
| O | 1.3136065 | -1.3136065 | 4.965708 |
| O | 4.965708 | -1.3136065 | 1.3136065 |
| O | 1.3136065 | -4.965708 | 1.3136065 |
| H | -3.443533 | 3.443533 | 1.4084038 |
| H | -3.443533 | 1.4084038 | 3.443533 |
| H | -1.4084038 | 3.443533 | 3.443533 |
| H | 1.4084038 | 3.443533 | -3.443533 |
| H | 3.443533 | 3.443533 | -1.4084038 |
| H | 3.443533 | 1.4084038 | -3.443533 |
| H | -3.443533 | -1.4084038 | -3.443533 |
| H | -1.4084038 | -3.443533 | -3.443533 |
| H | -3.443533 | -3.443533 | -1.4084038 |
| H | 3.443533 | -3.443533 | 1.4084038 |
| H | 1.4084038 | -3.443533 | 3.443533 |
| H | 3.443533 | -1.4084038 | 3.443533 |
| H | -3.3345018 | 1.4919255 | -1.4919255 |
| H | -3.3345018 | -1.4919255 | 1.4919255 |
| H | 1.4919255 | -1.4919255 | -3.3345018 |
| H | -1.4919255 | 1.4919255 | -3.3345018 |
| H | -1.4919255 | 3.3345018 | -1.4919255 |
| H | 1.4919255 | 3.3345018 | 1.4919255 |
| H | 1.4919255 | 1.4919255 | 3.3345018 |
| H | -1.4919255 | -1.4919255 | 3.3345018 |
| H | -1.4919255 | -3.3345018 | 1.4919255 |
| H | 1.4919255 | -3.3345018 | -1.4919255 |
| H | 3.3345018 | -1.4919255 | -1.4919255 |
| H | 3.3345018 | 1.4919255 | 1.4919255 |
| H | -1.6494865 | 0.5321459 | 5.4617314 |
| H | -0.5321459 | 1.6494865 | 5.4617314 |
| H | -0.5321459 | 5.4617314 | 1.6494865 |
| H | -1.6494865 | 5.4617314 | 0.5321459 |
| H | -5.4617314 | 1.6494865 | 0.5321459 |
| H | -5.4617314 | 0.5321459 | 1.6494865 |

| | | | |
|---|---|---|---|
| H | 5.4617314 | 1.6494865 | -0.5321459 |
| H | 5.4617314 | 0.5321459 | -1.6494865 |
| H | 1.6494865 | 0.5321459 | -5.4617314 |
| H | 0.5321459 | 1.6494865 | -5.4617314 |
| H | 0.5321459 | 5.4617314 | -1.6494865 |
| H | 1.6494865 | 5.4617314 | -0.5321459 |
| H | -0.5321459 | -5.4617314 | -1.6494865 |
| H | -1.6494865 | -5.4617314 | -0.5321459 |
| H | -5.4617314 | -1.6494865 | -0.5321459 |
| H | -5.4617314 | -0.5321459 | -1.6494865 |
| H | -1.6494865 | -0.5321459 | -5.4617314 |
| H | -0.5321459 | -1.6494865 | -5.4617314 |
| H | 1.6494865 | -0.5321459 | 5.4617314 |
| H | 0.5321459 | -1.6494865 | 5.4617314 |
| H | 5.4617314 | -1.6494865 | 0.5321459 |
| H | 5.4617314 | -0.5321459 | 1.6494865 |
| H | 0.5321459 | -5.4617314 | 1.6494865 |
| H | 1.6494865 | -5.4617314 | 0.5321459 |

Table S18. $GaAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Ga | 0 | 0 | 0 |
| Al | -1.0205261 | 1.0205261 | 3.0517848 |
| Al | -1.0205261 | 3.0517848 | 1.0205261 |
| Al | -3.0517848 | 1.0205261 | 1.0205261 |
| Al | 3.0517848 | 1.0205261 | -1.0205261 |
| Al | 1.0205261 | 1.0205261 | -3.0517848 |
| Al | 1.0205261 | 3.0517848 | -1.0205261 |
| Al | -1.0205261 | -3.0517848 | -1.0205261 |
| Al | -3.0517848 | -1.0205261 | -1.0205261 |
| Al | -1.0205261 | -1.0205261 | -3.0517848 |
| Al | 1.0205261 | -1.0205261 | 3.0517848 |
| Al | 3.0517848 | -1.0205261 | 1.0205261 |
| Al | 1.0205261 | -3.0517848 | 1.0205261 |
| O | 1.0909637 | -1.0909637 | 1.0909637 |
| O | -1.0909637 | 1.0909637 | 1.0909637 |
| O | 1.0909637 | 1.0909637 | -1.0909637 |
| O | -1.0909637 | -1.0909637 | -1.0909637 |
| O | -2.8689081 | 2.8689081 | 0.8795357 |
| O | -2.8689081 | 0.8795357 | 2.8689081 |
| O | -0.8795357 | 2.8689081 | 2.8689081 |
| O | 0.8795357 | 2.8689081 | -2.8689081 |
| O | 2.8689081 | 2.8689081 | -0.8795357 |
| O | 2.8689081 | 0.8795357 | -2.8689081 |
| O | -2.8689081 | -0.8795357 | -2.8689081 |

