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Crystal structure of ω-Al_4Cr

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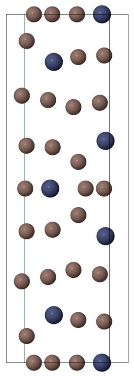
The new polymorph of tetraaluminium chromium, Al_4Cr, designated as the ω-phase, was obtained as the product from a high-pressure sintering (HPS) process of a stoichiometric Al_4Cr mixture. The crystal structure is isotypic with Al_4Mo and Al_4W. The unit cell of ω-Al_4Cr is much smaller than any of the other reported Al_4Cr polymorphs, containing 30 rather than several hundred atoms.

3D view



Structure description

Several polymorphs of Al_4Cr have been extensively investigated since the discovery of the icosahedral quasicrystal in rapidly solidified Al-Mn and Al-Cr alloys (Shechtman *et al.*, 1984). The orthorhombic ε-Al_4Cr phase was originally determined by electron diffraction in space group *Bbmm* with a = 34.6, b = 20.0, c = 12.4 Å and at elevated temperature shows a transformation to another phase (named ε') in space group *Pbmm* with the same lattice parameters (Wen *et al.*, 1992). Later, the crystal structure of the ε-Al_4Cr phase was refined by single-crystal X-ray diffraction with lattice parameters a = 12.521 (1), b = 34.705 (2), c = 20.223 (1) Å in the space group *Cmcm* (Li *et al.*, 1997). The hexagonal μ-Al_4Cr pholymorph, isostructural with μ-Al_4Mn, was also reported. It crystallizes in space group $P6_3/mmc$ with $a \simeq 20.0$, $c \simeq 24.7$ Å as determined by electron diffraction (Wen *et al.*, 1992) and single-crystal X-ray diffraction (Cao & Kuo, 2008). Both the ε-Al_4Cr and the μ-Al_4Cr phase have rather large unit cells, containing 682 and 566 atoms, respectively.

In contrast to the orthorhombic ε- and the hexagonal μ-polymorphs, the unit cell of the new ω-Al_4Cr phase contains only 30 atoms (24 Al and 6 Cr atoms; Z = 6). The crystal structure is isotypic with Al_4W (Bland & Clark, 1958)) and Al_4Mo (Leake, 1964). The Al and Cr atoms are arranged in sets of almost close-packed puckered planes arranged perpendicular to [010]. Fig. 1 shows the coordination polyhedra around the two distinct chromium atoms, Cr1 and Cr2. The first chromium atom is located on a general site (4*b*) and connects to eleven aluminium atoms whereas Cr2 atom is located on a site with

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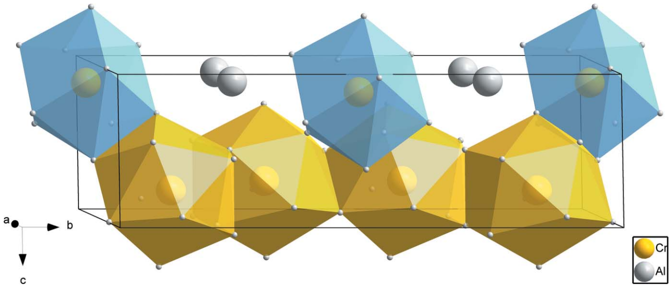

Figure 1
The crystal structure of ω-Al_4Cr with coordination polyhedra displayed for Cr1 (gold) and Cr2 (pale blue).

mirror symmetry ($2a$) and is connected to ten Al atoms (Fig. 2). Two (Al1 and Al2) of the seven unique aluminium atoms are also located on a mirror plane.

Synthesis and crystallization

The elements Al (purity 99.8%, product No. 00010 from Alfa Aesar) and Cr (purity 99.95%, product No. 13796 from Alfa Aesar) were mixed in the stoichiometric ratio 4:1 and initially ground in an agate mortar. The blended powders were then put into a grinding tool with a diameter of 9.6 mm and pressed into a tablet at 3–4 MPa slowly and continuously for about 5 min. A cylindrical block with 9.6 mm in diameter and 10.0 mm in height was obtained without cracks or deformations defects. The cylindrical block was then inserted into a six-anvil high-pressure apparatus for HPS experiments, pressurized up to 5 GPa and heated to 1299 K for 30 minutes, cooled to 1169 K and held at that temperature for 2 h, and then rapidly cooled down to room temperature. A fragment was selected and mounted on a glass fiber for single-crystal X-ray diffraction measurements.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The crystal was refined as an inversion twin with a ratio of 0.84 (7):0.16 (7) for the two twin components.

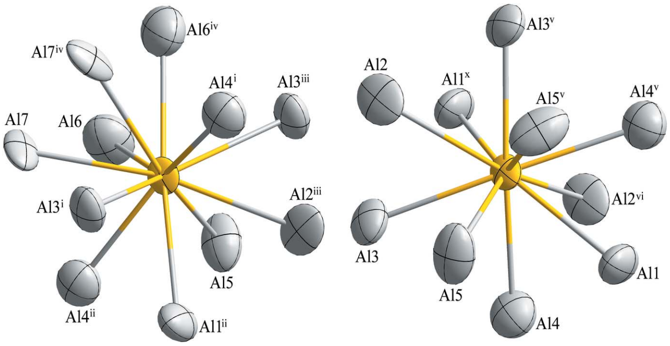

Figure 2
Details of the coordination polyhedra around Cr1 (left) and Cr2 (right). Displacement ellipsoids are given at the 99.8% probability level. [Symmetry codes: (i) $1 + x, y, 1 + z$; (ii) $x, y, 1 + z$; (iii) $1 + x, y, z$; (iv) $\frac{1}{2} + x, \frac{1}{2} - y, z$; (v) $x, 1 - y, z$; (vi) $x, y, -1 + z$; (x) $-1 + x, y, z$.]

Table 1
Experimental details.

