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 $\text{Al}_{48.18}\text{Cr}_{22.78}\text{Fe}_{4.04}\text{Si}_3$ Xinyu Liang,^a Changzeng Fan,^{a,b*} Bin Wen^a and Lifeng Zhang^{a,c}

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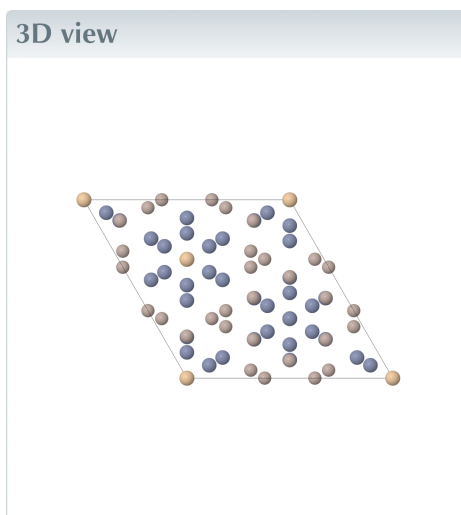
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Structural data: full structural data are available from iucrdata.iucr.org

A mixture with the initial chemical composition $\text{Al}_{59}\text{Cr}_{21}\text{Fe}_{10}\text{Si}_{10}$ was subjected to high-pressure sintering, resulting in the unexpected synthesis of an intermetallic compound with the composition $\text{Al}_{48.18}\text{Cr}_{22.78}\text{Fe}_{4.04}\text{Si}_3$, which adopts the $\text{Cr}_{0.88}\text{Fe}_{0.12}\text{Ga}$ structure type in the space group $R\bar{3}m$. Structural analysis indicates that Al, Cr and Fe jointly occupy a special position (Wyckoff site $18h$), with refined site occupancy factors of 0.676 (6), 0.17 (2) and 0.16 (2), respectively. Cr and Fe share another special position (Wyckoff site $3b$), with refined site occupancy factors of 0.60 (6) and 0.40 (6), respectively. Other atoms in the crystal (Al and Si) fully occupy their sites.



Structure description

Quaternary decagonal quasicrystals (DQC) have been discovered in a few systems, for example, Ga–Fe–Cu–Si, Ga–V–Ni–Si and Al–Mn–Fe–Ge. However, there have been far fewer detailed studies of the stability of quaternary DQCs and correspondingly, there is far less atomic-scale structural information. The quaternary Al–Cr–Fe–Si DQCs exhibit distinctive structural characteristics, thereby constituting a novel structural class of DQCs. Specifically, the presence of multiple types of 2-nm decagons exhibiting both perfect and destructive tenfold symmetry within Al–Cr–Fe–Si DQCs is noteworthy, as such a phenomenon is rarely observed in other DQCs. This observation is likely to generate considerable interest, as the 2-nm decagons constitute the most significant structural element of DQCs. Therefore, it is imperative that an exhaustive study of the thermodynamic stability and the corresponding atomic-scale structural information to be conducted.

Ma *et al.* (2018, 2020) discovered the DQC $\text{Al}_{59}\text{Cr}_{21}\text{Fe}_{10}\text{Si}_{10}$ by melting the quaternary alloy $\text{Al}_{60}\text{Cr}_{20}\text{Fe}_{10}\text{Si}_{10}$ in an induction furnace under an argon atmosphere, using high-purity elements. The molten alloy was then poured into a graphite crucible in the furnace



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Refinement

Table 1 shows the details of data collection and structural refinement. The labelling scheme and atomic coordinates of $\text{Al}_{48.18}\text{Cr}_{22.78}\text{Fe}_{4.04}\text{Si}_3$ were adapted from $\text{Cr}_{0.88}\text{Fe}_{0.12}\text{Ga}$ for better comparison. One site is co-occupied by Al, Cr and Fe atoms (Al1/Cr3/Fe1), and site occupancies were refined to 0.676 (6) for Al, 0.17 (2) for Cr and 0.16 (2) for Fe. Another site is co-occupied by Cr and Fe (Cr2/Fe2), and site occupancies were refined to 0.60 (6) for Cr and 0.40 (6) for Fe. Atoms sharing the same position were constrained to have identical coordinates and displacement parameters. The maximum and minimum residual electron densities in the last difference map are located 1.18 Å from atom Si1 and 0.75 Å from atom Al3, respectively.

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References

- Brandenburg, K. & Putz, H. (2017). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2023). *APEX5* and *SAINT*. Bruker AXS Inc. Madison, Wisconsin, USA, 2008.
- Hu, Q., Wen, B. & Fan, C. (2021). *IUCrData* **6**, x210988.
- Ko, H., Gourdon, O., Gout, D., Mun, E.-D., Thimmaiah, S. & Miller, G. J. (2010). *Inorg. Chem.* **49**, 11505–11515.
- Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
- Liu, C. & Fan, C. (2018). *IUCrData* **3**, x180363.
- Ma, H., He, Z., Hou, L. & Steurer, W. (2018). *J. Alloys Compd.* **765**, 753–756.
- Ma, H., You, L. & He, Z. (2020). *Mater. Charact.* **166**, 110424.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

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Aluminium chromium iron silicide