| | | | |
|---|---|---|---|
| O | -0.8795357 | -2.8689081 | -2.8689081 |
| O | -2.8689081 | -2.8689081 | -0.8795357 |
| O | 2.8689081 | -2.8689081 | 0.8795357 |
| O | 0.8795357 | -2.8689081 | 2.8689081 |
| O | 2.8689081 | -0.8795357 | 2.8689081 |
| O | -3.1670378 | 0.8130332 | -0.8130332 |
| O | -3.1670378 | -0.8130332 | 0.8130332 |
| O | -0.8130332 | 0.8130332 | -3.1670378 |
| O | 0.8130332 | -0.8130332 | -3.1670378 |
| O | -0.8130332 | 3.1670378 | -0.8130332 |
| O | 0.8130332 | 3.1670378 | 0.8130332 |
| O | 0.8130332 | 0.8130332 | 3.1670378 |
| O | -0.8130332 | -0.8130332 | 3.1670378 |
| O | -0.8130332 | -3.1670378 | 0.8130332 |
| O | 0.8130332 | -3.1670378 | -0.8130332 |
| O | 3.1670378 | -0.8130332 | -0.8130332 |
| O | 3.1670378 | 0.8130332 | 0.8130332 |
| O | -1.3046254 | 1.3046254 | 4.9680603 |
| O | -1.3046254 | 4.9680603 | 1.3046254 |
| O | -4.9680603 | 1.3046254 | 1.3046254 |
| O | 4.9680603 | 1.3046254 | -1.3046254 |
| O | 1.3046254 | 1.3046254 | -4.9680603 |
| O | 1.3046254 | 4.9680603 | -1.3046254 |
| O | -1.3046254 | -4.9680603 | -1.3046254 |
| O | -4.9680603 | -1.3046254 | -1.3046254 |
| O | -1.3046254 | -1.3046254 | -4.9680603 |
| O | 1.3046254 | -1.3046254 | 4.9680603 |
| O | 4.9680603 | -1.3046254 | 1.3046254 |
| O | 1.3046254 | -4.9680603 | 1.3046254 |
| H | -3.449601 | 3.449601 | 1.4124671 |
| H | -3.449601 | 1.4124671 | 3.449601 |
| H | -1.4124671 | 3.449601 | 3.449601 |
| H | 1.4124671 | 3.449601 | -3.449601 |
| H | 3.449601 | 3.449601 | -1.4124671 |
| H | 3.449601 | 1.4124671 | -3.449601 |
| H | -3.449601 | -1.4124671 | -3.449601 |
| H | -1.4124671 | -3.449601 | -3.449601 |
| H | -3.449601 | -3.449601 | -1.4124671 |
| H | 3.449601 | -3.449601 | 1.4124671 |
| H | 1.4124671 | -3.449601 | 3.449601 |
| H | 3.449601 | -1.4124671 | 3.449601 |
| H | -3.3290155 | 1.4909707 | -1.4909707 |
| H | -3.3290155 | -1.4909707 | 1.4909707 |
| H | 1.4909707 | -1.4909707 | -3.3290155 |
| H | -1.4909707 | 1.4909707 | -3.3290155 |

| | | | |
|---|---|---|---|
| H | -1.4909707 | 3.3290155 | -1.4909707 |
| H | 1.4909707 | 3.3290155 | 1.4909707 |
| H | 1.4909707 | 1.4909707 | 3.3290155 |
| H | -1.4909707 | -1.4909707 | 3.3290155 |
| H | -1.4909707 | -3.3290155 | 1.4909707 |
| H | 1.4909707 | -3.3290155 | -1.4909707 |
| H | 3.3290155 | -1.4909707 | -1.4909707 |
| H | 3.3290155 | 1.4909707 | 1.4909707 |
| H | -1.6482741 | 0.5299868 | 5.4692213 |
| H | -0.5299868 | 1.6482741 | 5.4692213 |
| H | -0.5299868 | 5.4692213 | 1.6482741 |
| H | -1.6482741 | 5.4692213 | 0.5299868 |
| H | -5.4692213 | 1.6482741 | 0.5299868 |
| H | -5.4692213 | 0.5299868 | 1.6482741 |
| H | 5.4692213 | 1.6482741 | -0.5299868 |
| H | 5.4692213 | 0.5299868 | -1.6482741 |
| H | 1.6482741 | 0.5299868 | -5.4692213 |
| H | 0.5299868 | 1.6482741 | -5.4692213 |
| H | 0.5299868 | 5.4692213 | -1.6482741 |
| H | 1.6482741 | 5.4692213 | -0.5299868 |
| H | -0.5299868 | -5.4692213 | -1.6482741 |
| H | -1.6482741 | -5.4692213 | -0.5299868 |
| H | -5.4692213 | -1.6482741 | -0.5299868 |
| H | -5.4692213 | -0.5299868 | -1.6482741 |
| H | -1.6482741 | -0.5299868 | -5.4692213 |
| H | -0.5299868 | -1.6482741 | -5.4692213 |
| H | 1.6482741 | -0.5299868 | 5.4692213 |
| H | 0.5299868 | -1.6482741 | 5.4692213 |
| H | 5.4692213 | -1.6482741 | 0.5299868 |
| H | 5.4692213 | -0.5299868 | 1.6482741 |
| H | 0.5299868 | -5.4692213 | 1.6482741 |
| H | 1.6482741 | -5.4692213 | 0.5299868 |

Table S19. $GeAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Ge | 0 | 0 | 0 |
| Al | -1.0138964 | 1.0138964 | 3.088978 |
| Al | -1.0138964 | 3.088978 | 1.0138964 |
| Al | -3.088978 | 1.0138964 | 1.0138964 |
| Al | 3.088978 | 1.0138964 | -1.0138964 |
| Al | 1.0138964 | 1.0138964 | -3.088978 |
| Al | 1.0138964 | 3.088978 | -1.0138964 |
| Al | -1.0138964 | -3.088978 | -1.0138964 |
| Al | -3.088978 | -1.0138964 | -1.0138964 |
| Al | -1.0138964 | -1.0138964 | -3.088978 |

| | | | |
|---|---|---|---|
| Al | 1.0138964 | -1.0138964 | 3.088978 |
| Al | 3.088978 | -1.0138964 | 1.0138964 |
| Al | 1.0138964 | -3.088978 | 1.0138964 |
| O | 1.042911 | -1.042911 | 1.042911 |
| O | -1.042911 | 1.042911 | 1.042911 |
| O | 1.042911 | 1.042911 | -1.042911 |
| O | -1.042911 | -1.042911 | -1.042911 |
| O | -2.845658 | 2.845658 | 0.8831759 |
| O | -2.845658 | 0.8831759 | 2.845658 |
| O | -0.8831759 | 2.845658 | 2.845658 |
| O | 0.8831759 | 2.845658 | -2.845658 |
| O | 2.845658 | 2.845658 | -0.8831759 |
| O | 2.845658 | 0.8831759 | -2.845658 |
| O | -2.845658 | -0.8831759 | -2.845658 |
| O | -0.8831759 | -2.845658 | -2.845658 |
| O | -2.845658 | -2.845658 | -0.8831759 |
| O | 2.845658 | -2.845658 | 0.8831759 |
| O | 0.8831759 | -2.845658 | 2.845658 |
| O | 2.845658 | -0.8831759 | 2.845658 |
| O | -3.143568 | 0.8154819 | -0.8154819 |
| O | -3.143568 | -0.8154819 | 0.8154819 |
| O | -0.8154819 | 0.8154819 | -3.143568 |
| O | 0.8154819 | -0.8154819 | -3.143568 |
| O | -0.8154819 | 3.143568 | -0.8154819 |
| O | 0.8154819 | 3.143568 | 0.8154819 |
| O | 0.8154819 | 0.8154819 | 3.143568 |
| O | -0.8154819 | -0.8154819 | 3.143568 |
| O | -0.8154819 | -3.143568 | 0.8154819 |
| O | 0.8154819 | -3.143568 | -0.8154819 |
| O | 3.143568 | -0.8154819 | -0.8154819 |
| O | 3.143568 | 0.8154819 | 0.8154819 |
| O | -1.3041635 | 1.3041635 | 4.979617 |
| O | -1.3041635 | 4.979617 | 1.3041635 |
| O | -4.979617 | 1.3041635 | 1.3041635 |
| O | 4.979617 | 1.3041635 | -1.3041635 |
| O | 1.3041635 | 1.3041635 | -4.979617 |
| O | 1.3041635 | 4.979617 | -1.3041635 |
| O | -1.3041635 | -4.979617 | -1.3041635 |
| O | -4.979617 | -1.3041635 | -1.3041635 |
| O | -1.3041635 | -1.3041635 | -4.979617 |
| O | 1.3041635 | -1.3041635 | 4.979617 |
| O | 4.979617 | -1.3041635 | 1.3041635 |
| O | 1.3041635 | -4.979617 | 1.3041635 |
| H | -3.4328181 | 3.4328181 | 1.4039918 |
| H | -3.4328181 | 1.4039918 | 3.4328181 |