Crystal data	
Chemical formula	Al_4Cr
M_r	159.92
Crystal system, space group	Monoclinic, *Cm*
Temperature (K)	293
a, b, c (Å)	5.1574 (6), 17.413 (2), 5.1107 (7)
β (°)	100.357 (4)
V (Å^3)	451.49 (10)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.65
Crystal size (mm)	0.07 × 0.05 × 0.03
Data collection	
Diffractometer	Bruker APEXII Photon 100 COMS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.757, 0.870
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4792, 1200, 967
R_{int}	0.068
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.681
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.090, 1.05
No. of reflections	1200
No. of parameters	74
No. of restraints	2
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.85, −1.20
Absolute structure	Flack (1983); 584 Friedel pairs
Absolute structure parameter	0.16 (7)

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

Acknowledgements

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full crystallographic data

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Crystal structure of ω-Al_4Cr

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Tetraaluminium chromium

Crystal data

Al_4Cr
$M_r = 159.92$
Monoclinic, *Cm*
$a = 5.1574$ (6) Å
$b = 17.413$ (2) Å
$c = 5.1107$ (7) Å
$\beta = 100.357$ (4)°
$V = 451.49$ (10) Å^3
$Z = 6$

$F(000) = 456$
$D_x = 3.529$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1199 reflections
$\theta = 4.1–27.0°$
$\mu = 4.65$ mm^{-1}
$T = 293$ K
Fragment, metallic
0.07 × 0.05 × 0.03 mm

Data collection

Bruker APEXII Photon 100 COMS diffractometer
Graphite monochromator
Detector resolution: 10.4167 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{min} = 0.757$, $T_{max} = 0.870$

4792 measured reflections
1200 independent reflections
967 reflections with $I > 2\sigma(I)$
$R_{int} = 0.068$
$\theta_{max} = 28.9°$, $\theta_{min} = 2.3°$
$h = -6 \rightarrow 7$
$k = -23 \rightarrow 21$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.090$
$S = 1.05$
1200 reflections
74 parameters
2 restraints

$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 2.4184P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.85$ e Å^{-3}
$\Delta\rho_{min} = -1.20$ e Å^{-3}
Absolute structure: Flack (1983); 584 Friedel pairs
Absolute structure parameter: 0.16 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component inversion twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cr1	0.9253 (3)	0.36325 (9)	0.8089 (3)	0.0047 (4)
Al1	0.7655 (11)	0.5	−0.0048 (11)	0.0092 (13)
Cr2	0.2728 (5)	0.5	0.1495 (5)	0.0055 (6)
Al2	0.1177 (11)	0.5	0.6353 (10)	0.0099 (13)
Al4	0.4332 (8)	0.3817 (2)	−0.0771 (7)	0.0098 (9)
Al3	0.0753 (7)	0.3773 (2)	0.3243 (7)	0.0090 (9)
Al5	0.6001 (9)	0.4235 (2)	0.4558 (8)	0.0114 (8)
Al6	0.5715 (7)	0.2664 (2)	0.5621 (8)	0.0126 (9)
Al7	0.7391 (7)	0.2538 (2)	1.0760 (8)	0.0087 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0051 (10)	0.0072 (8)	0.0011 (8)	−0.0002 (8)	−0.0012 (7)	0.0000 (7)
Al1	0.007 (3)	0.009 (3)	0.013 (3)	0	0.005 (2)	0
Cr2	0.0089 (16)	0.0057 (11)	0.0017 (14)	0	0.0009 (11)	0
Al2	0.016 (4)	0.011 (3)	0.002 (3)	0	−0.001 (2)	0
Al4	0.012 (2)	0.0110 (18)	0.007 (2)	−0.0003 (14)	0.0014 (17)	−0.0007 (15)
Al3	0.012 (2)	0.0102 (18)	0.005 (2)	−0.0015 (14)	0.0033 (17)	−0.0007 (14)
Al5	0.0087 (16)	0.0168 (18)	0.0079 (17)	−0.0003 (15)	−0.0006 (13)	0.0049 (15)
Al6	0.014 (2)	0.0132 (18)	0.011 (2)	−0.0018 (15)	0.0029 (18)	−0.0032 (16)
Al7	0.0030 (19)	0.0126 (17)	0.011 (2)	0.0026 (15)	0.0031 (14)	0.0046 (14)

Geometric parameters (Å, º)

Cr1—Al5	2.467 (5)	Al2—Al5$^{\mathrm{xi}}$	2.977 (7)
Cr1—Al4$^{\mathrm{i}}$	2.599 (5)	Al4—Cr1$^{\mathrm{xiv}}$	2.599 (5)
Cr1—Al3$^{\mathrm{i}}$	2.620 (4)	Al4—Cr1$^{\mathrm{vi}}$	2.723 (5)
Cr1—Al7	2.625 (4)	Al4—Al7$^{\mathrm{xv}}$	2.731 (5)
Cr1—Al6	2.634 (4)	Al4—Al7$^{\mathrm{vi}}$	2.759 (6)
Cr1—Al4$^{\mathrm{ii}}$	2.723 (5)	Al4—Al5$^{\mathrm{vi}}$	2.777 (6)
Cr1—Al3$^{\mathrm{iii}}$	2.735 (4)	Al4—Al5	2.801 (5)
Cr1—Al1$^{\mathrm{ii}}$	2.745 (3)	Al4—Al2$^{\mathrm{vi}}$	2.862 (6)
Cr1—Al6$^{\mathrm{iv}}$	2.757 (4)	Al4—Al6$^{\mathrm{vi}}$	2.900 (5)
Cr1—Al2$^{\mathrm{iii}}$	2.786 (3)	Al4—Al3	2.997 (5)
Cr1—Al7$^{\mathrm{iv}}$	2.800 (4)	Al3—Cr1$^{\mathrm{xiv}}$	2.620 (4)
Al1—Cr2$^{\mathrm{iii}}$	2.593 (6)	Al3—Cr1$^{\mathrm{x}}$	2.735 (4)
Al1—Al4	2.663 (5)	Al3—Al5$^{\mathrm{x}}$	2.775 (6)
Al1—Al4$^{\mathrm{v}}$	2.663 (5)	Al3—Al6$^{\mathrm{xvi}}$	2.783 (5)
Al1—Cr1$^{\mathrm{vi}}$	2.745 (3)	Al3—Al5	2.788 (6)
Al1—Cr1$^{\mathrm{vii}}$	2.745 (3)	Al3—Al7$^{\mathrm{xv}}$	2.814 (5)
Al1—Cr2	2.793 (6)	Al3—Al7$^{\mathrm{xiv}}$	2.907 (5)
Al1—Al2$^{\mathrm{viii}}$	2.808 (7)	Al3—Al1$^{\mathrm{x}}$	2.997 (5)
Al1—Al5$^{\mathrm{v}}$	2.960 (7)	Al5—Al5$^{\mathrm{v}}$	2.663 (7)
Al1—Al5	2.960 (7)	Al5—Al3$^{\mathrm{iii}}$	2.775 (6)