Crystal data

$$\text{Al}_{48.18}\text{Cr}_{22.78}\text{Fe}_{4.04}\text{Si}_3$$

$$M_r = 2794.43$$

Trigonal, $R\bar{3}m:H$

$$a = 12.5478 (9) \text{ \AA}$$

$$c = 7.9296 (9) \text{ \AA}$$

$$V = 1081.2 (2) \text{ \AA}^3$$

$$Z = 1$$

$$F(000) = 1320$$

$$D_x = 4.292 \text{ Mg m}^{-3}$$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2885 reflections

$$\theta = 3.2\text{--}28.5^\circ$$

$$\mu = 7.85 \text{ mm}^{-1}$$

$$T = 296 \text{ K}$$

Lump, grey

$$0.08 \times 0.06 \times 0.06 \text{ mm}$$

Data collection

Bruker D8 Venture Photon 100 CMOS
diffractometer

phi and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$$T_{\min} = 0.574, T_{\max} = 0.746$$

10693 measured reflections

417 independent reflections

338 reflections with $I > 2\sigma(I)$

$$R_{\text{int}} = 0.099$$

$$\theta_{\max} = 30.5^\circ, \theta_{\min} = 3.2^\circ$$

$$h = -17 \rightarrow 17$$

$$k = -17 \rightarrow 17$$

$$l = -11 \rightarrow 11$$

Refinement

Refinement on F^2

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.031$$

$$wR(F^2) = 0.047$$

$$S = 1.13$$

417 reflections

32 parameters

1 restraint

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

$$w = 1/[\sigma^2(F_o^2) + (0.0136P)^2 + 4.4686P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} = 0.004$$

$$\Delta\rho_{\max} = 0.55 \text{ e \AA}^{-3}$$

$$\Delta\rho_{\min} = -1.03 \text{ e \AA}^{-3}$$
Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|--------------|--------------|--------------|----------------------------------|-----------|
| Al1 | −0.07243 (4) | 0.07243 (4) | 0.24743 (10) | 0.0082 (3) | 0.676 (6) |
| Al2 | 0.37822 (10) | 0.37822 (10) | 0.500000 | 0.0096 (3) | |
| Al3 | 0.23539 (11) | 0.11769 (5) | 0.57349 (15) | 0.0108 (3) | |
| Cr3 | −0.07243 (4) | 0.07243 (4) | 0.24743 (10) | 0.0082 (3) | 0.17 (2) |
| Si1 | 0.000000 | 0.000000 | 0.000000 | 0.0127 (6) | |
| Fe1 | −0.07243 (4) | 0.07243 (4) | 0.24743 (10) | 0.0082 (3) | 0.16 (2) |
| Cr1 | 0.43537 (5) | 0.21768 (3) | 0.40484 (7) | 0.00680 (18) | |

| | | | | | |
|-----|----------|----------|----------|------------|----------|
| Cr2 | 0.000000 | 0.000000 | 0.500000 | 0.0035 (4) | 0.60 (6) |
| Fe2 | 0.000000 | 0.000000 | 0.500000 | 0.0035 (4) | 0.40 (6) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|-------------|--------------|---------------|--------------|
| Al1 | 0.0089 (4) | 0.0089 (4) | 0.0056 (4) | 0.0033 (4) | −0.00109 (17) | 0.00109 (17) |
| Al2 | 0.0107 (5) | 0.0107 (5) | 0.0092 (5) | 0.0068 (5) | 0.0011 (2) | −0.0011 (2) |
| Al3 | 0.0066 (6) | 0.0125 (5) | 0.0114 (6) | 0.0033 (3) | −0.0012 (5) | −0.0006 (2) |
| Cr3 | 0.0089 (4) | 0.0089 (4) | 0.0056 (4) | 0.0033 (4) | −0.00109 (17) | 0.00109 (17) |
| Si1 | 0.0162 (9) | 0.0162 (9) | 0.0057 (12) | 0.0081 (5) | 0.000 | 0.000 |
| Fe1 | 0.0089 (4) | 0.0089 (4) | 0.0056 (4) | 0.0033 (4) | −0.00109 (17) | 0.00109 (17) |
| Cr1 | 0.0084 (3) | 0.0068 (3) | 0.0057 (3) | 0.00420 (17) | 0.0003 (2) | 0.00016 (12) |
| Cr2 | 0.0035 (5) | 0.0035 (5) | 0.0036 (7) | 0.0017 (3) | 0.000 | 0.000 |
| Fe2 | 0.0035 (5) | 0.0035 (5) | 0.0036 (7) | 0.0017 (3) | 0.000 | 0.000 |

Geometric parameters (Å, °)

