IUCrData

ISSN 2414-3146

Crystal structure of the Al_8Cr_5-type intermetallic $Al_{7.85}Cr_{5.16}$

Xu Geng, Bin Wen and Changzeng Fan*

State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, People's Republic of China. *Correspondence e-mail: chzfan@ysu.edu.cn

Received 24 December 2019
Accepted 27 March 2020

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

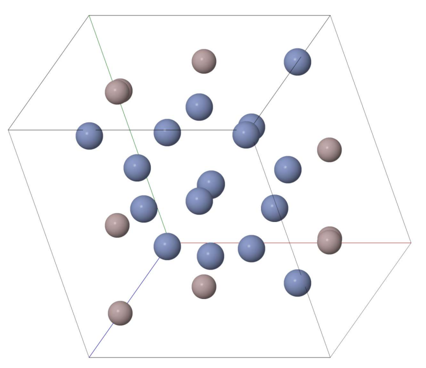
Keywords: crystal structure; high-pressure sintering; intermetallic; γ-brass phase.

CCDC reference: 1993113

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

An aluminium-deficient Al_8Cr_5-type intermetallic with formula $Al_{7.85}Cr_{5.16}$ (octaaluminium pentachromium) was uncovered when high-pressure sintering of a mixture with composition $Al_{11}Cr_4$ was carried out. Structure analysis reveals that there are three co-occupied positions with refined occupancy factors for Al atoms being 0.958, 0.772 and 1/2. The present phase is confirmed to be isotypic with the previously reported rhombohedral Al_8Cr_5 ordered phase [Bradley & Lu (1937). *Z. Kristallogr.* **96**, 20–37] and structurally closely related to the disordered phases of rhombohedral $Al_{16}Cr_{9.5}$ and cubic Al_8Cr_5.

3D view



Structure description

The γ_2-Al_8Cr_5 phase (hereafter named as the γ_2 phase) was determined to have a γ-brass-like structure by powder diffraction photographs. This phase was found in slowly cooled chromium–aluminium alloys (Bradley & Lu, 1937). Although the same clusters of 26 atoms are found in the γ_2 phase, the atomic arrangement in the γ_2 phase is much more complex than that of the γ-brass, and results in a rhombohedral rather than cubic symmetry (Bradley & Lu, 1937). A high-temperature γ_1 phase was also reported to be stable between 1350 and 980°C at the same composition (Bradley & Lu, 1937) and its structure has been redetermined by single-crystal methods for a sample sintered at 1000°C for 6 h and re-annealed at 1215°C for 287 h (Brandon *et al.*, 1977). As a result of the close agreement of Brandon's analysis with that of Bradley & Lu, it was suggested that either the structure of γ_1 and γ_2 are very similar, or that in the former case the crystals decomposed to γ_2 on quenching. In another work, the high-temperature γ_1 phase prepared by splat cooling was reported to be of the same type as Cu_5Zn_8, by using power diffraction data combined with electron diffraction patterns (Braun *et al.*, 1992). When comparing the three aforementioned models (see Table S1 of the supporting information), it was found that there are one vacancy position and three co-occupied positions in

https://doi.org/10.1107/S2414314620004228

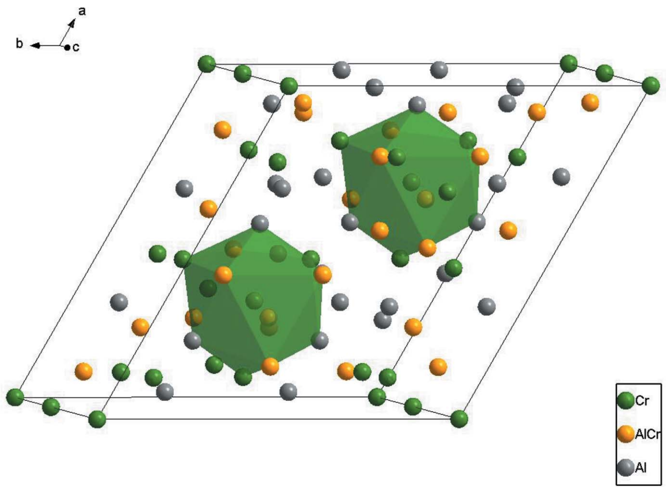


Figure 1
The crystal structure of $Al_{7.85}Cr_{5.16}$. The icosahedra centred on Cr4 are emphasized.

the Brandon model, while all atomic sites are fully occupied in Bradley & Lu's model. For the convenience of comparison, the cubic Braun model was transformed to the rhombohedral description, and it was found that there are two co-occupied positions. In the study reported herein, the crystal structure of a third type of Al_8Cr_5 phase, with the refined chemical composition $Al_{7.85}Cr_{5.16}$ and hereafter named as γ_2'-Al_8Cr_5 phase, was determined by single-crystal X-ray diffraction measurements.