Al1—Al3^{ix}	2.997 (5)	Al5—Al4^{ii}	2.777 (6)
Al1—Al3^{iii}	2.997 (5)	Al5—Al6	2.799 (5)
Cr2—Al5	2.474 (5)	Al5—Al2^{iii}	2.977 (7)
Cr2—Al5^{v}	2.474 (5)	Al6—Al7	2.622 (5)
Cr2—Al4	2.572 (4)	Al6—Al6^{xvi}	2.6413 (17)
Cr2—Al4^{v}	2.572 (4)	Al6—Al6^{iv}	2.6413 (17)
Cr2—Al1^{x}	2.593 (6)	Al6—Cr1^{xvi}	2.757 (4)
Cr2—Al3	2.594 (4)	Al6—Al7^{xv}	2.776 (5)
Cr2—Al3^{v}	2.594 (4)	Al6—Al7^{vi}	2.782 (5)
Cr2—Al2^{vi}	2.606 (6)	Al6—Al3^{iv}	2.783 (5)
Cr2—Al2	2.742 (6)	Al6—Al4^{ii}	2.900 (5)
Al2—Cr2^{ii}	2.606 (6)	Al7—Al7^{xvi}	2.5821 (5)
Al2—Al3	2.648 (4)	Al7—Al7^{iv}	2.5821 (5)
Al2—Al3^{v}	2.648 (4)	Al7—Al4^{xvii}	2.731 (5)
Al2—Cr1^{x}	2.786 (3)	Al7—Al4^{ii}	2.759 (6)
Al2—Cr1^{xi}	2.786 (3)	Al7—Al6^{xvii}	2.776 (5)
Al2—Al1^{xii}	2.808 (7)	Al7—Al6^{ii}	2.782 (5)
Al2—Al4^{xiii}	2.862 (6)	Al7—Cr1^{xvi}	2.800 (4)
Al2—Al4^{ii}	2.862 (6)	Al7—Al3^{xvii}	2.814 (5)
Al2—Al5^{x}	2.977 (7)	Al7—Al3^{i}	2.907 (5)

Al5—Cr1—Al4^{i}	129.56 (15)	Al1—Al4—Al5	65.55 (16)
Al5—Cr1—Al3^{i}	137.30 (14)	Cr1^{vi}—Al4—Al5	95.93 (16)
Al4^{i}—Cr1—Al3^{i}	70.10 (12)	Al7^{xv}—Al4—Al5	90.61 (17)
Al5—Cr1—Al7	115.17 (14)	Al7^{vi}—Al4—Al5	82.78 (15)
Al4^{i}—Cr1—Al7	114.91 (13)	Al5^{vi}—Al4—Al5	132.8 (2)
Al3^{i}—Cr1—Al7	67.32 (13)	Cr2—Al4—Al2^{vi}	57.00 (13)
Al5—Cr1—Al6	66.46 (13)	Cr1^{xiv}—Al4—Al2^{vi}	61.11 (13)
Al4^{i}—Cr1—Al6	140.34 (15)	Al1—Al4—Al2^{vi}	78.84 (17)
Al3^{i}—Cr1—Al6	126.53 (15)	Cr1^{vi}—Al4—Al2^{vi}	116.13 (19)
Al7—Cr1—Al6	59.83 (12)	Al7^{xv}—Al4—Al2^{vi}	124.41 (18)
Al5—Cr1—Al4^{ii}	64.48 (14)	Al7^{vi}—Al4—Al2^{vi}	165.8 (2)
Al4^{i}—Cr1—Al4^{ii}	151.41 (17)	Al5^{vi}—Al4—Al2^{vi}	66.73 (17)
Al3^{i}—Cr1—Al4^{ii}	83.80 (14)	Al5—Al4—Al2^{vi}	111.02 (18)
Al7—Cr1—Al4^{ii}	62.09 (13)	Cr2—Al4—Al6^{vi}	167.55 (18)
Al6—Cr1—Al4^{ii}	65.53 (13)	Cr1^{xiv}—Al4—Al6^{vi}	97.20 (15)
Al5—Cr1—Al3^{iii}	64.23 (13)	Al1—Al4—Al6^{vi}	113.44 (16)
Al4^{i}—Cr1—Al3^{iii}	75.77 (13)	Cr1^{vi}—Al4—Al6^{vi}	55.75 (10)
Al3^{i}—Cr1—Al3^{iii}	145.25 (18)	Al7^{xv}—Al4—Al6^{vi}	74.30 (14)
Al7—Cr1—Al3^{iii}	136.50 (13)	Al7^{vi}—Al4—Al6^{vi}	55.14 (13)
Al6—Cr1—Al3^{iii}	84.71 (13)	Al5^{vi}—Al4—Al6^{vi}	59.02 (12)
Al4^{ii}—Cr1—Al3^{iii}	127.55 (13)	Al5—Al4—Al6^{vi}	136.94 (19)
Al5—Cr1—Al1^{ii}	71.19 (15)	Al2^{vi}—Al4—Al6^{vi}	110.72 (16)
Al4^{i}—Cr1—Al1^{ii}	99.70 (15)	Cr2—Al4—Al3	54.88 (12)
Al3^{i}—Cr1—Al1^{ii}	67.87 (15)	Cr1^{xiv}—Al4—Al3	55.28 (12)
Al7—Cr1—Al1^{ii}	106.78 (14)	Al1—Al4—Al3	112.64 (17)
Al6—Cr1—Al1^{ii}	119.74 (17)	Cr1^{vi}—Al4—Al3	148.85 (17)
Al4^{ii}—Cr1—Al1^{ii}	58.29 (14)	Al7^{xv}—Al4—Al3	58.63 (13)