| | | | |
|---|-------------|--|--------------|
| Al1—Si1 | 2.5154 (9) | Al2—Al2 ^{ix} | 2.8175 (8) |
| Al1—Fe2 | 2.5473 (8) | Al2—Al3 | 2.8947 (12) |
| Al1—Cr2 | 2.5473 (8) | Al2—Al3 ^{iv} | 2.8948 (12) |
| Al1—Cr1 ⁱ | 2.6048 (7) | Al3—Cr1 | 2.5516 (13) |
| Al1—Cr1 ⁱⁱ | 2.6048 (7) | Al3—Al3 ^{xi} | 2.591 (2) |
| Al1—Al2 ⁱ | 2.6344 (10) | Al3—Fe2 | 2.6234 (12) |
| Al1—Al2 ⁱⁱⁱ | 2.6344 (10) | Al3—Cr2 | 2.6234 (12) |
| Al1—Al3 ^{iv} | 2.6478 (11) | Al3—Al3 ^{iv} | 2.8108 (14) |
| Al1—Al3 ^v | 2.6478 (11) | Al3—Al3 ^{xii} | 2.8108 (14) |
| Al1—Cr1 ^{vi} | 2.6979 (10) | Al3—Cr1 ^{xi} | 2.8154 (14) |
| Al1—Al1 ^{vii} | 2.7264 (16) | Si1—Cr1 ^{xiii} | 2.5766 (6) |
| Al1—Al1 ^{viii} | 2.7264 (16) | Si1—Cr1 ⁱⁱ | 2.5766 (6) |
| Al2—Cr1 ^{iv} | 2.5663 (4) | Si1—Cr1 ⁱ | 2.5766 (6) |
| Al2—Cr1 | 2.5663 (4) | Si1—Cr1 ^{xiv} | 2.5766 (6) |
| Al2—Cr1 ^{ix} | 2.6705 (8) | Cr1—Cr1 ^x | 2.7575 (7) |
| Al2—Cr1 ^x | 2.6705 (8) | Cr1—Cr1 ^{xv} | 2.7576 (7) |
| Al2—Al2 ⁱⁱ | 2.8175 (8) | | |
| Si1—Al1—Fe2 | 103.10 (3) | Al1 ^{xix} —Si1—Cr1 ^{xiii} | 116.03 (2) |
| Si1—Al1—Cr2 | 103.10 (3) | Al1 ^{viii} —Si1—Cr1 ^{xiii} | 63.97 (2) |
| Si1—Al1—Cr1 ⁱ | 60.40 (2) | Al1—Si1—Cr1 ^{xiii} | 118.481 (11) |
| Cr2—Al1—Cr1 ⁱ | 110.23 (2) | Al1 ^{xvii} —Si1—Cr1 ⁱⁱ | 118.482 (11) |
| Si1—Al1—Cr1 ⁱⁱ | 60.40 (2) | Al1 ^{vii} —Si1—Cr1 ⁱⁱ | 61.518 (11) |
| Fe2—Al1—Cr1 ⁱⁱ | 110.23 (2) | Al1 ^{xviii} —Si1—Cr1 ⁱⁱ | 118.481 (11) |
| Cr2—Al1—Cr1 ⁱⁱ | 110.23 (2) | Al1 ^{xix} —Si1—Cr1 ⁱⁱ | 63.97 (2) |
| Cr1 ⁱ —Al1—Cr1 ⁱⁱ | 113.37 (4) | Al1 ^{viii} —Si1—Cr1 ⁱⁱ | 116.03 (2) |
| Si1—Al1—Al2 ⁱ | 107.27 (3) | Al1—Si1—Cr1 ⁱⁱ | 61.519 (11) |
| Cr2—Al1—Al2 ⁱ | 132.19 (3) | Cr1 ^{xiii} —Si1—Cr1 ⁱⁱ | 180.0 |
| Cr1 ⁱ —Al1—Al2 ⁱ | 58.65 (2) | Al1 ^{xvii} —Si1—Cr1 ⁱ | 63.97 (2) |
| Cr1 ⁱⁱ —Al1—Al2 ⁱ | 116.70 (4) | Al1 ^{vii} —Si1—Cr1 ⁱ | 116.03 (2) |