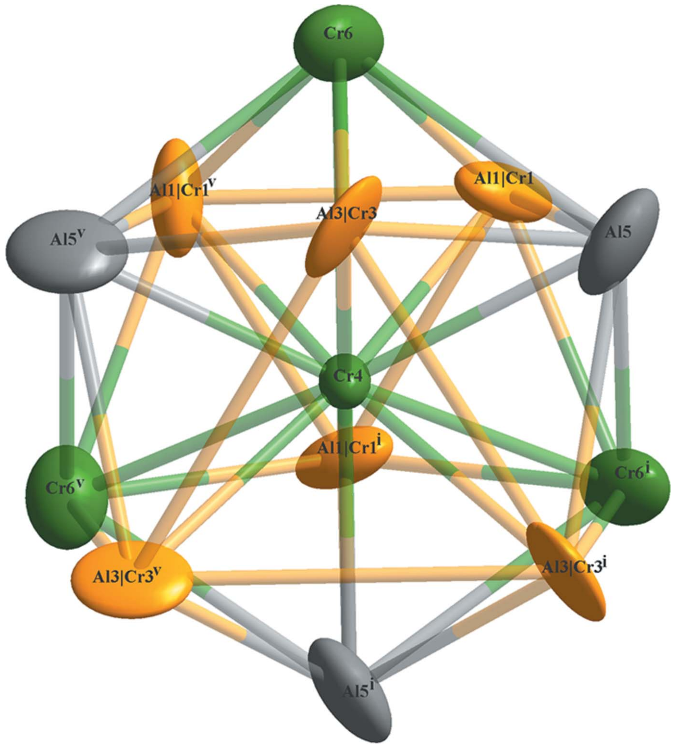


Figure 2
The environment of the Cr4 atom. Displacement ellipsoids are given at the 99% probability level. [Symmetry codes: (i) y, z, x; (v) y, z, x.]

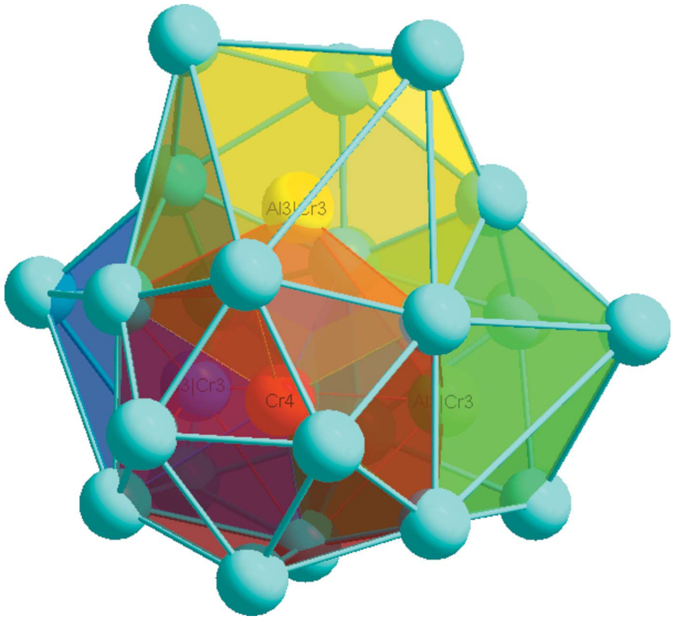


Figure 3
26-atom γ-brass-type cluster represented as four interpenetrating distorted icosahedra centred at one Cr4 and three Al3/Cr3 sites.

Fig. 1 shows the crystal structure of γ_2'-Al_8Cr_5 based on the standardized crystal data in the primitive trigonal setting (see Tables S2 and S3 of the supporting information). There are 78 atoms in the unit cell ($a = b = 12.8717$ Å, $c = 7.8408$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$), whose volume is three times that of the refined model (trigonal cell, rhombohedral axes, see Table 1). For simplicity, only two distorted icosahedra centred at Wyckoff sites $3a$ (Cr4, with coordinates 0, 0, z) are illustrated in Fig. 1, and the environment of the Cr4 atoms is shown in Fig. 2. The twelve vertices include three Al atoms (Al5), three Cr atoms (Cr6) along with six co-occupied Al/Cr sites (Al1/Cr1 and Al3/Cr3), for which the refined site occupancies converged to 0.772 (4) and 0.958 (4) for Al atoms Al1 and Al3.

The principle building blocks in the structure can also be represented by four interpenetrating distorted icosahedra centred at one Cr4 and three Al3/Cr3 atomic sites, as shown in Fig. 3, similarly to the building blocks of the I-cell (space group $I\bar{4}3m$) of the γ-brass phase (Pankova *et al.*, 2013). According to the topological analysis of the structure model with the 'nanocluster' method available in the *ToposPro* package (Akhmetshina & Blatov, 2017), these one Cr4 and three Al3/Cr3 sites form an inner tetrahedron (IT), followed by an outer tetrahedron (OT), an octahedron (OH), whose vertices are projected onto the edges of the outer tetrahedron, and finally a distorted cuboctahedron (CO) with vertices located above the edges of the octahedron, as illustrated in Fig. 4.

The present rhombohedral γ_2'-Al_8Cr_5 phase is thus confirmed to be isotypic to the previously reported ordered Al_8Cr_5 phase (Bradley & Lu, 1937), and closely related to the the disordered rhombohedral $Al_{16}Cr_{9.5}$ phase (Brandon *et al.*, 1977) and the disordered cubic Al_8Cr_5 phase (Braun *et al.*, 1992).

Synthesis and crystallization

The high-purity elements Al (indicated purity 99.8%, 0.588 g) and Cr (indicated purity 99.95%, 0.539 g) were mixed uniformly in the stoichiometric ratio 11:4 and thoroughly ground in an agate mortar. The blended powders were then placed in a cemented carbide grinding mould of 5 mm diameter, and pressed into a tablet at about 4 MPa for 5 min. A cylindrical block (5 mm in diameter and 3 mm in height) was obtained without deformations or cracks. Details of the high-pressure sintering experiment using a six-anvil high-temperature high-pressure apparatus can be found elsewhere (Liu & Fan, 2018). The samples were pressurized up to 5 GPa and heated to 1400°C for 30 minutes, slowly cooled to 660°C and held at this temperature for 2 h, and then rapidly cooled to room temperature by turning off the furnace power. Subsequently, a small amount of powder sample was uniformly placed on the inner wall of a quartz tube, annealed in a vacuum environment, heated to 300°C for 24 h, and then cooled within the furnace. A piece of a single crystal ($0.13 \times 0.06 \times 0.05$ mm^3) was selected and mounted on a glass fibre for single-crystal X-ray diffraction measurements.