Al3^{iii}—Cr1—Al1^{ii}	112.82 (14)	Al7^{vi}—Al4—Al3	100.16 (16)
Al5—Cr1—Al6^{iv}	102.70 (13)	Al5^{vi}—Al4—Al3	156.84 (19)
Al4^{i}—Cr1—Al6^{iv}	81.72 (14)	Al5—Al4—Al3	57.35 (14)
Al3^{i}—Cr1—Al6^{iv}	118.74 (12)	Al2^{vi}—Al4—Al3	90.38 (17)
Al7—Cr1—Al6^{iv}	78.41 (12)	Al6^{vi}—Al4—Al3	132.06 (19)
Al6—Cr1—Al6^{iv}	58.63 (6)	Cr2—Al3—Cr1^{xiv}	78.09 (12)
Al4^{ii}—Cr1—Al6^{iv}	122.44 (13)	Cr2—Al3—Al2	63.06 (14)
Al3^{iii}—Cr1—Al6^{iv}	60.90 (13)	Cr1^{xiv}—Al3—Al2	131.01 (16)
Al1^{ii}—Cr1—Al6^{iv}	173.15 (16)	Cr2—Al3—Cr1^{x}	125.32 (15)
Al5—Cr1—Al2^{iii}	68.74 (15)	Cr1^{xiv}—Al3—Cr1^{x}	145.25 (18)
Al4^{i}—Cr1—Al2^{iii}	64.12 (15)	Al2—Al3—Cr1^{x}	62.30 (11)
Al3^{i}—Cr1—Al2^{iii}	100.53 (14)	Cr2—Al3—Al5^{x}	105.24 (15)
Al7—Cr1—Al2^{iii}	166.17 (15)	Cr1^{xiv}—Al3—Al5^{x}	99.00 (15)
Al6—Cr1—Al2^{iii}	130.59 (15)	Al2—Al3—Al5^{x}	66.54 (15)
Al4^{ii}—Cr1—Al2^{iii}	111.51 (15)	Cr1^{x}—Al3—Al5^{x}	53.19 (12)
Al3^{iii}—Cr1—Al2^{iii}	57.33 (13)	Cr2—Al3—Al6^{xvi}	157.66 (18)
Al1^{ii}—Cr1—Al2^{iii}	61.01 (13)	Cr1^{xiv}—Al3—Al6^{xvi}	109.33 (15)
Al6^{iv}—Cr1—Al2^{iii}	114.33 (15)	Al2—Al3—Al6^{xvi}	118.01 (14)
Al5—Cr1—Al7^{iv}	157.49 (13)	Cr1^{x}—Al3—Al6^{xvi}	59.94 (11)
Al4^{i}—Cr1—Al7^{iv}	60.64 (11)	Al5^{x}—Al3—Al6^{xvi}	94.56 (15)
Al3^{i}—Cr1—Al7^{iv}	62.45 (12)	Cr2—Al3—Al5	54.60 (13)
Al7—Cr1—Al7^{iv}	56.73 (6)	Cr1^{xiv}—Al3—Al5	111.56 (17)
Al6—Cr1—Al7^{iv}	93.29 (13)	Al2—Al3—Al5	69.54 (16)
Al4^{ii}—Cr1—Al7^{iv}	117.42 (13)	Cr1^{x}—Al3—Al5	103.18 (15)
Al3^{iii}—Cr1—Al7^{iv}	105.89 (12)	Al5^{x}—Al3—Al5	136.00 (19)
Al1^{ii}—Cr1—Al7^{iv}	130.20 (15)	Al6^{xvi}—Al3—Al5	103.72 (16)
Al6^{iv}—Cr1—Al7^{iv}	56.31 (12)	Cr2—Al3—Al7^{xv}	110.15 (17)
Al2^{iii}—Cr1—Al7^{iv}	124.73 (15)	Cr1^{xiv}—Al3—Al7^{xv}	61.92 (12)
Cr2^{iii}—Al1—Al4	129.13 (11)	Al2—Al3—Al7^{xv}	157.80 (19)
Cr2^{iii}—Al1—Al4^{v}	129.13 (11)	Cr1^{x}—Al3—Al7^{xv}	119.51 (15)
Al4—Al1—Al4^{v}	101.4 (2)	Al5^{x}—Al3—Al7^{xv}	133.98 (17)
Cr2^{iii}—Al1—Cr1^{vi}	75.88 (13)	Al6^{xvi}—Al3—Al7^{xv}	59.59 (13)
Al4—Al1—Cr1^{vi}	60.44 (11)	Al5—Al3—Al7^{xv}	89.19 (16)
Al4^{v}—Al1—Cr1^{vi}	148.1 (2)	Cr2—Al3—Al7^{xiv}	134.37 (17)
Cr2^{iii}—Al1—Cr1^{vii}	75.88 (13)	Cr1^{xiv}—Al3—Al7^{xiv}	56.42 (11)
Al4—Al1—Cr1^{vii}	148.1 (2)	Al2—Al3—Al7^{xiv}	146.85 (17)
Al4^{v}—Al1—Cr1^{vii}	60.44 (11)	Cr1^{x}—Al3—Al7^{xiv}	94.91 (14)
Cr1^{vi}—Al1—Cr1^{vii}	120.3 (2)	Al5^{x}—Al3—Al7^{xiv}	80.61 (14)
Cr2^{iii}—Al1—Cr2	146.5 (2)	Al6^{xvi}—Al3—Al7^{xiv}	58.34 (12)
Al4—Al1—Cr2	56.19 (11)	Al5—Al3—Al7^{xiv}	142.75 (18)
Al4^{v}—Al1—Cr2	56.19 (11)	Al7^{xv}—Al3—Al7^{xiv}	53.63 (8)
Cr1^{vi}—Al1—Cr2	116.29 (13)	Cr2—Al3—Al1^{x}	54.69 (12)
Cr1^{vii}—Al1—Cr2	116.29 (13)	Cr1^{xiv}—Al3—Al1^{x}	58.06 (12)
Cr2^{iii}—Al1—Al2^{viii}	57.52 (17)	Al2—Al3—Al1^{x}	74.92 (14)
Al4—Al1—Al2^{viii}	112.66 (15)	Cr1^{x}—Al3—Al1^{x}	111.29 (16)
Al4^{v}—Al1—Al2^{viii}	112.65 (15)	Al5^{x}—Al3—Al1^{x}	61.57 (16)
Cr1^{vi}—Al1—Al2^{viii}	60.20 (12)	Al6^{xvi}—Al3—Al1^{x}	147.27 (18)
Cr1^{vii}—Al1—Al2^{viii}	60.20 (12)	Al5—Al3—Al1^{x}	109.01 (16)