| | | | |
|---|--------------|--|--------------|
| Si1—Al1—Al2 ⁱⁱⁱ | 107.27 (3) | Al1 ^{xviii} —Si1—Cr1 ⁱ | 118.481 (11) |
| Cr2—Al1—Al2 ⁱⁱⁱ | 132.19 (3) | Al1 ^{xix} —Si1—Cr1 ⁱ | 118.482 (11) |
| Cr1 ⁱ —Al1—Al2 ⁱⁱⁱ | 116.70 (4) | Al1 ^{viii} —Si1—Cr1 ⁱ | 61.518 (11) |
| Cr1 ⁱⁱ —Al1—Al2 ⁱⁱⁱ | 58.65 (2) | Al1—Si1—Cr1 ⁱ | 61.519 (11) |
| Al2 ⁱ —Al1—Al2 ⁱⁱⁱ | 70.91 (5) | Cr1 ^{xiii} —Si1—Cr1 ⁱ | 64.698 (9) |
| Si1—Al1—Al3 ^{iv} | 110.40 (3) | Cr1 ⁱⁱ —Si1—Cr1 ⁱ | 115.302 (9) |
| Cr2—Al1—Al3 ^{iv} | 60.62 (3) | Al1 ^{xvii} —Si1—Cr1 ^{xiv} | 116.03 (2) |
| Cr1 ⁱ —Al1—Al3 ^{iv} | 166.60 (4) | Al1 ^{vii} —Si1—Cr1 ^{xiv} | 63.97 (2) |
| Cr1 ⁱⁱ —Al1—Al3 ^{iv} | 64.82 (3) | Al1 ^{xviii} —Si1—Cr1 ^{xiv} | 61.519 (11) |
| Al2 ⁱ —Al1—Al3 ^{iv} | 134.61 (4) | Al1 ^{xix} —Si1—Cr1 ^{xiv} | 61.518 (11) |
| Al2 ⁱⁱⁱ —Al1—Al3 ^{iv} | 74.44 (3) | Al1 ^{viii} —Si1—Cr1 ^{xiv} | 118.482 (11) |
| Si1—Al1—Al3 ^v | 110.40 (3) | Al1—Si1—Cr1 ^{xiv} | 118.481 (11) |
| Cr2—Al1—Al3 ^v | 60.62 (3) | Cr1 ^{xiii} —Si1—Cr1 ^{xiv} | 115.302 (9) |
| Cr1 ⁱ —Al1—Al3 ^v | 64.82 (3) | Cr1 ⁱⁱ —Si1—Cr1 ^{xiv} | 64.698 (9) |
| Cr1 ⁱⁱ —Al1—Al3 ^v | 166.60 (4) | Cr1 ⁱ —Si1—Cr1 ^{xiv} | 180.000 (16) |
| Al2 ⁱ —Al1—Al3 ^v | 74.44 (3) | Al3—Cr1—Al2 ^{xii} | 68.89 (3) |
| Al2 ⁱⁱⁱ —Al1—Al3 ^v | 134.61 (4) | Al3—Cr1—Al2 | 68.89 (3) |
| Al3 ^{iv} —Al1—Al3 ^v | 113.57 (6) | Al2 ^{xii} —Cr1—Al2 | 135.23 (5) |
| Si1—Al1—Cr1 ^{vi} | 59.12 (2) | Al3—Cr1—Si1 ^{xvi} | 161.11 (3) |
| Cr2—Al1—Cr1 ^{vi} | 162.21 (4) | Al2 ^{xii} —Cr1—Si1 ^{xvi} | 107.50 (3) |
| Cr1 ⁱ —Al1—Cr1 ^{vi} | 62.639 (19) | Al2—Cr1—Si1 ^{xvi} | 107.50 (3) |
| Cr1 ⁱⁱ —Al1—Cr1 ^{vi} | 62.639 (19) | Al3—Cr1—Al1 ^{ix} | 106.49 (3) |
| Al2 ⁱ —Al1—Cr1 ^{vi} | 60.09 (2) | Al2 ^{xii} —Cr1—Al1 ^{ix} | 61.25 (3) |
| Al2 ⁱⁱⁱ —Al1—Cr1 ^{vi} | 60.09 (2) | Al2—Cr1—Al1 ^{ix} | 119.13 (3) |