Refinement

Table 1 shows the details of data collection and structural refinement. Three sites are co-occupied by Al and Cr atoms (Al1/Cr1, Al2/Cr2, Al3/Cr3). Site occupancies were refined, and then fixed to their as-found values, 0.772, 0.5 and 0.958 for Al1, Al2 and Al3, respectively, assuming full occupancy for each site. Atoms sharing the same site were constrained to have the same coordinates and displacement parameters. Moreover, disordered atoms were restrained to be isotropic, with standard deviations of 0.01 Å^2 (Sheldrick, 2015*b*). The maximum and minimum residual electron densities in the last difference map are located 1.68 Å from atom Cr3 and 0.36 Å from atom Cr4, respectively. The crystal was considered as a sample twinned by inversion (Parsons *et al.*, 2013), and the batch scale factor converged to $x = 0.3$ (2).

Table 1
Experimental details.

Crystal data	
Chemical formula	$Al_{7.85}Cr_{5.16}$
M_r	479.72
Crystal system, space group	Trigonal, *R*3*m*:*R*
Temperature (K)	296
a (Å)	7.8777 (5), 7.8777 (5)
α (°)	109.566 (2)
V (Å^3)	375.01 (7)
Z	2
Radiation type	Mo *Kα*
μ (mm^{-1})	8.05
Crystal size (mm)	$0.13 \times 0.06 \times 0.05$
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.496, 0.523
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7330, 576, 547
R_{int}	0.090
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.068, 0.178, 1.16
No. of reflections	576
No. of parameters	53
No. of restraints	37
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.02, −1.27
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.3 (2)

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2017/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2017) and *publCIF* (Westrip, 2010).

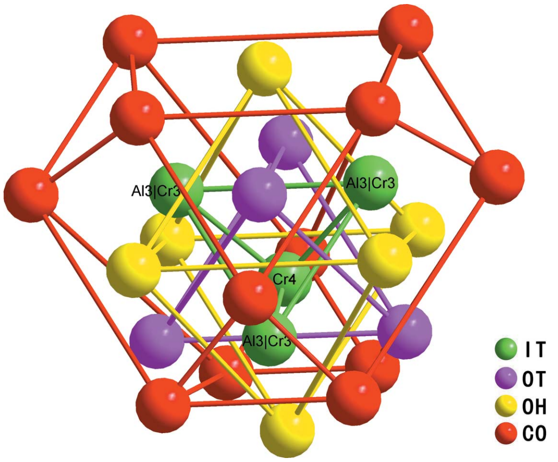


Figure 4
26-atom γ-brass-type cluster represented as a sequence of polyhedral shells.

Funding information

Funding for this research was provided by: Research Foundation of Education Bureau of Hebei Province (grant No. ZD2018069); The National Natural Science Foundation of China (grant No. 51771165).

References

Akhmetshina, T. G. & Blatov, V. A. (2017). *Z. Kristallogr.* **232**, 497–506.
Bradley, A. J. & Lu, S. S. (1937). *Z. Kristallogr.* **96**, 20–37.
Brandenburg, K. & Putz, H. (2017). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Brandon, J. K., Pearson, W. B., Riley, P. W., Chieh, C. & Stokhuyzen, R. (1977). *Acta Cryst.* B**33**, 1088–1095.
Braun, J., Ellner, M. & Predel, B. (1992). *J. Alloys Compd.* **183**, 444–448.
Bruker (2015). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, C. & Fan, C. (2018). *IUCrData*, **3**, x180363.
Pankova, A. A., Blatov, V. A., Ilyushin, G. D. & Proserpio, D. M. (2013). *Inorg. Chem.* **52**, 13094–13107.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2020). **5**, x200422 [https://doi.org/10.1107/S2414314620004228]

Crystal structure of the Al_8Cr_5-type intermetallic $Al_{7.85}Cr_{5.16}$

Xu Geng, Bin Wen and Changzeng Fan

Octaaluminium pentachromium

Crystal data

$Al_{7.85}Cr_{5.16}$
M_r = 479.72
Trigonal, $R3m$:R
a = 7.8777 (5) Å
α = 109.566 (2)°
V = 375.01 (7) Å^3
Z = 2
F(000) = 451
D_x = 4.248 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2208 reflections
θ = 3.2–26.3°
μ = 8.05 mm^{-1}
T = 296 K
Graininess, metallic silver
0.13 × 0.06 × 0.05 mm

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.496, T_{max} = 0.523
7330 measured reflections
576 independent reflections
547 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 26.8°, θ_{min} = 3.2°
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.178
S = 1.16
576 reflections
53 parameters
37 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 19.1482P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −1.27 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.3 (2)

Special details

Refinement. Refined as a two-component inversion twin

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Al1	0.2998 (14)	0.2998 (14)	0.0928 (15)	0.0108 (19)	0.772
Cr1	0.2998 (14)	0.2998 (14)	0.0928 (15)	0.0108 (19)	0.228
Al2	1.3096 (13)	0.6646 (11)	0.6646 (11)	0.0117 (19)	0.5
Cr2	1.3096 (13)	0.6646 (11)	0.6646 (11)	0.0117 (19)	0.5