| | | | |
|---|---|---|---|
| H | -1.4039918 | 3.4328181 | 3.4328181 |
| H | 1.4039918 | 3.4328181 | -3.4328181 |
| H | 3.4328181 | 3.4328181 | -1.4039918 |
| H | 3.4328181 | 1.4039918 | -3.4328181 |
| H | -3.4328181 | -1.4039918 | -3.4328181 |
| H | -1.4039918 | -3.4328181 | -3.4328181 |
| H | -3.4328181 | -3.4328181 | -1.4039918 |
| H | 3.4328181 | -3.4328181 | 1.4039918 |
| H | 1.4039918 | -3.4328181 | 3.4328181 |
| H | 3.4328181 | -1.4039918 | 3.4328181 |
| H | -3.364309 | 1.4860644 | -1.4860644 |
| H | -3.364309 | -1.4860644 | 1.4860644 |
| H | 1.4860644 | -1.4860644 | -3.364309 |
| H | -1.4860644 | 1.4860644 | -3.364309 |
| H | -1.4860644 | 3.364309 | -1.4860644 |
| H | 1.4860644 | 3.364309 | 1.4860644 |
| H | 1.4860644 | 1.4860644 | 3.364309 |
| H | -1.4860644 | -1.4860644 | 3.364309 |
| H | -1.4860644 | -3.364309 | 1.4860644 |
| H | 1.4860644 | -3.364309 | -1.4860644 |
| H | 3.364309 | -1.4860644 | -1.4860644 |
| H | 3.364309 | 1.4860644 | 1.4860644 |
| H | -1.6934293 | 0.5714255 | 5.509721 |
| H | -0.5714255 | 1.6934293 | 5.509721 |
| H | -0.5714255 | 5.509721 | 1.6934293 |
| H | -1.6934293 | 5.509721 | 0.5714255 |
| H | -5.509721 | 1.6934293 | 0.5714255 |
| H | -5.509721 | 0.5714255 | 1.6934293 |
| H | 5.509721 | 1.6934293 | -0.5714255 |
| H | 5.509721 | 0.5714255 | -1.6934293 |
| H | 1.6934293 | 0.5714255 | -5.509721 |
| H | 0.5714255 | 1.6934293 | -5.509721 |
| H | 0.5714255 | 5.509721 | -1.6934293 |
| H | 1.6934293 | 5.509721 | -0.5714255 |
| H | -0.5714255 | -5.509721 | -1.6934293 |
| H | -1.6934293 | -5.509721 | -0.5714255 |
| H | -5.509721 | -1.6934293 | -0.5714255 |
| H | -5.509721 | -0.5714255 | -1.6934293 |
| H | -1.6934293 | -0.5714255 | -5.509721 |
| H | -0.5714255 | -1.6934293 | -5.509721 |
| H | 1.6934293 | -0.5714255 | 5.509721 |
| H | 0.5714255 | -1.6934293 | 5.509721 |
| H | 5.509721 | -1.6934293 | 0.5714255 |
| H | 5.509721 | -0.5714255 | 1.6934293 |
| H | 0.5714255 | -5.509721 | 1.6934293 |

| | | | |
|---|---|---|---|
| H | 1.6934293 | -5.509721 | 0.5714255 |

Table S20. $BeAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Be | 0 | 0 | 0 |
| Al | -1.0064223 | 1.0064223 | 3.0036229 |
| Al | -1.0064223 | 3.0036229 | 1.0064223 |
| Al | -3.0036229 | 1.0064223 | 1.0064223 |
| Al | 3.0036229 | 1.0064223 | -1.0064223 |
| Al | 1.0064223 | 1.0064223 | -3.0036229 |
| Al | 1.0064223 | 3.0036229 | -1.0064223 |
| Al | -1.0064223 | -3.0036229 | -1.0064223 |
| Al | -3.0036229 | -1.0064223 | -1.0064223 |
| Al | -1.0064223 | -1.0064223 | -3.0036229 |
| Al | 1.0064223 | -1.0064223 | 3.0036229 |
| Al | 3.0036229 | -1.0064223 | 1.0064223 |
| Al | 1.0064223 | -3.0036229 | 1.0064223 |
| O | 1.0328568 | -1.0328568 | 1.0328568 |
| O | -1.0328568 | 1.0328568 | 1.0328568 |
| O | 1.0328568 | 1.0328568 | -1.0328568 |
| O | -1.0328568 | -1.0328568 | -1.0328568 |
| O | -2.8497109 | 2.8497109 | 0.8571518 |
| O | -2.8497109 | 0.8571518 | 2.8497109 |
| O | -0.8571518 | 2.8497109 | 2.8497109 |
| O | 0.8571518 | 2.8497109 | -2.8497109 |
| O | 2.8497109 | 2.8497109 | -0.8571518 |
| O | 2.8497109 | 0.8571518 | -2.8497109 |
| O | -2.8497109 | -0.8571518 | -2.8497109 |
| O | -0.8571518 | -2.8497109 | -2.8497109 |
| O | -2.8497109 | -2.8497109 | -0.8571518 |
| O | 2.8497109 | -2.8497109 | 0.8571518 |
| O | 0.8571518 | -2.8497109 | 2.8497109 |
| O | 2.8497109 | -0.8571518 | 2.8497109 |
| O | -3.2917735 | 0.8110054 | -0.8110054 |
| O | -3.2917735 | -0.8110054 | 0.8110054 |
| O | -0.8110054 | 0.8110054 | -3.2917735 |
| O | 0.8110054 | -0.8110054 | -3.2917735 |
| O | -0.8110054 | 3.2917735 | -0.8110054 |
| O | 0.8110054 | 3.2917735 | 0.8110054 |
| O | 0.8110054 | 0.8110054 | 3.2917735 |
| O | -0.8110054 | -0.8110054 | 3.2917735 |
| O | -0.8110054 | -3.2917735 | 0.8110054 |
| O | 0.8110054 | -3.2917735 | -0.8110054 |
| O | 3.2917735 | -0.8110054 | -0.8110054 |
| O | 3.2917735 | 0.8110054 | 0.8110054 |