| Al3 ^{iv} —Al1—Cr1 ^{vi} | 122.79 (3) | Si1 ^{xvi} —Cr1—Al1 ^{ix} | 58.08 (2) |
| Al3 ^v —Al1—Cr1 ^{vi} | 122.79 (3) | Al3—Cr1—Al1 ^{xvi} | 106.49 (3) |
| Si1—Al1—Al1 ^{vii} | 57.184 (16) | Al2 ^{xii} —Cr1—Al1 ^{xvi} | 119.13 (3) |
| Fe2—Al1—Al1 ^{vii} | 57.646 (16) | Al2—Cr1—Al1 ^{xvi} | 61.25 (3) |
| Cr2—Al1—Al1 ^{vii} | 57.646 (16) | Si1 ^{xvi} —Cr1—Al1 ^{xvi} | 58.08 (2) |
| Cr1 ⁱ —Al1—Al1 ^{vii} | 108.20 (2) | Al1 ^{ix} —Cr1—Al1 ^{xvi} | 63.11 (4) |
| Cr1 ⁱⁱ —Al1—Al1 ^{vii} | 58.44 (2) | Al3—Cr1—Al2 ⁱⁱ | 90.98 (3) |
| Al2 ⁱ —Al1—Al1 ^{vii} | 164.434 (19) | Al2 ^{xii} —Cr1—Al2 ⁱⁱ | 129.54 (2) |
| Al2 ⁱⁱⁱ —Al1—Al1 ^{vii} | 112.54 (2) | Al2—Cr1—Al2 ⁱⁱ | 65.06 (3) |
| Al3 ^{iv} —Al1—Al1 ^{vii} | 59.01 (2) | Si1 ^{xvi} —Cr1—Al2 ⁱⁱ | 104.440 (18) |
| Al3 ^v —Al1—Al1 ^{vii} | 108.77 (3) | Al1 ^{ix} —Cr1—Al2 ⁱⁱ | 162.44 (3) |
| Cr1 ^{vi} —Al1—Al1 ^{vii} | 107.55 (2) | Al1 ^{xvi} —Cr1—Al2 ⁱⁱ | 110.76 (3) |
| Si1—Al1—Al1 ^{viii} | 57.184 (16) | Al3—Cr1—Al2 ^{xv} | 90.98 (3) |
| Cr2—Al1—Al1 ^{viii} | 57.646 (16) | Al2 ^{xii} —Cr1—Al2 ^{xv} | 65.06 (3) |
| Cr1 ⁱ —Al1—Al1 ^{viii} | 58.44 (2) | Al2—Cr1—Al2 ^{xv} | 129.54 (2) |
| Cr1 ⁱⁱ —Al1—Al1 ^{viii} | 108.20 (2) | Si1 ^{xvi} —Cr1—Al2 ^{xv} | 104.441 (18) |
| Al2 ⁱ —Al1—Al1 ^{viii} | 112.54 (2) | Al1 ^{ix} —Cr1—Al2 ^{xv} | 110.76 (3) |
| Al2 ⁱⁱⁱ —Al1—Al1 ^{viii} | 164.434 (19) | Al1 ^{xvi} —Cr1—Al2 ^{xv} | 162.44 (3) |
| Al3 ^{iv} —Al1—Al1 ^{viii} | 108.77 (3) | Al2 ⁱⁱ —Cr1—Al2 ^{xv} | 69.81 (5) |
| Al3 ^v —Al1—Al1 ^{viii} | 59.01 (2) | Al3—Cr1—Al1 ^{xx} | 141.98 (4) |
| Cr1 ^{vi} —Al1—Al1 ^{viii} | 107.55 (2) | Al2 ^{xii} —Cr1—Al1 ^{xx} | 111.094 (17) |
| Al1 ^{vii} —Al1—Al1 ^{viii} | 60.0 | Al2—Cr1—Al1 ^{xx} | 111.092 (17) |
| Cr1 ^{iv} —Al2—Cr1 | 150.72 (6) | Si1 ^{xvi} —Cr1—Al1 ^{xx} | 56.91 (2) |
| Cr1 ^{iv} —Al2—Al1 ^{xvi} | 142.35 (3) | Al1 ^{ix} —Cr1—Al1 ^{xx} | 105.74 (3) |