Al3	0.9238 (18)	0.6488 (14)	0.6488 (14)	0.012 (2)	0.958
Cr3	0.9238 (18)	0.6488 (14)	0.6488 (14)	0.012 (2)	0.042
Cr4	−0.0434 (12)	−0.0434 (12)	−0.0434 (12)	0.006 (2)	
Cr5	0.6391 (8)	0.3060 (8)	0.3060 (8)	0.0028 (10)	
Cr6	1.3001 (10)	0.9464 (8)	0.9464 (8)	0.0108 (14)	
Cr7	0.5198 (13)	0.5198 (13)	0.5198 (13)	0.008 (2)	
Al4	0.5500 (17)	−0.0607 (15)	0.2804 (16)	0.018 (2)	
Al5	0.0366 (18)	0.0366 (18)	−0.313 (2)	0.015 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.007 (3)	0.007 (3)	0.019 (5)	0.005 (3)	0.006 (3)	0.006 (3)
Cr1	0.007 (3)	0.007 (3)	0.019 (5)	0.005 (3)	0.006 (3)	0.006 (3)
Al2	0.008 (4)	0.008 (3)	0.008 (3)	0.000 (3)	0.000 (3)	0.001 (3)
Cr2	0.008 (4)	0.008 (3)	0.008 (3)	0.000 (3)	0.000 (3)	0.001 (3)
Al3	0.013 (5)	0.010 (3)	0.010 (3)	0.007 (3)	0.007 (3)	−0.001 (3)
Cr3	0.013 (5)	0.010 (3)	0.010 (3)	0.007 (3)	0.007 (3)	−0.001 (3)
Cr4	0.007 (4)	0.007 (4)	0.007 (4)	0.005 (4)	0.005 (4)	0.005 (4)
Cr5	0.001 (2)	0.0034 (18)	0.0034 (18)	0.0001 (17)	0.0001 (17)	0.002 (2)
Cr6	0.016 (3)	0.008 (3)	0.008 (3)	0.006 (3)	0.006 (3)	0.003 (3)
Cr7	0.006 (3)	0.006 (3)	0.006 (3)	0.000 (4)	0.000 (4)	0.000 (4)
Al4	0.024 (5)	0.021 (4)	0.031 (5)	0.016 (3)	0.021 (4)	0.021 (4)
Al5	0.015 (4)	0.015 (4)	0.017 (5)	0.004 (5)	0.011 (4)	0.011 (4)

Geometric parameters (Å, º)

Al1—Cr5	2.611 (7)	Cr2—Al5^{xi}	2.930 (16)
Al1—Cr5^{i}	2.611 (7)	Al3—Cr5	2.572 (12)
Al1—Cr6^{ii}	2.634 (7)	Al3—Cr6	2.606 (11)
Al1—Cr6^{iii}	2.634 (7)	Al3—Cr4^{xiii}	2.655 (12)
Al1—Cr4	2.644 (11)	Al3—Cr7	2.678 (13)
Al1—Al4^{i}	2.654 (11)	Al3—Al5^{xiii}	2.758 (11)
Al1—Al4^{iv}	2.654 (11)	Al3—Al5^{xiv}	2.758 (11)
Al1—Al5	2.659 (17)	Al3—Al4^{xii}	2.798 (12)
Al1—Al1^{i}	2.665 (16)	Al3—Al4^{ix}	2.798 (12)
Al1—Al1^{v}	2.665 (16)	Cr3—Cr5	2.572 (12)
Al1—Cr7	2.739 (11)	Cr3—Cr6	2.606 (11)
Cr1—Cr5	2.611 (7)	Cr3—Cr4^{xiii}	2.655 (12)
Cr1—Cr5^{i}	2.611 (7)	Cr3—Cr7	2.678 (13)
Cr1—Cr6^{ii}	2.634 (7)	Cr3—Al5^{xiii}	2.758 (11)
Cr1—Cr6^{iii}	2.634 (7)	Cr3—Al5^{xiv}	2.758 (11)
Cr1—Cr4	2.644 (11)	Cr3—Al4^{xii}	2.798 (12)
Cr1—Al4^{i}	2.654 (11)	Cr3—Al4^{ix}	2.798 (12)
Cr1—Al4^{iv}	2.654 (11)	Cr4—Al5	2.616 (10)
Cr1—Al5	2.659 (17)	Cr4—Al5^{v}	2.616 (10)
Cr1—Cr7	2.739 (11)	Cr4—Al5^{i}	2.616 (10)
Al2—Cr6	2.604 (9)	Cr4—Cr6^{iii}	2.761 (7)

Al2—Cr7$^{\mathrm{vi}}$	2.647 (9)
Al2—Al4$^{\mathrm{vii}}$	2.656 (9)
Al2—Al4$^{\mathrm{viii}}$	2.656 (9)
Al2—Cr5$^{\mathrm{ix}}$	2.754 (6)
Al2—Cr5$^{\mathrm{x}}$	2.754 (6)
Al2—Al5$^{\mathrm{xi}}$	2.930 (16)
Al2—Al4$^{\mathrm{xii}}$	2.996 (10)
Al2—Al4$^{\mathrm{ix}}$	2.996 (10)
Cr2—Cr6	2.604 (9)
Cr2—Cr7$^{\mathrm{vi}}$	2.647 (9)
Cr2—Al4$^{\mathrm{vii}}$	2.656 (9)
Cr2—Al4$^{\mathrm{viii}}$	2.656 (9)
Cr2—Cr5$^{\mathrm{ix}}$	2.754 (6)
Cr2—Cr5$^{\mathrm{x}}$	2.754 (6)
Cr4—Cr6$^{\mathrm{ii}}$	2.761 (7)
Cr5—Cr7	2.603 (7)
Cr5—Al4$^{\mathrm{xii}}$	2.620 (10)
Cr5—Al4$^{\mathrm{ix}}$	2.620 (10)
Cr5—Al4$^{\mathrm{iv}}$	2.652 (9)
Cr5—Al4	2.652 (9)
Cr5—Al5$^{\mathrm{x}}$	2.683 (12)
Cr6—Al5$^{\mathrm{xi}}$	2.654 (12)
Cr6—Al4$^{\mathrm{xv}}$	2.739 (11)
Cr6—Al4$^{\mathrm{xiii}}$	2.739 (11)
Cr6—Al5$^{\mathrm{xiv}}$	2.849 (8)
Al4—Al5$^{\mathrm{x}}$	2.693 (12)
Al4—Al4$^{\mathrm{ix}}$	2.726 (5)
Al4—Al4$^{\mathrm{xvi}}$	2.726 (5)