Cr2—Al1—Al2^{viii}	156.0 (2)
Cr2^{iii}—Al1—Al5^{v}	100.2 (2)
Al4—Al1—Al5^{v}	100.83 (18)
Al4^{v}—Al1—Al5^{v}	59.47 (12)
Cr1^{vi}—Al1—Al5^{v}	144.40 (18)
Cr1^{vii}—Al1—Al5^{v}	91.89 (10)
Cr2—Al1—Al5^{v}	50.84 (13)
Al2^{viii}—Al1—Al5^{v}	146.48 (16)
Cr2^{iii}—Al1—Al5	100.2 (2)
Al4—Al1—Al5	59.47 (12)
Al4^{v}—Al1—Al5	100.83 (18)
Cr1^{vi}—Al1—Al5	91.89 (10)
Cr1^{vii}—Al1—Al5	144.40 (18)
Cr2—Al1—Al5	50.84 (13)
Al2^{viii}—Al1—Al5	146.48 (16)
Al5^{v}—Al1—Al5	53.45 (17)
Cr2^{iii}—Al1—Al3^{ix}	54.72 (12)
Al4—Al1—Al3^{ix}	153.4 (2)
Al4^{v}—Al1—Al3^{ix}	77.94 (11)
Cr1^{vi}—Al1—Al3^{ix}	130.5 (2)
Cr1^{vii}—Al1—Al3^{ix}	54.08 (10)
Cr2—Al1—Al3^{ix}	105.18 (15)
Al2^{viii}—Al1—Al3^{ix}	91.45 (17)
Al5^{v}—Al1—Al3^{ix}	55.51 (13)
Al5—Al1—Al3^{ix}	94.30 (18)
Cr2^{iii}—Al1—Al3^{iii}	54.72 (12)
Al4—Al1—Al3^{iii}	77.94 (11)
Al4^{v}—Al1—Al3^{iii}	153.4 (2)
Cr1^{vi}—Al1—Al3^{iii}	54.08 (10)
Cr1^{vii}—Al1—Al3^{iii}	130.5 (2)
Cr2—Al1—Al3^{iii}	105.18 (15)
Al2^{viii}—Al1—Al3^{iii}	91.45 (17)
Al5^{v}—Al1—Al3^{iii}	94.30 (18)
Al5—Al1—Al3^{iii}	55.51 (13)
Al3^{ix}—Al1—Al3^{iii}	91.0 (2)
Al5—Cr2—Al5^{v}	65.10 (18)
Al5—Cr2—Al4	67.40 (13)
Al5^{v}—Cr2—Al4	118.54 (17)
Al5—Cr2—Al4^{v}	118.54 (17)
Al5^{v}—Cr2—Al4^{v}	67.40 (13)
Al4—Cr2—Al4^{v}	106.5 (2)
Al5—Cr2—Al1^{x}	136.77 (15)
Al5^{v}—Cr2—Al1^{x}	136.77 (15)
Al4—Cr2—Al1^{x}	104.58 (13)
Al4^{v}—Cr2—Al1^{x}	104.58 (13)
Al5—Cr2—Al3	66.69 (13)
Al5^{v}—Cr2—Al3	119.39 (15)
Al4—Cr2—Al3	70.93 (11)
Al7^{xv}—Al3—Al1^{x}	119.87 (16)
Al7^{xiv}—Al3—Al1^{x}	93.81 (16)
Cr2—Al3—Al4	54.20 (12)
Cr1^{xiv}—Al3—Al4	54.62 (12)
Al2—Al3—Al4	113.30 (17)
Cr1^{x}—Al3—Al4	158.64 (17)
Al5^{x}—Al3—Al4	146.91 (18)
Al6^{xvi}—Al3—Al4	112.03 (17)
Al5—Al3—Al4	57.78 (13)
Al7^{xv}—Al3—Al4	55.96 (13)
Al7^{xiv}—Al3—Al4	96.45 (16)
Al1^{x}—Al3—Al4	85.95 (14)
Cr1—Al5—Cr2	171.39 (18)
Cr1—Al5—Al5^{v}	115.19 (9)
Cr2—Al5—Al5^{v}	57.45 (9)
Cr1—Al5—Al3^{iii}	62.58 (13)
Cr2—Al5—Al3^{iii}	122.34 (19)
Al5^{v}—Al5—Al3^{iii}	106.88 (10)
Cr1—Al5—Al4^{ii}	62.24 (13)
Cr2—Al5—Al4^{ii}	113.8 (2)
Al5^{v}—Al5—Al4^{ii}	105.23 (11)
Al3^{iii}—Al5—Al4^{ii}	123.76 (18)
Cr1—Al5—Al3	123.80 (17)
Cr2—Al5—Al3	58.71 (14)
Al5^{v}—Al5—Al3	106.79 (10)
Al3^{iii}—Al5—Al3	136.00 (19)
Al4^{ii}—Al5—Al3	72.16 (16)
Cr1—Al5—Al6	59.63 (11)
Cr2—Al5—Al6	126.52 (17)
Al5^{v}—Al5—Al6	167.87 (12)
Al3^{iii}—Al5—Al6	80.95 (15)
Al4^{ii}—Al5—Al6	62.68 (14)
Al3—Al5—Al6	71.44 (14)
Cr1—Al5—Al4	130.56 (18)
Cr2—Al5—Al4	57.96 (13)
Al5^{v}—Al5—Al4	105.09 (11)
Al3^{iii}—Al5—Al4	79.60 (16)
Al4^{ii}—Al5—Al4	132.8 (2)
Al3—Al5—Al4	64.86 (14)
Al6—Al5—Al4	85.21 (15)
Cr1—Al5—Al1	121.2 (2)
Cr2—Al5—Al1	61.08 (15)
Al5^{v}—Al5—Al1	63.27 (8)
Al3^{iii}—Al5—Al1	62.91 (15)
Al4^{ii}—Al5—Al1	168.50 (18)
Al3—Al5—Al1	110.15 (19)
Al6—Al5—Al1	128.82 (17)
Al4—Al5—Al1	54.98 (14)