| | | | |
|--|--------------|---|-------------|
| Cr1—Al2—Al1 ^{xvi} | 60.10 (2) | Al1 ^{xvi} —Cr1—Al1 ^{xx} | 105.74 (3) |
| Cr1 ^{iv} —Al2—Al1 ⁱⁱⁱ | 60.10 (2) | Al2 ⁱⁱ —Cr1—Al1 ^{xx} | 58.77 (2) |
| Cr1—Al2—Al1 ⁱⁱⁱ | 142.35 (3) | Al2 ^{xv} —Cr1—Al1 ^{xx} | 58.77 (2) |
| Al1 ^{xvi} —Al2—Al1 ⁱⁱⁱ | 109.09 (5) | Al3—Cr1—Cr1 ^x | 127.136 (8) |
| Cr1 ^{iv} —Al2—Cr1 ^{ix} | 63.51 (2) | Al2 ^{xii} —Cr1—Cr1 ^x | 163.97 (3) |
| Cr1—Al2—Cr1 ^{ix} | 137.33 (3) | Al2—Cr1—Cr1 ^x | 60.09 (2) |
| Al1 ^{xvi} —Al2—Cr1 ^{ix} | 79.57 (3) | Si1 ^{xvi} —Cr1—Cr1 ^x | 57.649 (5) |
| Al1 ⁱⁱⁱ —Al2—Cr1 ^{ix} | 61.13 (3) | Al1 ^{ix} —Cr1—Cr1 ^x | 109.35 (2) |
| Cr1 ^{iv} —Al2—Cr1 ^x | 137.33 (3) | Al1 ^{xvi} —Cr1—Cr1 ^x | 60.33 (2) |
| Cr1—Al2—Cr1 ^x | 63.51 (2) | Al2 ⁱⁱ —Cr1—Cr1 ^x | 56.40 (2) |
| Al1 ^{xvi} —Al2—Cr1 ^x | 61.13 (3) | Al2 ^{xv} —Cr1—Cr1 ^x | 110.49 (4) |
| Al1 ⁱⁱⁱ —Al2—Cr1 ^x | 79.57 (3) | Al1 ^{xx} —Cr1—Cr1 ^x | 57.03 (2) |
| Cr1 ^{ix} —Al2—Cr1 ^x | 110.19 (5) | Al3—Cr1—Cr1 ^{xv} | 127.134 (8) |
| Cr1 ^{iv} —Al2—Al2 ⁱⁱ | 111.077 (13) | Al2 ^{xii} —Cr1—Cr1 ^{xv} | 60.09 (2) |
| Cr1—Al2—Al2 ⁱⁱ | 59.25 (3) | Al2—Cr1—Cr1 ^{xv} | 163.97 (3) |
| Al1 ^{xvi} —Al2—Al2 ⁱⁱ | 105.509 (18) | Si1 ^{xvi} —Cr1—Cr1 ^{xv} | 57.652 (5) |
| Al1 ⁱⁱⁱ —Al2—Al2 ⁱⁱ | 94.62 (3) | Al1 ^{ix} —Cr1—Cr1 ^{xv} | 60.34 (2) |
| Cr1 ^{ix} —Al2—Al2 ⁱⁱ | 155.09 (5) | Al1 ^{xvi} —Cr1—Cr1 ^{xv} | 109.35 (2) |
| Cr1 ^x —Al2—Al2 ⁱⁱ | 55.681 (11) | Al2 ⁱⁱ —Cr1—Cr1 ^{xv} | 110.49 (4) |
| Cr1 ^{iv} —Al2—Al2 ^{ix} | 59.25 (3) | Al2 ^{xv} —Cr1—Cr1 ^{xv} | 56.40 (2) |
| Cr1—Al2—Al2 ^{ix} | 111.078 (13) | Al1 ^{xx} —Cr1—Cr1 ^{xv} | 57.03 (2) |
| Al1 ^{xvi} —Al2—Al2 ^{ix} | 94.62 (3) | Cr1 ^x —Cr1—Cr1 ^{xv} | 104.26 (3) |
| Al1 ⁱⁱⁱ —Al2—Al2 ^{ix} | 105.509 (18) | Al3—Cr1—Al3 ^{xi} | 57.49 (4) |
| Cr1 ^{ix} —Al2—Al2 ^{ix} | 55.681 (11) | Al2 ^{xii} —Cr1—Al3 ^{xi} | 72.675 (14) |
| Cr1 ^x —Al2—Al2 ^{ix} | 155.09 (5) | Al2—Cr1—Al3 ^{xi} | 72.673 (14) |
| Al2 ⁱⁱ —Al2—Al2 ^{ix} | 145.10 (7) | Si1 ^{xvi} —Cr1—Al3 ^{xi} | 103.62 (3) |
| Cr1 ^{iv} —Al2—Al3 | 97.30 (4) | Al1 ^{ix} —Cr1—Al3 ^{xi} | 58.33 (3) |
| Cr1—Al2—Al3 | 55.32 (3) | Al1 ^{xvi} —Cr1—Al3 ^{xi} | 58.33 (3) |
| Al1 ^{xvi} —Al2—Al3 | 96.58 (3) | Al2 ⁱⁱ —Cr1—Al3 ^{xi} | 134.48 (3) |
| Al1 ⁱⁱⁱ —Al2—Al3 | 154.10 (4) | Al2 ^{xv} —Cr1—Al3 ^{xi} | 134.48 (3) |
| Cr1 ^{ix} —Al2—Al3 | 122.77 (3) | Al1 ^{xx} —Cr1—Al3 ^{xi} | 160.53 (4) |
| Cr1 ^x —Al2—Al3 | 117.33 (3) | Cr1 ^x —Cr1—Al3 ^{xi} | 114.73 (3) |
| Al2 ⁱⁱ —Al2—Al3 | 81.39 (5) | Cr1 ^{xv} —Cr1—Al3 ^{xi} | 114.74 (3) |
| Al2 ^{ix} —Al2—Al3 | 68.01 (3) | Al1 ^{xii} —Cr2—Al1 ^{viii} | 180.0 |
| Cr1 ^{iv} —Al2—Al3 ^{iv} | 55.32 (3) | Al1 ^{xii} —Cr2—Al1 ^v | 64.71 (3) |
| Cr1—Al2—Al3 ^{iv} | 97.30 (4) | Al1 ^{viii} —Cr2—Al1 ^v | 115.29 (3) |
| Al1 ^{xvi} —Al2—Al3 ^{iv} | 154.09 (4) | Al1 ^{xii} —Cr2—Al1 ^{iv} | 64.71 (3) |
| Al1 ⁱⁱⁱ —Al2—Al3 ^{iv} | 96.58 (3) | Al1 ^{viii} —Cr2—Al1 ^{iv} | 115.29 (3) |
| Cr1 ^{ix} —Al2—Al3 ^{iv} | 117.33 (3) | Al1 ^v —Cr2—Al1 ^{iv} | 64.71 (3) |
| Cr1 ^x —Al2—Al3 ^{iv} | 122.77 (3) | Al1 ^{xii} —Cr2—Al1 ^{vii} | 115.29 (3) |
| Al2 ⁱⁱ —Al2—Al3 ^{iv} | 68.01 (3) | Al1 ^{viii} —Cr2—Al1 ^{vii} | 64.71 (3) |
| Al2 ^{ix} —Al2—Al3 ^{iv} | 81.39 (5) | Al1 ^v —Cr2—Al1 ^{vii} | 115.29 (3) |
| Al3—Al2—Al3 ^{iv} | 58.09 (5) | Al1 ^{iv} —Cr2—Al1 ^{vii} | 180.0 |
| Cr1—Al3—Al3 ^{xi} | 66.38 (5) | Al1 ^{xii} —Cr2—Al1 | 115.29 (3) |
| Cr1—Al3—Fe2 | 135.56 (5) | Al1 ^{viii} —Cr2—Al1 | 64.71 (3) |
| Al3 ^{xi} —Al3—Fe2 | 158.07 (8) | Al1 ^v —Cr2—Al1 | 180.0 |
| Cr1—Al3—Cr2 | 135.56 (5) | Al1 ^{iv} —Cr2—Al1 | 115.29 (3) |
| Al3 ^{xi} —Al3—Cr2 | 158.07 (8) | Al1 ^{vii} —Cr2—Al1 | 64.71 (3) |