| | | | |
|---|---|---|---|
| O | -1.3355599 | 1.3355599 | 4.935761 |
| O | -1.3355599 | 4.935761 | 1.3355599 |
| O | -4.935761 | 1.3355599 | 1.3355599 |
| O | 4.935761 | 1.3355599 | -1.3355599 |
| O | 1.3355599 | 1.3355599 | -4.935761 |
| O | 1.3355599 | 4.935761 | -1.3355599 |
| O | -1.3355599 | -4.935761 | -1.3355599 |
| O | -4.935761 | -1.3355599 | -1.3355599 |
| O | -1.3355599 | -1.3355599 | -4.935761 |
| O | 1.3355599 | -1.3355599 | 4.935761 |
| O | 4.935761 | -1.3355599 | 1.3355599 |
| O | 1.3355599 | -4.935761 | 1.3355599 |
| H | -3.4265871 | 3.4265871 | 1.39807 |
| H | -3.4265871 | 1.39807 | 3.4265871 |
| H | -1.39807 | 3.4265871 | 3.4265871 |
| H | 1.39807 | 3.4265871 | -3.4265871 |
| H | 3.4265871 | 3.4265871 | -1.39807 |
| H | 3.4265871 | 1.39807 | -3.4265871 |
| H | -3.4265871 | -1.39807 | -3.4265871 |
| H | -1.39807 | -3.4265871 | -3.4265871 |
| H | -3.4265871 | -3.4265871 | -1.39807 |
| H | 3.4265871 | -3.4265871 | 1.39807 |
| H | 1.39807 | -3.4265871 | 3.4265871 |
| H | 3.4265871 | -1.39807 | 3.4265871 |
| H | -3.2417732 | 1.4968087 | -1.4968087 |
| H | -3.2417732 | -1.4968087 | 1.4968087 |
| H | 1.4968087 | -1.4968087 | -3.2417732 |
| H | -1.4968087 | 1.4968087 | -3.2417732 |
| H | -1.4968087 | 3.2417732 | -1.4968087 |
| H | 1.4968087 | 3.2417732 | 1.4968087 |
| H | 1.4968087 | 1.4968087 | 3.2417732 |
| H | -1.4968087 | -1.4968087 | 3.2417732 |
| H | -1.4968087 | -3.2417732 | 1.4968087 |
| H | 1.4968087 | -3.2417732 | -1.4968087 |
| H | 3.2417732 | -1.4968087 | -1.4968087 |
| H | 3.2417732 | 1.4968087 | 1.4968087 |
| H | -1.637781 | 0.5236836 | 5.4033562 |
| H | -0.5236836 | 1.637781 | 5.4033562 |
| H | -0.5236836 | 5.4033562 | 1.637781 |
| H | -1.637781 | 5.4033562 | 0.5236836 |
| H | -5.4033562 | 1.637781 | 0.5236836 |
| H | -5.4033562 | 0.5236836 | 1.637781 |
| H | 5.4033562 | 1.637781 | -0.5236836 |
| H | 5.4033562 | 0.5236836 | -1.637781 |
| H | 1.637781 | 0.5236836 | -5.4033562 |

| | | | |
|---|---|---|---|
| H | 0.5236836 | 1.637781 | -5.4033562 |
| H | 0.5236836 | 5.4033562 | -1.637781 |
| H | 1.637781 | 5.4033562 | -0.5236836 |
| H | -0.5236836 | -5.4033562 | -1.637781 |
| H | -1.637781 | -5.4033562 | -0.5236836 |
| H | -5.4033562 | -1.637781 | -0.5236836 |
| H | -5.4033562 | -0.5236836 | -1.637781 |
| H | -1.637781 | -0.5236836 | -5.4033562 |
| H | -0.5236836 | -1.637781 | -5.4033562 |
| H | 1.637781 | -0.5236836 | 5.4033562 |
| H | 0.5236836 | -1.637781 | 5.4033562 |
| H | 5.4033562 | -1.637781 | 0.5236836 |
| H | 5.4033562 | -0.5236836 | 1.637781 |
| H | 0.5236836 | -5.4033562 | 1.637781 |
| H | 1.637781 | -5.4033562 | 0.5236836 |

Table S21. $MgAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Mg | 0 | 0 | 0 |
| Al | -1.0386476 | 1.0386476 | 3.0448816 |
| Al | -1.0386476 | 3.0448816 | 1.0386476 |
| Al | -3.0448816 | 1.0386476 | 1.0386476 |
| Al | 3.0448816 | 1.0386476 | -1.0386476 |
| Al | 1.0386476 | 1.0386476 | -3.0448816 |
| Al | 1.0386476 | 3.0448816 | -1.0386476 |
| Al | -1.0386476 | -3.0448816 | -1.0386476 |
| Al | -3.0448816 | -1.0386476 | -1.0386476 |
| Al | -1.0386476 | -1.0386476 | -3.0448816 |
| Al | 1.0386476 | -1.0386476 | 3.0448816 |
| Al | 3.0448816 | -1.0386476 | 1.0386476 |
| Al | 1.0386476 | -3.0448816 | 1.0386476 |
| O | 1.1463952 | -1.1463952 | 1.1463952 |
| O | -1.1463952 | 1.1463952 | 1.1463952 |
| O | 1.1463952 | 1.1463952 | -1.1463952 |
| O | -1.1463952 | -1.1463952 | -1.1463952 |
| O | -2.9020321 | 2.9020321 | 0.873512 |
| O | -2.9020321 | 0.873512 | 2.9020321 |
| O | -0.873512 | 2.9020321 | 2.9020321 |
| O | 0.873512 | 2.9020321 | -2.9020321 |
| O | 2.9020321 | 2.9020321 | -0.873512 |
| O | 2.9020321 | 0.873512 | -2.9020321 |
| O | -2.9020321 | -0.873512 | -2.9020321 |
| O | -0.873512 | -2.9020321 | -2.9020321 |
| O | -2.9020321 | -2.9020321 | -0.873512 |
| O | 2.9020321 | -2.9020321 | 0.873512 |