Al4^{v}—Cr2—Al3	173.21 (17)	Cr1—Al5—Al2^{iii}	60.70 (12)
Al1^{x}—Cr2—Al3	70.59 (12)	Cr2—Al5—Al2^{iii}	115.24 (16)
Al5—Cr2—Al3^{v}	119.39 (15)	Al5^{v}—Al5—Al2^{iii}	63.43 (9)
Al5^{v}—Cr2—Al3^{v}	66.69 (13)	Al3^{iii}—Al5—Al2^{iii}	54.70 (14)
Al4—Cr2—Al3^{v}	173.21 (17)	Al4^{ii}—Al5—Al2^{iii}	104.59 (18)
Al4^{v}—Cr2—Al3^{v}	70.92 (11)	Al3—Al5—Al2^{iii}	168.98 (19)
Al1^{x}—Cr2—Al3^{v}	70.59 (12)	Al6—Al5—Al2^{iii}	116.93 (16)
Al3—Cr2—Al3^{v}	110.9 (2)	Al4—Al5—Al2^{iii}	121.2 (2)
Al5—Cr2—Al2^{vi}	133.53 (15)	Al1—Al5—Al2^{iii}	70.93 (17)
Al5^{v}—Cr2—Al2^{vi}	133.53 (15)	Al7—Al6—Cr1	59.92 (12)
Al4—Cr2—Al2^{vi}	67.12 (12)	Al7—Al6—Al6^{xvi}	97.34 (13)
Al4^{v}—Cr2—Al2^{vi}	67.12 (12)	Cr1—Al6—Al6^{xvi}	136.96 (18)
Al1^{x}—Cr2—Al2^{vi}	65.38 (17)	Al7—Al6—Al6^{iv}	80.56 (13)
Al3—Cr2—Al2^{vi}	106.21 (13)	Cr1—Al6—Al6^{iv}	63.02 (12)
Al3^{v}—Cr2—Al2^{vi}	106.21 (12)	Al6^{xvi}—Al6—Al6^{iv}	155.0 (3)
Al5—Cr2—Al2	72.78 (16)	Al7—Al6—Cr1^{xvi}	62.68 (13)
Al5^{v}—Cr2—Al2	72.78 (16)	Cr1—Al6—Cr1^{xvi}	121.88 (17)
Al4—Cr2—Al2	125.27 (10)	Al6^{xvi}—Al6—Cr1^{xvi}	58.35 (14)
Al4^{v}—Cr2—Al2	125.27 (10)	Al6^{iv}—Al6—Cr1^{xvi}	99.80 (19)
Al1^{x}—Cr2—Al2	80.38 (19)	Al7—Al6—Al7^{xv}	157.7 (2)
Al3—Cr2—Al2	59.44 (11)	Cr1—Al6—Al7^{xv}	140.64 (18)
Al3^{v}—Cr2—Al2	59.44 (11)	Al6^{xvi}—Al6—Al7^{xv}	61.74 (11)
Al2^{vi}—Cr2—Al2	145.8 (3)	Al6^{iv}—Al6—Al7^{xv}	114.75 (13)
Al5—Cr2—Al1	68.08 (16)	Cr1^{xvi}—Al6—Al7^{xv}	97.46 (15)
Al5^{v}—Cr2—Al1	68.08 (16)	Al7—Al6—Al7^{vi}	142.0 (2)
Al4—Cr2—Al1	59.35 (11)	Cr1—Al6—Al7^{vi}	100.29 (16)
Al4^{v}—Cr2—Al1	59.35 (11)	Al6^{xvi}—Al6—Al7^{vi}	116.29 (12)
Al1^{x}—Cr2—Al1	146.5 (2)	Al6^{iv}—Al6—Al7^{vi}	61.50 (12)
Al3—Cr2—Al1	122.06 (10)	Cr1^{xvi}—Al6—Al7^{vi}	119.89 (15)
Al3^{v}—Cr2—Al1	122.06 (10)	Al7^{xv}—Al6—Al7^{vi}	55.37 (10)
Al2^{vi}—Cr2—Al1	81.1 (2)	Al7—Al6—Al3^{iv}	109.57 (18)
Al2—Cr2—Al1	133.15 (19)	Cr1—Al6—Al3^{iv}	136.57 (17)
Cr2^{ii}—Al2—Al3	125.62 (10)	Al6^{xvi}—Al6—Al3^{iv}	83.61 (18)
Cr2^{ii}—Al2—Al3^{v}	125.62 (10)	Al6^{iv}—Al6—Al3^{iv}	73.86 (18)
Al3—Al2—Al3^{v}	107.6 (2)	Cr1^{xvi}—Al6—Al3^{iv}	59.16 (13)
Cr2^{ii}—Al2—Cr2	145.8 (3)	Al7^{xv}—Al6—Al3^{iv}	63.06 (13)
Al3—Al2—Cr2	57.50 (10)	Al7^{vi}—Al6—Al3^{iv}	60.76 (12)
Al3^{v}—Al2—Cr2	57.50 (10)	Al7—Al6—Al5	104.89 (15)
Cr2^{ii}—Al2—Cr1^{x}	74.99 (13)	Cr1—Al6—Al5	53.91 (11)
Al3—Al2—Cr1^{x}	60.38 (9)	Al6^{xvi}—Al6—Al5	107.3 (2)
Al3^{v}—Al2—Cr1^{x}	152.3 (2)	Al6^{iv}—Al6—Al5	97.3 (2)
Cr2—Al2—Cr1^{x}	117.84 (11)	Cr1^{xvi}—Al6—Al5	156.61 (19)
Cr2^{ii}—Al2—Cr1^{xi}	74.99 (13)	Al7^{xv}—Al6—Al5	89.76 (16)
Al3—Al2—Cr1^{xi}	152.3 (2)	Al7^{vi}—Al6—Al5	82.42 (16)
Al3^{v}—Al2—Cr1^{xi}	60.38 (9)	Al3^{iv}—Al6—Al5	142.13 (18)
Cr2—Al2—Cr1^{xi}	117.84 (11)	Al7—Al6—Al4^{ii}	59.71 (13)
Cr1^{x}—Al2—Cr1^{xi}	117.5 (2)	Cr1—Al6—Al4^{ii}	58.72 (13)
Cr2^{ii}—Al2—Al1^{xii}	57.10 (17)	Al6^{xvi}—Al6—Al4^{ii}	78.34 (14)