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| Cr1—Al3—Al1 ^{xii} | 148.29 (3) | Al1 ^{xii} —Cr2—Al3 ^v | 118.42 (2) |
| Al3 ^{xi} —Al3—Al1 ^{xii} | 104.10 (6) | Al1 ^{viii} —Cr2—Al3 ^v | 61.58 (2) |
| Fe2—Al3—Al1 ^{xii} | 57.79 (3) | Al1 ^v —Cr2—Al3 ^v | 118.42 (2) |
| Cr2—Al3—Al1 ^{xii} | 57.79 (3) | Al1 ^{iv} —Cr2—Al3 ^v | 64.67 (3) |
| Cr1—Al3—Al1 ^v | 148.29 (3) | Al1 ^{vii} —Cr2—Al3 ^v | 115.33 (3) |
| Al3 ^{xi} —Al3—Al1 ^v | 104.10 (6) | Al1—Cr2—Al3 ^v | 61.58 (2) |
| Cr2—Al3—Al1 ^v | 57.79 (3) | Al1 ^{xii} —Cr2—Al3 ^{iv} | 64.67 (3) |
| Al1 ^{xii} —Al3—Al1 ^v | 61.97 (5) | Al1 ^{viii} —Cr2—Al3 ^{iv} | 115.33 (3) |
| Cr1—Al3—Al1 ^{vii} | 79.23 (4) | Al1 ^v —Cr2—Al3 ^{iv} | 118.42 (2) |
| Al3 ^{xi} —Al3—Al1 ^{vii} | 145.60 (8) | Al1 ^{iv} —Cr2—Al3 ^{iv} | 118.42 (2) |
| Fe2—Al3—Al1 ^{vii} | 56.33 (3) | Al1 ^{vii} —Cr2—Al3 ^{iv} | 61.58 (2) |
| Cr2—Al3—Al1 ^{vii} | 56.33 (3) | Al1—Cr2—Al3 ^{iv} | 61.58 (2) |
| Al1 ^{xii} —Al3—Al1 ^{vii} | 105.27 (4) | Al3 ^v —Cr2—Al3 ^{iv} | 115.213 (18) |
| Al1 ^v —Al3—Al1 ^{vii} | 105.27 (4) | Al1 ^{xii} —Cr2—Al3 ^{vii} | 115.33 (3) |
| Cr1—Al3—Al3 ^{iv} | 99.80 (4) | Al1 ^{viii} —Cr2—Al3 ^{vii} | 64.67 (3) |
| Al3 ^{xi} —Al3—Al3 ^{iv} | 127.604 (15) | Al1 ^v —Cr2—Al3 ^{vii} | 61.58 (2) |
| Cr2—Al3—Al3 ^{iv} | 57.606 (9) | Al1 ^{iv} —Cr2—Al3 ^{vii} | 61.58 (2) |
| Al1 ^{xii} —Al3—Al3 ^{iv} | 60.81 (3) | Al1 ^{vii} —Cr2—Al3 ^{vii} | 118.42 (2) |
| Al1 ^v —Al3—Al3 ^{iv} | 108.89 (3) | Al1—Cr2—Al3 ^{vii} | 118.42 (2) |
| Al1 ^{vii} —Al3—Al3 ^{iv} | 56.68 (4) | Al3 ^v —Cr2—Al3 ^{vii} | 64.787 (18) |
| Cr1—Al3—Al3 ^{xii} | 99.80 (4) | Al3 ^{iv} —Cr2—Al3 ^{vii} | 180.0 |
| Al3 ^{xi} —Al3—Al3 ^{xii} | 127.606 (15) | Al1 ^{xii} —Cr2—Al3 ^{viii} | 61.58 (2) |
| Fe2—Al3—Al3 ^{xii} | 57.606 (9) | Al1 ^{viii} —Cr2—Al3 ^{viii} | 118.42 (2) |
| Cr2—Al3—Al3 ^{xii} | 57.606 (9) | Al1 ^v —Cr2—Al3 ^{viii} | 115.33 (3) |
| Al1 ^{xii} —Al3—Al3 ^{xii} | 108.89 (3) | Al1 ^{iv} —Cr2—Al3 ^{viii} | 61.58 (2) |
| Al1 ^v —Al3—Al3 ^{xii} | 60.81 (3) | Al1 ^{vii} —Cr2—Al3 ^{viii} | 118.42 (2) |
| Al1 ^{vii} —Al3—Al3 ^{xii} | 56.68 (4) | Al1—Cr2—Al3 ^{viii} | 64.67 (3) |
| Al3 ^{iv} —Al3—Al3 ^{xii} | 104.01 (5) | Al3 ^v —Cr2—Al3 ^{viii} | 64.787 (18) |
| Cr1—Al3—Cr1 ^{xi} | 122.51 (4) | Al3 ^{iv} —Cr2—Al3 ^{viii} | 64.787 (18) |
| Al3 ^{xi} —Al3—Cr1 ^{xi} | 56.13 (4) | Al3 ^{vii} —Cr2—Al3 ^{viii} | 115.213 (18) |
| Cr2—Al3—Cr1 ^{xi} | 101.93 (4) | Al1 ^{xii} —Fe2—Al1 ^{viii} | 180.0 |
| Al1 ^{xii} —Al3—Cr1 ^{xi} | 56.85 (3) | Al1 ^{xii} —Fe2—Al1 ^v | 64.71 (3) |
| Al1 ^v —Al3—Cr1 ^{xi} | 56.85 (3) | Al1 ^{viii} —Fe2—Al1 ^v | 115.29 (3) |
| Al1 ^{vii} —Al3—Cr1 ^{xi} | 158.26 (5) | Al1 ^{xii} —Fe2—Al1 ^{iv} | 64.71 (3) |
| Al3 ^{iv} —Al3—Cr1 ^{xi} | 114.04 (5) | Al1 ^{viii} —Fe2—Al1 ^{iv} | 115.29 (3) |
| Al3 ^{xii} —Al3—Cr1 ^{xi} | 114.04 (5) | Al1 ^v —Fe2—Al1 ^{iv} | 64.71 (3) |
| Cr1—Al3—Al2 ^{xii} | 55.79 (2) | Al1 ^{xii} —Fe2—Al1 ^{vii} | 115.29 (3) |
| Al3 ^{xi} —Al3—Al2 ^{xii} | 70.99 (3) | Al1 ^{viii} —Fe2—Al1 ^{vii} | 64.71 (3) |
| Fe2—Al3—Al2 ^{xii} | 118.56 (3) | Al1 ^v —Fe2—Al1 ^{vii} | 115.29 (3) |
| Cr2—Al3—Al2 ^{xii} | 118.56 (3) | Al1 ^{iv} —Fe2—Al1 ^{vii} | 180.0 |
| Al1 ^{xii} —Al3—Al2 ^{xii} | 152.70 (4) | Al1 ^{xii} —Fe2—Al1 | 115.29 (3) |
| Al1 ^v —Al3—Al2 ^{xii} | 92.55 (2) | Al1 ^{viii} —Fe2—Al1 | 64.71 (3) |
| Al1 ^{vii} —Al3—Al2 ^{xii} | 90.15 (3) | Al1 ^v —Fe2—Al1 | 180.0 |
| Al3 ^{iv} —Al3—Al2 ^{xii} | 143.76 (7) | Al1 ^{iv} —Fe2—Al1 | 115.29 (3) |
| Al3 ^{xii} —Al3—Al2 ^{xii} | 60.95 (2) | Al1 ^{vii} —Fe2—Al1 | 64.71 (3) |
| Cr1 ^{xi} —Al3—Al2 ^{xii} | 102.11 (3) | Al1 ^{xii} —Fe2—Al3 ^v | 118.42 (2) |
| Cr1—Al3—Al2 | 55.79 (2) | Al1 ^{viii} —Fe2—Al3 ^v | 61.58 (2) |
| Al3 ^{xi} —Al3—Al2 | 70.99 (3) | Al1 ^v —Fe2—Al3 ^v | 118.42 (2) |