| | | | |
|---|---|---|---|
| O | 0.873512 | -2.9020321 | 2.9020321 |
| O | 2.9020321 | -0.873512 | 2.9020321 |
| O | -3.2540942 | 0.8045618 | -0.8045618 |
| O | -3.2540942 | -0.8045618 | 0.8045618 |
| O | -0.8045618 | 0.8045618 | -3.2540942 |
| O | 0.8045618 | -0.8045618 | -3.2540942 |
| O | -0.8045618 | 3.2540942 | -0.8045618 |
| O | 0.8045618 | 3.2540942 | 0.8045618 |
| O | 0.8045618 | 0.8045618 | 3.2540942 |
| O | -0.8045618 | -0.8045618 | 3.2540942 |
| O | -0.8045618 | -3.2540942 | 0.8045618 |
| O | 0.8045618 | -3.2540942 | -0.8045618 |
| O | 3.2540942 | -0.8045618 | -0.8045618 |
| O | 3.2540942 | 0.8045618 | 0.8045618 |
| O | -1.3321026 | 1.3321026 | 4.9748381 |
| O | -1.3321026 | 4.9748381 | 1.3321026 |
| O | -4.9748381 | 1.3321026 | 1.3321026 |
| O | 4.9748381 | 1.3321026 | -1.3321026 |
| O | 1.3321026 | 1.3321026 | -4.9748381 |
| O | 1.3321026 | 4.9748381 | -1.3321026 |
| O | -1.3321026 | -4.9748381 | -1.3321026 |
| O | -4.9748381 | -1.3321026 | -1.3321026 |
| O | -1.3321026 | -1.3321026 | -4.9748381 |
| O | 1.3321026 | -1.3321026 | 4.9748381 |
| O | 4.9748381 | -1.3321026 | 1.3321026 |
| O | 1.3321026 | -4.9748381 | 1.3321026 |
| H | -3.4862625 | 3.4862625 | 1.3974704 |
| H | -3.4862625 | 1.3974704 | 3.4862625 |
| H | -1.3974704 | 3.4862625 | 3.4862625 |
| H | 1.3974704 | 3.4862625 | -3.4862625 |
| H | 3.4862625 | 3.4862625 | -1.3974704 |
| H | 3.4862625 | 1.3974704 | -3.4862625 |
| H | -3.4862625 | -1.3974704 | -3.4862625 |
| H | -1.3974704 | -3.4862625 | -3.4862625 |
| H | -3.4862625 | -3.4862625 | -1.3974704 |
| H | 3.4862625 | -3.4862625 | 1.3974704 |
| H | 1.3974704 | -3.4862625 | 3.4862625 |
| H | 3.4862625 | -1.3974704 | 3.4862625 |
| H | -3.2447278 | 1.4922523 | -1.4922523 |
| H | -3.2447278 | -1.4922523 | 1.4922523 |
| H | 1.4922523 | -1.4922523 | -3.2447278 |
| H | -1.4922523 | 1.4922523 | -3.2447278 |
| H | -1.4922523 | 3.2447278 | -1.4922523 |
| H | 1.4922523 | 3.2447278 | 1.4922523 |
| H | 1.4922523 | 1.4922523 | 3.2447278 |

| | | | |
|---|---|---|---|
| H | -1.4922523 | -1.4922523 | 3.2447278 |
| H | -1.4922523 | -3.2447278 | 1.4922523 |
| H | 1.4922523 | -3.2447278 | -1.4922523 |
| H | 3.2447278 | -1.4922523 | -1.4922523 |
| H | 3.2447278 | 1.4922523 | 1.4922523 |
| H | -1.6374068 | 0.5216138 | 5.4426887 |
| H | -0.5216138 | 1.6374068 | 5.4426887 |
| H | -0.5216138 | 5.4426887 | 1.6374068 |
| H | -1.6374068 | 5.4426887 | 0.5216138 |
| H | -5.4426887 | 1.6374068 | 0.5216138 |
| H | -5.4426887 | 0.5216138 | 1.6374068 |
| H | 5.4426887 | 1.6374068 | -0.5216138 |
| H | 5.4426887 | 0.5216138 | -1.6374068 |
| H | 1.6374068 | 0.5216138 | -5.4426887 |
| H | 0.5216138 | 1.6374068 | -5.4426887 |
| H | 0.5216138 | 5.4426887 | -1.6374068 |
| H | 1.6374068 | 5.4426887 | -0.5216138 |
| H | -0.5216138 | -5.4426887 | -1.6374068 |
| H | -1.6374068 | -5.4426887 | -0.5216138 |
| H | -5.4426887 | -1.6374068 | -0.5216138 |
| H | -5.4426887 | -0.5216138 | -1.6374068 |
| H | -1.6374068 | -0.5216138 | -5.4426887 |
| H | -0.5216138 | -1.6374068 | -5.4426887 |
| H | 1.6374068 | -0.5216138 | 5.4426887 |
| H | 0.5216138 | -1.6374068 | 5.4426887 |
| H | 5.4426887 | -1.6374068 | 0.5216138 |
| H | 5.4426887 | -0.5216138 | 1.6374068 |
| H | 0.5216138 | -5.4426887 | 1.6374068 |
| H | 1.6374068 | -5.4426887 | 0.5216138 |

Table S22. $ZnAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Zn | 0 | 0 | 0 |
| Al | -1.0313881 | 1.0313881 | 3.0349067 |
| Al | -1.0313881 | 3.0349067 | 1.0313881 |
| Al | -3.0349067 | 1.0313881 | 1.0313881 |
| Al | 3.0349067 | 1.0313881 | -1.0313881 |
| Al | 1.0313881 | 1.0313881 | -3.0349067 |
| Al | 1.0313881 | 3.0349067 | -1.0313881 |
| Al | -1.0313881 | -3.0349067 | -1.0313881 |
| Al | -3.0349067 | -1.0313881 | -1.0313881 |
| Al | -1.0313881 | -1.0313881 | -3.0349067 |
| Al | 1.0313881 | -1.0313881 | 3.0349067 |
| Al | 3.0349067 | -1.0313881 | 1.0313881 |
| Al | 1.0313881 | -3.0349067 | 1.0313881 |