Al3—Al2—Al1^{xii}	113.55 (14)	Al6^{iv}—Al6—Al4^{ii}	120.11 (16)
Al3^{v}—Al2—Al1^{xii}	113.55 (14)	Cr1^{xvi}—Al6—Al4^{ii}	99.03 (15)
Cr2—Al2—Al1^{xii}	157.1 (3)	Al7^{xv}—Al6—Al4^{ii}	118.28 (17)
Cr1^{x}—Al2—Al1^{xii}	58.79 (11)	Al7^{vi}—Al6—Al4^{ii}	140.71 (17)
Cr1^{xi}—Al2—Al1^{xii}	58.79 (11)	Al3^{iv}—Al6—Al4^{ii}	157.15 (18)
Cr2^{ii}—Al2—Al4^{xiii}	55.88 (12)	Al5—Al6—Al4^{ii}	58.30 (13)
Al3—Al2—Al4^{xiii}	150.1 (2)	Al7^{xvi}—Al7—Al7^{iv}	174.1 (3)
Al3^{v}—Al2—Al4^{xiii}	72.86 (11)	Al7^{xvi}—Al7—Al6	81.67 (12)
Cr2—Al2—Al4^{xiii}	103.51 (17)	Al7^{iv}—Al7—Al6	98.83 (12)
Cr1^{x}—Al2—Al4^{xiii}	130.8 (2)	Al7^{xvi}—Al7—Cr1	119.74 (17)
Cr1^{xi}—Al2—Al4^{xiii}	54.77 (10)	Al7^{iv}—Al7—Cr1	65.06 (13)
Al1^{xii}—Al2—Al4^{xiii}	92.21 (16)	Al6—Al7—Cr1	60.25 (12)
Cr2^{ii}—Al2—Al4^{ii}	55.88 (12)	Al7^{xvi}—Al7—Al4^{xvii}	111.92 (19)
Al3—Al2—Al4^{ii}	72.86 (11)	Al7^{iv}—Al7—Al4^{xvii}	62.50 (16)
Al3^{v}—Al2—Al4^{ii}	150.1 (2)	Al6—Al7—Al4^{xvii}	81.79 (16)
Cr2—Al2—Al4^{ii}	103.51 (17)	Cr1—Al7—Al4^{xvii}	106.91 (15)
Cr1^{x}—Al2—Al4^{ii}	54.77 (10)	Al7^{xvi}—Al7—Al4^{ii}	61.40 (14)
Cr1^{xi}—Al2—Al4^{ii}	130.8 (2)	Al7^{iv}—Al7—Al4^{ii}	124.2 (2)
Al1^{xii}—Al2—Al4^{ii}	92.21 (16)	Al6—Al7—Al4^{ii}	65.15 (14)
Al4^{xiii}—Al2—Al4^{ii}	92.1 (2)	Cr1—Al7—Al4^{ii}	60.70 (13)
Cr2^{ii}—Al2—Al5^{x}	114.0 (2)	Al4^{xvii}—Al7—Al4^{ii}	146.7 (2)
Al3—Al2—Al5^{x}	58.76 (12)	Al7^{xvi}—Al7—Al6^{xvii}	116.73 (12)
Al3^{v}—Al2—Al5^{x}	101.71 (18)	Al7^{iv}—Al7—Al6^{xvii}	62.43 (12)
Cr2—Al2—Al5^{x}	96.44 (18)	Al6—Al7—Al6^{xvii}	161.1 (2)
Cr1^{x}—Al2—Al5^{x}	50.56 (11)	Cr1—Al7—Al6^{xvii}	109.43 (16)
Cr1^{xi}—Al2—Al5^{x}	97.43 (19)	Al4^{xvii}—Al7—Al6^{xvii}	87.00 (15)
Al1^{xii}—Al2—Al5^{x}	63.38 (18)	Al4^{ii}—Al7—Al6^{xvii}	125.86 (18)
Al4^{xiii}—Al2—Al5^{x}	151.1 (2)	Al7^{xvi}—Al7—Al6^{ii}	62.19 (12)
Al4^{ii}—Al2—Al5^{x}	103.40 (12)	Al7^{iv}—Al7—Al6^{ii}	118.33 (12)
Cr2^{ii}—Al2—Al5^{xi}	114.0 (2)	Al6—Al7—Al6^{ii}	142.0 (2)
Al3—Al2—Al5^{xi}	101.71 (18)	Cr1—Al7—Al6^{ii}	127.48 (16)
Al3^{v}—Al2—Al5^{xi}	58.76 (12)	Al4^{xvii}—Al7—Al6^{ii}	120.85 (16)
Cr2—Al2—Al5^{xi}	96.44 (18)	Al4^{ii}—Al7—Al6^{ii}	86.33 (16)
Cr1^{x}—Al2—Al5^{xi}	97.43 (19)	Al6^{xvii}—Al7—Al6^{ii}	56.76 (11)
Cr1^{xi}—Al2—Al5^{xi}	50.56 (11)	Al7^{xvi}—Al7—Cr1^{xvi}	58.21 (12)
Al1^{xii}—Al2—Al5^{xi}	63.38 (18)	Al7^{iv}—Al7—Cr1^{xvi}	116.89 (18)
Al4^{xiii}—Al2—Al5^{xi}	103.40 (12)	Al6—Al7—Cr1^{xvi}	61.01 (13)
Al4^{ii}—Al2—Al5^{xi}	151.1 (2)	Cr1—Al7—Cr1^{xvi}	120.55 (16)
Al5^{x}—Al2—Al5^{xi}	53.13 (18)	Al4^{xvii}—Al7—Cr1^{xvi}	56.03 (11)
Cr2—Al4—Cr1^{xiv}	78.87 (14)	Al4^{ii}—Al7—Cr1^{xvi}	101.43 (14)
Cr2—Al4—Al1	64.46 (15)	Al6^{xvii}—Al7—Cr1^{xvi}	123.63 (16)
Cr1^{xiv}—Al4—Al1	136.39 (17)	Al6^{ii}—Al7—Cr1^{xvi}	104.35 (14)
Cr2—Al4—Cr1^{vi}	125.33 (17)	Al7^{xvi}—Al7—Al3^{xvii}	65.02 (15)
Cr1^{xiv}—Al4—Cr1^{vi}	151.41 (17)	Al7^{iv}—Al7—Al3^{xvii}	109.8 (2)
Al1—Al4—Cr1^{vi}	61.28 (11)	Al6—Al7—Al3^{xvii}	116.62 (18)
Cr2—Al4—Al7^{xv}	113.50 (17)	Cr1—Al7—Al3^{xvii}	172.32 (17)
Cr1^{xiv}—Al4—Al7^{xv}	63.33 (12)	Al4^{xvii}—Al7—Al3^{xvii}	65.41 (12)
Al1—Al4—Al7^{xv}	152.67 (18)	Al4^{ii}—Al7—Al3^{xvii}	125.43 (18)