Cr5—Al1—Cr5$^{\mathrm{i}}$	110.4 (5)
Cr5—Al1—Cr6$^{\mathrm{ii}}$	63.75 (14)
Cr5$^{\mathrm{i}}$—Al1—Cr6$^{\mathrm{ii}}$	167.7 (4)
Cr5—Al1—Cr6$^{\mathrm{iii}}$	167.7 (4)
Cr5$^{\mathrm{i}}$—Al1—Cr6$^{\mathrm{iii}}$	63.75 (14)
Cr6$^{\mathrm{ii}}$—Al1—Cr6$^{\mathrm{iii}}$	119.6 (5)
Cr5—Al1—Cr4	112.8 (3)
Cr5$^{\mathrm{i}}$—Al1—Cr4	112.8 (3)
Cr6$^{\mathrm{ii}}$—Al1—Cr4	63.1 (2)
Cr6$^{\mathrm{iii}}$—Al1—Cr4	63.1 (2)
Cr5—Al1—Al4$^{\mathrm{i}}$	125.5 (4)
Cr5$^{\mathrm{i}}$—Al1—Al4$^{\mathrm{i}}$	60.5 (2)
Cr6$^{\mathrm{ii}}$—Al1—Al4$^{\mathrm{i}}$	131.8 (4)
Cr6$^{\mathrm{iii}}$—Al1—Al4$^{\mathrm{i}}$	62.4 (2)
Cr4—Al1—Al4$^{\mathrm{i}}$	120.0 (3)
Cr5—Al1—Al4$^{\mathrm{iv}}$	60.5 (2)
Cr5$^{\mathrm{i}}$—Al1—Al4$^{\mathrm{iv}}$	125.5 (4)
Cr6$^{\mathrm{ii}}$—Al1—Al4$^{\mathrm{iv}}$	62.4 (2)
Cr6$^{\mathrm{iii}}$—Al1—Al4$^{\mathrm{iv}}$	131.8 (4)
Cr4—Al1—Al4$^{\mathrm{iv}}$	120.0 (3)
Al4$^{\mathrm{i}}$—Al1—Al4$^{\mathrm{iv}}$	81.7 (5)
Cr5—Al1—Al5	124.0 (2)
Cr5$^{\mathrm{i}}$—Al1—Al5	124.0 (2)
Cr6$^{\mathrm{ii}}$—Al1—Al5	65.1 (3)
Cr6$^{\mathrm{iii}}$—Al1—Al5	65.1 (3)
Cr4—Al1—Al5	59.1 (3)
Al4$^{\mathrm{i}}$—Al1—Al5	76.7 (3)
Al4$^{\mathrm{iv}}$—Al1—Al5	76.7 (3)
Cr5—Al1—Al1$^{\mathrm{i}}$	108.1 (2)
Cr5$^{\mathrm{i}}$—Al1—Al1$^{\mathrm{i}}$	59.3 (2)
Cr6$^{\mathrm{ii}}$—Al1—Al1$^{\mathrm{i}}$	111.0 (2)
Cr6$^{\mathrm{iii}}$—Al1—Al1$^{\mathrm{i}}$	59.6 (2)
Cr4—Al1—Al1$^{\mathrm{i}}$	59.73 (18)
Cr3—Cr5—Cr7	62.3 (4)
Al3—Cr5—Cr7	62.3 (4)
Cr3—Cr5—Al1$^{\mathrm{v}}$	116.2 (4)
Al3—Cr5—Al1$^{\mathrm{v}}$	116.2 (4)
Cr7—Cr5—Al1$^{\mathrm{v}}$	63.4 (3)
Cr7—Cr5—Al1	63.4 (3)
Al1$^{\mathrm{v}}$—Cr5—Al1	61.4 (4)
Cr7—Cr5—Cr1	63.4 (3)
Cr3—Cr5—Al4$^{\mathrm{xii}}$	65.2 (3)
Al3—Cr5—Al4$^{\mathrm{xii}}$	65.2 (3)
Cr7—Cr5—Al4$^{\mathrm{xii}}$	110.8 (3)
Al1$^{\mathrm{v}}$—Cr5—Al4$^{\mathrm{xii}}$	168.9 (3)
Al1—Cr5—Al4$^{\mathrm{xii}}$	107.8 (3)
Cr1—Cr5—Al4$^{\mathrm{xii}}$	107.8 (3)
Cr3—Cr5—Al4$^{\mathrm{ix}}$	65.2 (3)
Al3—Cr5—Al4$^{\mathrm{ix}}$	65.2 (3)
Cr7—Cr5—Al4$^{\mathrm{ix}}$	110.8 (3)
Al1$^{\mathrm{v}}$—Cr5—Al4$^{\mathrm{ix}}$	107.8 (3)
Al1—Cr5—Al4$^{\mathrm{ix}}$	168.9 (3)
Cr1—Cr5—Al4$^{\mathrm{ix}}$	168.9 (3)
Al4$^{\mathrm{xii}}$—Cr5—Al4$^{\mathrm{ix}}$	83.0 (5)
Cr3—Cr5—Al4$^{\mathrm{iv}}$	121.2 (3)
Al3—Cr5—Al4$^{\mathrm{iv}}$	121.2 (3)
Cr7—Cr5—Al4$^{\mathrm{iv}}$	115.6 (3)
Al1$^{\mathrm{v}}$—Cr5—Al4$^{\mathrm{iv}}$	110.7 (4)
Al1—Cr5—Al4$^{\mathrm{iv}}$	60.5 (3)
Cr1—Cr5—Al4$^{\mathrm{iv}}$	60.5 (3)
Al4$^{\mathrm{xii}}$—Cr5—Al4$^{\mathrm{iv}}$	62.3 (2)
Al4$^{\mathrm{ix}}$—Cr5—Al4$^{\mathrm{iv}}$	129.1 (2)
Cr3—Cr5—Al4	121.2 (3)
Al3—Cr5—Al4	121.2 (3)
Cr7—Cr5—Al4	115.6 (3)
Al1$^{\mathrm{v}}$—Cr5—Al4	60.5 (3)