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| Fe ² —Al ³ —Al ² | 118.56 (3) | Al ^{1iv} —Fe ² —Al ^{3v} | 64.67 (3) |
| Cr ² —Al ³ —Al ² | 118.56 (3) | Al ^{1vii} —Fe ² —Al ^{3v} | 115.33 (3) |
| Al ^{1xii} —Al ³ —Al ² | 92.55 (2) | Al ¹ —Fe ² —Al ^{3v} | 61.58 (2) |
| Al ^{1v} —Al ³ —Al ² | 152.70 (4) | Al ^{1xii} —Fe ² —Al ^{3iv} | 64.67 (3) |
| Al ^{1vii} —Al ³ —Al ² | 90.15 (3) | Al ^{1viii} —Fe ² —Al ^{3iv} | 115.33 (3) |
| Al ^{3iv} —Al ³ —Al ² | 60.95 (2) | Al ^{1v} —Fe ² —Al ^{3iv} | 118.42 (2) |
| Al ^{3xii} —Al ³ —Al ² | 143.76 (7) | Al ^{1iv} —Fe ² —Al ^{3iv} | 118.42 (2) |
| Cr ^{1xi} —Al ³ —Al ² | 102.11 (3) | Al ^{1vii} —Fe ² —Al ^{3iv} | 61.58 (2) |
| Al ^{2xii} —Al ³ —Al ² | 110.12 (4) | Al ¹ —Fe ² —Al ^{3iv} | 61.58 (2) |
| Al ^{1xvii} —Si ¹ —Al ^{1vii} | 180.000 (16) | Al ^{3v} —Fe ² —Al ^{3iv} | 115.213 (18) |
| Al ^{1xvii} —Si ¹ —Al ^{1xviii} | 65.63 (3) | Al ^{1xii} —Fe ² —Al ^{3vii} | 115.33 (3) |
| Al ^{1vii} —Si ¹ —Al ^{1xviii} | 114.37 (3) | Al ^{1viii} —Fe ² —Al ^{3vii} | 64.67 (3) |
| Al ^{1xvii} —Si ¹ —Al ^{1xix} | 65.63 (3) | Al ^{1v} —Fe ² —Al ^{3vii} | 61.58 (2) |
| Al ^{1vii} —Si ¹ —Al ^{1xix} | 114.37 (3) | Al ^{1iv} —Fe ² —Al ^{3vii} | 61.58 (2) |
| Al ^{1xviii} —Si ¹ —Al ^{1xix} | 65.63 (3) | Al ^{1vii} —Fe ² —Al ^{3vii} | 118.42 (2) |
| Al ^{1xvii} —Si ¹ —Al ^{1viii} | 114.37 (3) | Al ¹ —Fe ² —Al ^{3vii} | 118.42 (2) |
| Al ^{1vii} —Si ¹ —Al ^{1viii} | 65.63 (3) | Al ^{3v} —Fe ² —Al ^{3vii} | 64.787 (18) |
| Al ^{1xviii} —Si ¹ —Al ^{1viii} | 114.37 (3) | Al ^{3iv} —Fe ² —Al ^{3vii} | 180.0 |
| Al ^{1xix} —Si ¹ —Al ^{1viii} | 180.00 (4) | Al ^{1xii} —Fe ² —Al ^{3viii} | 61.58 (2) |
| Al ^{1xvii} —Si ¹ —Al ¹ | 114.37 (3) | Al ^{1viii} —Fe ² —Al ^{3viii} | 118.42 (2) |
| Al ^{1vii} —Si ¹ —Al ¹ | 65.63 (3) | Al ^{1v} —Fe ² —Al ^{3viii} | 115.33 (3) |
| Al ^{1xviii} —Si ¹ —Al ¹ | 180.0 | Al ^{1iv} —Fe ² —Al ^{3viii} | 61.58 (2) |
| Al ^{1xix} —Si ¹ —Al ¹ | 114.37 (3) | Al ^{1vii} —Fe ² —Al ^{3viii} | 118.42 (2) |
| Al ^{1viii} —Si ¹ —Al ¹ | 65.63 (3) | Al ¹ —Fe ² —Al ^{3viii} | 64.67 (3) |
| Al ^{1xvii} —Si ¹ —Cr ^{1xiii} | 61.518 (11) | Al ^{3v} —Fe ² —Al ^{3viii} | 64.787 (18) |
| Al ^{1vii} —Si ¹ —Cr ^{1xiii} | 118.482 (11) | Al ^{3iv} —Fe ² —Al ^{3viii} | 64.787 (18) |
| Al ^{1xviii} —Si ¹ —Cr ^{1xiii} | 61.519 (11) | Al ^{3vii} —Fe ² —Al ^{3viii} | 115.213 (18) |

Symmetry codes: (i) $x-2/3, y-1/3, z-1/3$; (ii) $-x+y+1/3, -x+2/3, z-1/3$; (iii) $-x+1/3, -y+2/3, -z+2/3$; (iv) $x-y, x, -z+1$; (v) $-x, -y, -z+1$; (vi) $y-1/3, -x+y+1/3, -z+1/3$; (vii) $-x+y, -x, z$; (viii) $-y, x-y, z$; (ix) $-y+2/3, x-y+1/3, z+1/3$; (x) $y+1/3, -x+y+2/3, -z+2/3$; (xi) $-x+2/3, -y+1/3, -z+4/3$; (xii) $y, -x+y, -z+1$; (xiii) $x-y-1/3, x-2/3, -z+1/3$; (xiv) $-x+2/3, -y+1/3, -z+1/3$; (xv) $x-y+1/3, x-1/3, -z+2/3$; (xvi) $x+2/3, y+1/3, z+1/3$; (xvii) $x-y, x, -z$; (xviii) $-x, -y, -z$; (xix) $y, -x+y, -z$; (xx) $x-y+2/3, x+1/3, -z+1/3$.