Cr1$^{\text{vi}}$—Al4—Al7$^{\text{xv}}$	111.30 (15)
Cr2—Al4—Al7$^{\text{vi}}$	137.10 (18)
Cr1$^{\text{xiv}}$—Al4—Al7$^{\text{vi}}$	117.76 (18)
Al1—Al4—Al7$^{\text{vi}}$	105.31 (14)
Cr1$^{\text{vi}}$—Al4—Al7$^{\text{vi}}$	57.20 (10)
Al7$^{\text{xv}}$—Al4—Al7$^{\text{vi}}$	56.10 (9)
Cr2—Al4—Al5$^{\text{vi}}$	110.56 (17)
Cr1$^{\text{xiv}}$—Al4—Al5$^{\text{vi}}$	107.18 (16)
Al1—Al4—Al5$^{\text{vi}}$	67.96 (17)
Cr1$^{\text{vi}}$—Al4—Al5$^{\text{vi}}$	53.28 (13)
Al7$^{\text{xv}}$—Al4—Al5$^{\text{vi}}$	131.25 (17)
Al7$^{\text{vi}}$—Al4—Al5$^{\text{vi}}$	101.88 (17)
Cr2—Al4—Al5	54.64 (13)
Cr1$^{\text{xiv}}$—Al4—Al5	111.79 (18)
Al6$^{\text{xvii}}$—Al7—Al3$^{\text{xvii}}$	71.38 (15)
Al6$^{\text{ii}}$—Al7—Al3$^{\text{xvii}}$	59.65 (13)
Cr1$^{\text{xvi}}$—Al7—Al3$^{\text{xvii}}$	55.63 (11)
Al7$^{\text{xvi}}$—Al7—Al3$^{\text{i}}$	123.73 (19)
Al7$^{\text{iv}}$—Al7—Al3$^{\text{i}}$	61.35 (15)
Al6—Al7—Al3$^{\text{i}}$	116.01 (16)
Cr1—Al7—Al3$^{\text{i}}$	56.26 (11)
Al4$^{\text{xvii}}$—Al7—Al3$^{\text{i}}$	122.91 (17)
Al4$^{\text{ii}}$—Al7—Al3$^{\text{i}}$	78.04 (15)
Al6$^{\text{xvii}}$—Al7—Al3$^{\text{i}}$	58.60 (13)
Al6$^{\text{ii}}$—Al7—Al3$^{\text{i}}$	78.95 (15)
Cr1$^{\text{xvi}}$—Al7—Al3$^{\text{i}}$	176.65 (17)
Al3$^{\text{xvii}}$—Al7—Al3$^{\text{i}}$	127.4 (2)

Symmetry codes: (i) *x*+1, *y*, *z*+1; (ii) *x*, *y*, *z*+1; (iii) *x*+1, *y*, *z*; (iv) *x*+1/2, −*y*+1/2, *z*; (v) *x*, −*y*+1, *z*; (vi) *x*, *y*, *z*−1; (vii) *x*, −*y*+1, *z*−1; (viii) *x*+1, *y*, *z*−1; (ix) *x*+1, −*y*+1, *z*; (x) *x*−1, *y*, *z*; (xi) *x*−1, −*y*+1, *z*; (xii) *x*−1, *y*, *z*+1; (xiii) *x*, −*y*+1, *z*+1; (xiv) *x*−1, *y*, *z*−1; (xv) *x*−1/2, −*y*+1/2, *z*−1; (xvi) *x*−1/2, −*y*+1/2, *z*; (xvii) *x*+1/2, −*y*+1/2, *z*+1.