Al4^{i}—Al1—Al1^{i}	109.0 (2)
Al4^{iv}—Al1—Al1^{i}	168.2 (3)
Al5—Al1—Al1^{i}	110.2 (3)
Cr5—Al1—Al1^{v}	59.3 (2)
Cr5^{i}—Al1—Al1^{v}	108.1 (2)
Cr6^{ii}—Al1—Al1^{v}	59.6 (2)
Cr6^{iii}—Al1—Al1^{v}	111.0 (2)
Cr4—Al1—Al1^{v}	59.73 (18)
Al4^{i}—Al1—Al1^{v}	168.2 (3)
Al4^{iv}—Al1—Al1^{v}	109.0 (2)
Al5—Al1—Al1^{v}	110.2 (3)
Al1^{i}—Al1—Al1^{v}	60.000 (1)
Cr5—Al1—Cr7	58.2 (2)
Cr5^{i}—Al1—Cr7	58.2 (2)
Cr6^{ii}—Al1—Cr7	111.2 (3)
Cr6^{iii}—Al1—Cr7	111.2 (3)
Cr4—Al1—Cr7	110.2 (4)
Al4^{i}—Al1—Cr7	111.1 (3)
Al4^{iv}—Al1—Cr7	111.1 (3)
Al5—Al1—Cr7	169.4 (5)
Al1^{i}—Al1—Cr7	60.89 (18)
Al1^{v}—Al1—Cr7	60.89 (18)
Cr5—Cr1—Cr5^{i}	110.4 (5)
Cr5—Cr1—Cr6^{ii}	63.75 (14)
Cr5^{i}—Cr1—Cr6^{ii}	167.7 (4)
Cr5—Cr1—Cr6^{iii}	167.7 (4)
Cr5^{i}—Cr1—Cr6^{iii}	63.75 (14)
Cr6^{ii}—Cr1—Cr6^{iii}	119.6 (5)
Cr5—Cr1—Cr4	112.8 (3)
Cr5^{i}—Cr1—Cr4	112.8 (3)
Cr6^{ii}—Cr1—Cr4	63.1 (2)
Cr6^{iii}—Cr1—Cr4	63.1 (2)
Cr5—Cr1—Al4^{i}	125.5 (4)
Cr5^{i}—Cr1—Al4^{i}	60.5 (2)
Cr6^{ii}—Cr1—Al4^{i}	131.8 (4)
Cr6^{iii}—Cr1—Al4^{i}	62.4 (2)
Cr4—Cr1—Al4^{i}	120.0 (3)
Cr5—Cr1—Al4^{iv}	60.5 (2)
Cr5^{i}—Cr1—Al4^{iv}	125.5 (4)
Cr6^{ii}—Cr1—Al4^{iv}	62.4 (2)
Cr6^{iii}—Cr1—Al4^{iv}	131.8 (4)
Cr4—Cr1—Al4^{iv}	120.0 (3)
Al4^{i}—Cr1—Al4^{iv}	81.7 (5)
Cr5—Cr1—Al5	124.0 (2)
Cr5^{i}—Cr1—Al5	124.0 (2)
Cr6^{ii}—Cr1—Al5	65.1 (3)
Cr6^{iii}—Cr1—Al5	65.1 (3)
Cr4—Cr1—Al5	59.1 (3)
Al1—Cr5—Al4	110.7 (4)
Cr1—Cr5—Al4	110.7 (4)
Al4^{xii}—Cr5—Al4	129.1 (2)
Al4^{ix}—Cr5—Al4	62.3 (2)
Al4^{iv}—Cr5—Al4	111.7 (5)
Cr3—Cr5—Al5^{x}	128.3 (4)
Al3—Cr5—Al5^{x}	128.3 (4)
Cr7—Cr5—Al5^{x}	169.4 (4)
Al1^{v}—Cr5—Al5^{x}	107.8 (3)
Al1—Cr5—Al5^{x}	107.8 (3)
Cr1—Cr5—Al5^{x}	107.8 (3)
Al4^{xii}—Cr5—Al5^{x}	76.8 (3)
Al4^{ix}—Cr5—Al5^{x}	76.8 (3)
Al4^{iv}—Cr5—Al5^{x}	60.6 (3)
Al4—Cr5—Al5^{x}	60.6 (3)
Cr3—Cr5—Al2^{xvi}	64.3 (2)
Al3—Cr5—Al2^{xvi}	64.3 (2)
Cr7—Cr5—Al2^{xvi}	59.1 (2)
Al1^{v}—Cr5—Al2^{xvi}	60.5 (3)
Al1—Cr5—Al2^{xvi}	110.8 (3)
Cr1—Cr5—Al2^{xvi}	110.8 (3)
Al4^{xii}—Cr5—Al2^{xvi}	125.9 (4)
Al4^{ix}—Cr5—Al2^{xvi}	59.2 (3)
Al4^{iv}—Cr5—Al2^{xvi}	170.8 (4)
Al4—Cr5—Al2^{xvi}	67.3 (2)
Al5^{x}—Cr5—Al2^{xvi}	123.0 (2)
Cr2—Cr6—Al1^{xiii}	149.6 (2)
Al2—Cr6—Al1^{xiii}	149.6 (2)
Cr3—Cr6—Al1^{xiii}	108.9 (3)
Al3—Cr6—Al1^{xiii}	108.9 (3)
Al1^{xiii}—Cr6—Al1^{xiv}	60.8 (4)
Cr2—Cr6—Al5^{xi}	67.7 (4)
Al2—Cr6—Al5^{xi}	67.7 (4)
Cr3—Cr6—Al5^{xi}	136.9 (4)
Al3—Cr6—Al5^{xi}	136.9 (4)
Al1^{xiii}—Cr6—Al5^{xi}	108.0 (4)
Al1^{xiv}—Cr6—Al5^{xi}	108.0 (4)
Al1^{xiii}—Cr6—Al4^{xv}	59.2 (3)
Al1^{xiv}—Cr6—Al4^{xv}	107.4 (4)
Al5^{xi}—Cr6—Al4^{xv}	59.9 (3)
Cr2—Cr6—Al4^{xiii}	96.4 (3)
Al2—Cr6—Al4^{xiii}	96.4 (3)
Cr3—Cr6—Al4^{xiii}	126.1 (2)
Al3—Cr6—Al4^{xiii}	126.1 (2)
Al1^{xiii}—Cr6—Al4^{xiii}	107.4 (4)
Al1^{xiv}—Cr6—Al4^{xiii}	59.2 (3)
Al5^{xi}—Cr6—Al4^{xiii}	59.9 (3)
Al4^{xv}—Cr6—Al4^{xiii}	106.5 (5)