| | | | |
|---|---|---|---|
| O | 1.1298654 | -1.1298654 | 1.1298654 |
| O | -1.1298654 | 1.1298654 | 1.1298654 |
| O | 1.1298654 | 1.1298654 | -1.1298654 |
| O | -1.1298654 | -1.1298654 | -1.1298654 |
| O | -2.892002 | 2.892002 | 0.8724091 |
| O | -2.892002 | 0.8724091 | 2.892002 |
| O | -0.8724091 | 2.892002 | 2.892002 |
| O | 0.8724091 | 2.892002 | -2.892002 |
| O | 2.892002 | 2.892002 | -0.8724091 |
| O | 2.892002 | 0.8724091 | -2.892002 |
| O | -2.892002 | -0.8724091 | -2.892002 |
| O | -0.8724091 | -2.892002 | -2.892002 |
| O | -2.892002 | -2.892002 | -0.8724091 |
| O | 2.892002 | -2.892002 | 0.8724091 |
| O | 0.8724091 | -2.892002 | 2.892002 |
| O | 2.892002 | -0.8724091 | 2.892002 |
| O | -3.2452714 | 0.8067042 | -0.8067042 |
| O | -3.2452714 | -0.8067042 | 0.8067042 |
| O | -0.8067042 | 0.8067042 | -3.2452714 |
| O | 0.8067042 | -0.8067042 | -3.2452714 |
| O | -0.8067042 | 3.2452714 | -0.8067042 |
| O | 0.8067042 | 3.2452714 | 0.8067042 |
| O | 0.8067042 | 0.8067042 | 3.2452714 |
| O | -0.8067042 | -0.8067042 | 3.2452714 |
| O | -0.8067042 | -3.2452714 | 0.8067042 |
| O | 0.8067042 | -3.2452714 | -0.8067042 |
| O | 3.2452714 | -0.8067042 | -0.8067042 |
| O | 3.2452714 | 0.8067042 | 0.8067042 |
| O | -1.3283618 | 1.3283618 | 4.965259 |
| O | -1.3283618 | 4.965259 | 1.3283618 |
| O | -4.965259 | 1.3283618 | 1.3283618 |
| O | 4.965259 | 1.3283618 | -1.3283618 |
| O | 1.3283618 | 1.3283618 | -4.965259 |
| O | 1.3283618 | 4.965259 | -1.3283618 |
| O | -1.3283618 | -4.965259 | -1.3283618 |
| O | -4.965259 | -1.3283618 | -1.3283618 |
| O | -1.3283618 | -1.3283618 | -4.965259 |
| O | 1.3283618 | -1.3283618 | 4.965259 |
| O | 4.965259 | -1.3283618 | 1.3283618 |
| O | 1.3283618 | -4.965259 | 1.3283618 |
| H | -3.4729318 | 3.4729318 | 1.40389 |
| H | -3.4729318 | 1.40389 | 3.4729318 |
| H | -1.40389 | 3.4729318 | 3.4729318 |
| H | 1.40389 | 3.4729318 | -3.4729318 |
| H | 3.4729318 | 3.4729318 | -1.40389 |

| | | | |
|---|---|---|---|
| H | 3.4729318 | 1.40389 | -3.4729318 |
| H | -3.4729318 | -1.40389 | -3.4729318 |
| H | -1.40389 | -3.4729318 | -3.4729318 |
| H | -3.4729318 | -3.4729318 | -1.40389 |
| H | 3.4729318 | -3.4729318 | 1.40389 |
| H | 1.40389 | -3.4729318 | 3.4729318 |
| H | 3.4729318 | -1.40389 | 3.4729318 |
| H | -3.2352886 | 1.4941237 | -1.4941237 |
| H | -3.2352886 | -1.4941237 | 1.4941237 |
| H | 1.4941237 | -1.4941237 | -3.2352886 |
| H | -1.4941237 | 1.4941237 | -3.2352886 |
| H | -1.4941237 | 3.2352886 | -1.4941237 |
| H | 1.4941237 | 3.2352886 | 1.4941237 |
| H | 1.4941237 | 1.4941237 | 3.2352886 |
| H | -1.4941237 | -1.4941237 | 3.2352886 |
| H | -1.4941237 | -3.2352886 | 1.4941237 |
| H | 1.4941237 | -3.2352886 | -1.4941237 |
| H | 3.2352886 | -1.4941237 | -1.4941237 |
| H | 3.2352886 | 1.4941237 | 1.4941237 |
| H | -1.6377238 | 0.5217184 | 5.4370388 |
| H | -0.5217184 | 1.6377238 | 5.4370388 |
| H | -0.5217184 | 5.4370388 | 1.6377238 |
| H | -1.6377238 | 5.4370388 | 0.5217184 |
| H | -5.4370388 | 1.6377238 | 0.5217184 |
| H | -5.4370388 | 0.5217184 | 1.6377238 |
| H | 5.4370388 | 1.6377238 | -0.5217184 |
| H | 5.4370388 | 0.5217184 | -1.6377238 |
| H | 1.6377238 | 0.5217184 | -5.4370388 |
| H | 0.5217184 | 1.6377238 | -5.4370388 |
| H | 0.5217184 | 5.4370388 | -1.6377238 |
| H | 1.6377238 | 5.4370388 | -0.5217184 |
| H | -0.5217184 | -5.4370388 | -1.6377238 |
| H | -1.6377238 | -5.4370388 | -0.5217184 |
| H | -5.4370388 | -1.6377238 | -0.5217184 |
| H | -5.4370388 | -0.5217184 | -1.6377238 |
| H | -1.6377238 | -0.5217184 | -5.4370388 |
| H | -0.5217184 | -1.6377238 | -5.4370388 |
| H | 1.6377238 | -0.5217184 | 5.4370388 |
| H | 0.5217184 | -1.6377238 | 5.4370388 |
| H | 5.4370388 | -1.6377238 | 0.5217184 |
| H | 5.4370388 | -0.5217184 | 1.6377238 |
| H | 0.5217184 | -5.4370388 | 1.6377238 |
| H | 1.6377238 | -5.4370388 | 0.5217184 |