Al4^{i}—Cr1—Al5	76.7 (3)
Al4^{iv}—Cr1—Al5	76.7 (3)
Cr5—Cr1—Cr7	58.2 (2)
Cr5^{i}—Cr1—Cr7	58.2 (2)
Cr6^{ii}—Cr1—Cr7	111.2 (3)
Cr6^{iii}—Cr1—Cr7	111.2 (3)
Cr4—Cr1—Cr7	110.2 (4)
Al4^{i}—Cr1—Cr7	111.1 (3)
Al4^{iv}—Cr1—Cr7	111.1 (3)
Al5—Cr1—Cr7	169.4 (5)
Cr6—Al2—Cr7^{vi}	150.7 (4)
Cr6—Al2—Al4^{vii}	71.0 (2)
Cr7^{vi}—Al2—Al4^{vii}	108.3 (2)
Cr6—Al2—Al4^{viii}	71.0 (2)
Cr7^{vi}—Al2—Al4^{viii}	108.3 (2)
Al4^{vii}—Al2—Al4^{viii}	141.3 (4)
Cr6—Al2—Cr5^{ix}	128.85 (18)
Cr7^{vi}—Al2—Cr5^{ix}	57.6 (2)
Al4^{vii}—Al2—Cr5^{ix}	159.6 (4)
Al4^{viii}—Al2—Cr5^{ix}	57.9 (2)
Cr6—Al2—Cr5^{x}	128.85 (18)
Cr7^{vi}—Al2—Cr5^{x}	57.6 (2)
Al4^{vii}—Al2—Cr5^{x}	57.9 (2)
Al4^{viii}—Al2—Cr5^{x}	159.6 (4)
Cr5^{ix}—Al2—Cr5^{x}	102.2 (4)
Cr6—Al2—Al5^{xi}	56.9 (3)
Cr7^{vi}—Al2—Al5^{xi}	93.8 (4)
Al4^{vii}—Al2—Al5^{xi}	82.8 (3)
Al4^{viii}—Al2—Al5^{xi}	82.8 (3)
Cr5^{ix}—Al2—Al5^{xi}	111.2 (3)
Cr5^{x}—Al2—Al5^{xi}	111.2 (3)
Cr6—Al2—Al4^{xii}	99.9 (3)
Cr7^{vi}—Al2—Al4^{xii}	103.8 (3)
Al4^{vii}—Al2—Al4^{xii}	57.30 (18)
Al4^{viii}—Al2—Al4^{xii}	123.5 (4)
Cr5^{ix}—Al2—Al4^{xii}	108.9 (3)
Cr5^{x}—Al2—Al4^{xii}	54.7 (2)
Al5^{xi}—Al2—Al4^{xii}	139.6 (3)
Cr6—Al2—Al4^{ix}	99.9 (3)
Cr7^{vi}—Al2—Al4^{ix}	103.8 (3)
Al4^{vii}—Al2—Al4^{ix}	123.5 (4)
Al4^{viii}—Al2—Al4^{ix}	57.30 (18)
Cr5^{ix}—Al2—Al4^{ix}	54.7 (2)
Cr5^{x}—Al2—Al4^{ix}	108.9 (3)
Al5^{xi}—Al2—Al4^{ix}	139.6 (3)
Al4^{xii}—Al2—Al4^{ix}	70.8 (4)
Cr6—Cr2—Cr7^{vi}	150.7 (4)
Cr6—Cr2—Al4^{vii}	71.0 (2)
Al1^{xiii}—Cr6—Cr4^{xiii}	58.6 (2)
Al1^{xiv}—Cr6—Cr4^{xiii}	58.6 (2)
Al5^{xi}—Cr6—Cr4^{xiii}	163.9 (4)
Al4^{xv}—Cr6—Cr4^{xiii}	113.1 (3)
Al4^{xiii}—Cr6—Cr4^{xiii}	113.1 (3)
Cr2—Cr6—Cr5^{xiii}	127.0 (4)
Al2—Cr6—Cr5^{xiii}	127.0 (4)
Cr3—Cr6—Cr5^{xiii}	163.9 (3)
Al3—Cr6—Cr5^{xiii}	163.9 (3)
Al1^{xiii}—Cr6—Cr5^{xiii}	57.7 (2)
Al1^{xiv}—Cr6—Cr5^{xiii}	57.7 (2)
Al5^{xi}—Cr6—Cr5^{xiii}	59.2 (3)
Al4^{xv}—Cr6—Cr5^{xiii}	57.6 (2)
Al4^{xiii}—Cr6—Cr5^{xiii}	57.6 (3)
Cr4^{xiii}—Cr6—Cr5^{xiii}	104.7 (3)
Cr2—Cr6—Al5^{xiv}	99.6 (3)
Al2—Cr6—Al5^{xiv}	99.6 (3)
Cr3—Cr6—Al5^{xiv}	60.5 (3)
Al3—Cr6—Al5^{xiv}	60.5 (3)
Al1^{xiii}—Cr6—Al5^{xiv}	105.5 (3)
Al1^{xiv}—Cr6—Al5^{xiv}	57.8 (3)
Al5^{xi}—Cr6—Al5^{xiv}	127.5 (2)
Al4^{xv}—Cr6—Al5^{xiv}	164.0 (4)
Al4^{xiii}—Cr6—Al5^{xiv}	72.2 (3)
Cr4^{xiii}—Cr6—Al5^{xiv}	55.6 (2)
Cr5^{xiii}—Cr6—Al5^{xiv}	111.8 (3)
Cr5—Cr7—Cr5^{v}	110.9 (2)
Cr5—Cr7—Cr5^{i}	110.9 (2)
Cr5^{v}—Cr7—Cr5^{i}	110.9 (2)
Cr5—Cr7—Al2^{xviii}	166.5 (5)
Cr5^{v}—Cr7—Al2^{xviii}	63.27 (8)
Cr5^{i}—Cr7—Al2^{xviii}	63.27 (8)
Cr5—Cr7—Al2^{xix}	63.27 (8)
Cr5^{v}—Cr7—Al2^{xix}	166.5 (5)
Cr5^{i}—Cr7—Al2^{xix}	63.27 (8)
Cr5—Cr7—Al2^{xvi}	63.27 (8)
Cr5^{v}—Cr7—Al2^{xvi}	63.27 (8)
Cr5^{i}—Cr7—Al2^{xvi}	166.5 (5)
Al2^{xviii}—Cr7—Al2^{xvi}	119.39 (7)
Al2^{xix}—Cr7—Al2^{xvi}	119.39 (7)
Cr5—Cr7—Al3	58.3 (2)
Cr5^{v}—Cr7—Al3	124.25 (17)
Cr5^{i}—Cr7—Al3	124.25 (17)
Cr5—Cr7—Cr3	58.3 (2)
Cr5^{v}—Cr7—Cr3	124.25 (17)
Cr5^{i}—Cr7—Cr3	124.25 (17)
Cr5—Cr7—Al3^{i}	124.25 (17)
Cr5^{v}—Cr7—Al3^{i}	124.25 (17)