Table S23. $SiAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Si | 0 | 0 | 0 |
| Al | -1.0062193 | 1.0062193 | 3.0830438 |
| Al | -1.0062193 | 3.0830438 | 1.0062193 |
| Al | -3.0830438 | 1.0062193 | 1.0062193 |
| Al | 3.0830438 | 1.0062193 | -1.0062193 |
| Al | 1.0062193 | 1.0062193 | -3.0830438 |
| Al | 1.0062193 | 3.0830438 | -1.0062193 |
| Al | -1.0062193 | -3.0830438 | -1.0062193 |
| Al | -3.0830438 | -1.0062193 | -1.0062193 |
| Al | -1.0062193 | -1.0062193 | -3.0830438 |
| Al | 1.0062193 | -1.0062193 | 3.0830438 |
| Al | 3.0830438 | -1.0062193 | 1.0062193 |
| Al | 1.0062193 | -3.0830438 | 1.0062193 |
| O | 0.9856374 | -0.9856374 | 0.9856374 |
| O | -0.9856374 | 0.9856374 | 0.9856374 |
| O | 0.9856374 | 0.9856374 | -0.9856374 |
| O | -0.9856374 | -0.9856374 | -0.9856374 |
| O | -2.8297563 | 2.8297563 | 0.8779338 |
| O | -2.8297563 | 0.8779338 | 2.8297563 |
| O | -0.8779338 | 2.8297563 | 2.8297563 |
| O | 0.8779338 | 2.8297563 | -2.8297563 |
| O | 2.8297563 | 2.8297563 | -0.8779338 |
| O | 2.8297563 | 0.8779338 | -2.8297563 |
| O | -2.8297563 | -0.8779338 | -2.8297563 |
| O | -0.8779338 | -2.8297563 | -2.8297563 |
| O | -2.8297563 | -2.8297563 | -0.8779338 |
| O | 2.8297563 | -2.8297563 | 0.8779338 |
| O | 0.8779338 | -2.8297563 | 2.8297563 |
| O | 2.8297563 | -0.8779338 | 2.8297563 |
| O | -3.1727571 | 0.8157166 | -0.8157166 |
| O | -3.1727571 | -0.8157166 | 0.8157166 |
| O | -0.8157166 | 0.8157166 | -3.1727571 |
| O | 0.8157166 | -0.8157166 | -3.1727571 |
| O | -0.8157166 | 3.1727571 | -0.8157166 |
| O | 0.8157166 | 3.1727571 | 0.8157166 |
| O | 0.8157166 | 0.8157166 | 3.1727571 |
| O | -0.8157166 | -0.8157166 | 3.1727571 |
| O | -0.8157166 | -3.1727571 | 0.8157166 |
| O | 0.8157166 | -3.1727571 | -0.8157166 |
| O | 3.1727571 | -0.8157166 | -0.8157166 |
| O | 3.1727571 | 0.8157166 | 0.8157166 |
| O | -1.295541 | 1.295541 | 4.97717 |
| O | -1.295541 | 4.97717 | 1.295541 |
| O | -4.97717 | 1.295541 | 1.295541 |

| | | | |
|---|---|---|---|
| O | 4.97717 | 1.295541 | -1.295541 |
| O | 1.295541 | 1.295541 | -4.97717 |
| O | 1.295541 | 4.97717 | -1.295541 |
| O | -1.295541 | -4.97717 | -1.295541 |
| O | -4.97717 | -1.295541 | -1.295541 |
| O | -1.295541 | -1.295541 | -4.97717 |
| O | 1.295541 | -1.295541 | 4.97717 |
| O | 4.97717 | -1.295541 | 1.295541 |
| O | 1.295541 | -4.97717 | 1.295541 |
| H | -3.4188524 | 3.4188524 | 1.3944924 |
| H | -3.4188524 | 1.3944924 | 3.4188524 |
| H | -1.3944924 | 3.4188524 | 3.4188524 |
| H | 1.3944924 | 3.4188524 | -3.4188524 |
| H | 3.4188524 | 3.4188524 | -1.3944924 |
| H | 3.4188524 | 1.3944924 | -3.4188524 |
| H | -3.4188524 | -1.3944924 | -3.4188524 |
| H | -1.3944924 | -3.4188524 | -3.4188524 |
| H | -3.4188524 | -3.4188524 | -1.3944924 |
| H | 3.4188524 | -3.4188524 | 1.3944924 |
| H | 1.3944924 | -3.4188524 | 3.4188524 |
| H | 3.4188524 | -1.3944924 | 3.4188524 |
| H | -3.3671342 | 1.4899598 | -1.4899598 |
| H | -3.3671342 | -1.4899598 | 1.4899598 |
| H | 1.4899598 | -1.4899598 | -3.3671342 |
| H | -1.4899598 | 1.4899598 | -3.3671342 |
| H | -1.4899598 | 3.3671342 | -1.4899598 |
| H | 1.4899598 | 3.3671342 | 1.4899598 |
| H | 1.4899598 | 1.4899598 | 3.3671342 |
| H | -1.4899598 | -1.4899598 | 3.3671342 |
| H | -1.4899598 | -3.3671342 | 1.4899598 |
| H | 1.4899598 | -3.3671342 | -1.4899598 |
| H | 3.3671342 | -1.4899598 | -1.4899598 |
| H | 3.3671342 | 1.4899598 | 1.4899598 |
| H | -1.6585704 | 0.5387529 | 5.4930868 |
| H | -0.5387529 | 1.6585704 | 5.4930868 |
| H | -0.5387529 | 5.4930868 | 1.6585704 |
| H | -1.6585704 | 5.4930868 | 0.5387529 |
| H | -5.4930868 | 1.6585704 | 0.5387529 |
| H | -5.4930868 | 0.5387529 | 1.6585704 |
| H | 5.4930868 | 1.6585704 | -0.5387529 |
| H | 5.4930868 | 0.5387529 | -1.6585704 |
| H | 1.6585704 | 0.5387529 | -5.4930868 |
| H | 0.5387529 | 1.6585704 | -5.4930868 |
| H | 0.5387529 | 5.4930868 | -1.6585704 |
| H | 1.6585704 | 5.4930868 | -0.5387529 |

| | | | |
|---|---|---|---|
| H | -0.5387529 | -5.4930868 | -1.6585704 |
| H | -1.6585704 | -5.4930868 | -0.5387529 |
| H | -5.4930868 | -1.6585704 | -0.5387529 |
| H | -5.4930868 | -0.5387529 | -1.6585704 |
| H | -1.6585704 | -0.5387529 | -5.4930868 |
| H | -0.5387529 | -1.6585704 | -5.4930868 |
| H | 1.6585704 | -0.5387529 | 5.4930868 |
| H | 0.5387529 | -1.6585704 | 5.4930868 |
| H | 5.4930868 | -1.6585704 | 0.5387529 |
| H | 5.4930868 | -0.5387529 | 1.6585704 |
| H | 0.5387529 | -5.4930868 | 1.6585704 |
| H | 1.6585704 | -5.4930868 | 0.5387529 |

Table S24. $FeAl_{12}$:

| Symbol | X | Y | Z |
|---|---|---|---|
| Fe | -0.0020727 | 0.0106082 | -0.020595 |
| Al | -1.4979294 | 2.941831 | -0.5786737 |
| Al | 0.4579928 | 2.9785607 | 1.5629787 |
| Al | 1.317614 | 2.8917563 | -1.1735456 |
| Al | -1.016915 | -1.5655777 | 2.7976263 |
| Al | 1.7887282 | -1.848341 | 2.1372823 |
| Al | 0.8012671 | 0.6286174 | 3.2065116 |
| Al | 0.8877566 | -1.8321 | -2.6963772 |
| Al | 2.5278499 | 0.4805245 | -2.1813987 |
| Al | 2.7890035 | -1.8911074 | -0.5582815 |
| Al | -3.1478395 | 0.6454316 | -1.1304533 |
| Al | -2.9241994 | -1.6094969 | 0.6219111 |
| Al | -1.9295326 | -1.7961895 | -2.0702627 |
| O | -1.7133708 | -0.6022726 | -0.5479054 |
| O | 0.0544666 | 1.8907556 | -0.0350049 |
| O | 0.3227682 | -0.5960687 | 1.7374634 |
| O | 1.3261193 | -0.6957231 | -1.1714561 |
| O | 1.6382868 | 3.8360532 | 0.4168008 |
| O | -0.2357398 | 3.7992946 | -1.6628808 |
| O | -1.0987928 | 3.8300651 | 1.0128416 |
| O | 2.1725929 | -0.5906408 | 3.478763 |
| O | -0.5524015 | -0.3249679 | 4.0918113 |
| O | 0.4173431 | -2.7336603 | 3.0275922 |
| O | 3.8295403 | -0.6644826 | -1.4790467 |
| O | 2.24986 | -2.9087599 | -2.0367124 |
| O | 1.9761814 | -0.6077328 | -3.5921952 |
| O | -2.9709599 | -2.7497688 | -0.8605469 |
| O | -3.221112 | -0.5283484 | -2.5610701 |
| O | -4.1850986 | -0.3797041 | 0.0500439 |
| O | 2.7252881 | 1.7245377 | -0.8083783 |

| | | | |
|---|---|---|---|
| O | 1.2366343 | 1.7490907 | -2.6266252 |
| O | 3.0739457 | -1.0543368 | 1.0601514 |
| O | 1.6389949 | -2.8416762 | 0.5595135 |
| O | 1.8095499 | 1.766379 | 2.0983563 |
| O | -0.4269357 | 1.9563607 | 2.8205777 |
| O | -2.7752506 | 1.8490336 | 0.2339993 |
| O | -2.0092964 | 1.8270957 | -1.9951318 |
| O | -0.6715317 | -0.9501543 | -3.1493492 |
| O | -0.3789692 | -2.8079957 | -1.670754 |
| O | -1.6903366 | -2.665093 | 1.4750322 |
| O | -2.430834 | -0.4944072 | 2.0977052 |
| O | -2.7742509 | 4.3549267 | -0.9657631 |
| O | 0.76904 | 4.3963339 | 2.8534685 |
| O | 2.4048453 | 4.2518007 | -2.0358865 |
| O | -2.013094 | -2.507463 | 4.1757535 |
| O | 3.0063798 | -3.1033999 | 2.9927473 |
| O | 1.2535699 | 1.4413757 | 4.9179969 |
| O | 0.8339102 | -2.9147162 | -4.3035 |
| O | 3.9422966 | 1.2208409 | -3.291187 |
| O | 4.2932406 | -3.1121955 | -0.4327682 |
| O | -4.8199129 | 1.4596147 | -1.684711 |
| O | -4.3922665 | -2.5730492 | 1.4520779 |
| O | -2.5745758 | -2.9146094 | -3.5178852 |
| H | 1.5836576 | 4.8130011 | 0.3614014 |
| H | -0.2219465 | 4.7780636 | -1.6925811 |
| H | -1.1770024 | 4.8037735 | 1.0742083 |
| H | 2.3155731 | -0.9189289 | 4.3908338 |
| H | -0.3641614 | -0.6371318 | 5.0012957 |
| H | 0.5895126 | -3.1478481 | 3.8977426 |
| H | 4.5349234 | -0.9791172 | -2.080852 |
| H | 2.9630411 | -3.1930086 | -2.645642 |
| H | 2.61199 | -0.9383932 | -4.2588819 |
| H | -3.8193142 | -3.1521186 | -1.1379995 |
| H | -4.0891911 | -0.8228934 | -2.9047125 |
| H | -5.0346232 | -0.7218822 | -0.2987116 |
| H | 2.8007584 | 1.4314013 | 0.1302356 |
| H | 0.8871564 | 1.9493086 | -3.5157291 |
| H | 0.7893132 | -3.0406043 | 0.0961925 |
| H | 3.7962895 | -0.4691971 | 1.3564006 |
| H | 2.6971969 | 2.079667 | 2.3672752 |
| H | -1.3872255 | 1.8082935 | 2.9193859 |
| H | -2.6334396 | 1.4003813 | 1.101083 |
| H | -2.0033472 | 2.0846804 | -2.9373454 |
| H | -0.6874295 | 0.0287606 | -3.2173035 |
| H | -0.4030227 | -3.7868917 | -1.700702 |

| | | | |
|---|---|---|---|
| H | -1.2562108 | -3.4556064 | 1.1018338 |
| H | -3.14665 | -0.2324988 | 2.7151327 |
| H | -3.0744255 | 4.5017697 | -1.8911603 |
| H | -3.5701444 | 4.3913093 | -0.3873352 |
| H | 0.2080872 | 4.3969312 | 3.6616632 |
| H | 1.672351 | 4.6881741 | 3.109743 |
| H | 3.3339969 | 4.3062536 | -1.7148863 |
| H | 2.4251227 | 4.3168192 | -3.0171619 |
| H | -2.6284485 | -2.0797227 | 4.8119356 |
| H | -2.3460885 | -3.4123297 | 3.9846716 |
| H | 2.9561275 | -4.0337952 | 2.6746383 |
| H | 3.9590405 | -2.8638901 | 3.0487021 |
| H | 2.1513174 | 1.7826906 | 5.1295072 |
| H | 0.5972553 | 2.0894857 | 5.259965 |
| H | 0.7496989 | -3.8943818 | -4.288337 |
| H | 0.2923626 | -2.5710133 | -5.0494941 |
| H | 3.7184043 | 1.716569 | -4.1105482 |
| H | 4.6451784 | 1.7245778 | -2.8209035 |
| H | 5.0528875 | -2.8686549 | 0.1428715 |
| H | 4.0602215 | -4.0483009 | -0.2361491 |
| H | -5.3148219 | 1.9275573 | -0.9739052 |
| H | -4.8726313 | 2.0092569 | -2.4988203 |
| H | -4.1918637 | -3.4325656 | 1.8851855 |
| H | -5.0947755 | -2.1225087 | 1.972226 |
| H | -2.4709705 | -2.5536122 | -4.4274716 |
| H | -2.4358345 | -3.8874414 | -3.5595046 |

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