Cr7^{vi}—Cr2—Al4^{vii}	108.3 (2)
Cr6—Cr2—Al4^{viii}	71.0 (2)
Cr7^{vi}—Cr2—Al4^{viii}	108.3 (2)
Al4^{vii}—Cr2—Al4^{viii}	141.3 (4)
Cr6—Cr2—Cr5^{ix}	128.85 (18)
Cr7^{vi}—Cr2—Cr5^{ix}	57.6 (2)
Al4^{vii}—Cr2—Cr5^{ix}	159.6 (4)
Al4^{viii}—Cr2—Cr5^{ix}	57.9 (2)
Cr6—Cr2—Cr5^{x}	128.85 (18)
Cr7^{vi}—Cr2—Cr5^{x}	57.6 (2)
Al4^{vii}—Cr2—Cr5^{x}	57.9 (2)
Al4^{viii}—Cr2—Cr5^{x}	159.6 (4)
Cr5^{ix}—Cr2—Cr5^{x}	102.2 (4)
Cr6—Cr2—Al5^{xi}	56.9 (3)
Cr7^{vi}—Cr2—Al5^{xi}	93.8 (4)
Al4^{vii}—Cr2—Al5^{xi}	82.8 (3)
Al4^{viii}—Cr2—Al5^{xi}	82.8 (3)
Cr5^{ix}—Cr2—Al5^{xi}	111.2 (3)
Cr5^{x}—Cr2—Al5^{xi}	111.2 (3)
Cr5—Al3—Cr6	157.4 (4)
Cr5—Al3—Cr4^{xiii}	139.3 (5)
Cr6—Al3—Cr4^{xiii}	63.3 (3)
Cr5—Al3—Cr7	59.4 (3)
Cr6—Al3—Cr7	143.2 (4)
Cr4^{xiii}—Al3—Cr7	79.9 (4)
Cr5—Al3—Al5^{xiii}	123.2 (3)
Cr6—Al3—Al5^{xiii}	64.1 (3)
Cr4^{xiii}—Al3—Al5^{xiii}	57.8 (3)
Cr7—Al3—Al5^{xiii}	97.1 (3)
Cr5—Al3—Al5^{xiv}	123.2 (3)
Cr6—Al3—Al5^{xiv}	64.1 (3)
Cr4^{xiii}—Al3—Al5^{xiv}	57.8 (3)
Cr7—Al3—Al5^{xiv}	97.1 (3)
Al5^{xiii}—Al3—Al5^{xiv}	109.5 (6)
Cr5—Al3—Al4^{xii}	58.2 (3)
Cr6—Al3—Al4^{xii}	105.2 (4)
Cr4^{xiii}—Al3—Al4^{xii}	141.1 (3)
Cr7—Al3—Al4^{xii}	103.4 (4)
Al5^{xiii}—Al3—Al4^{xii}	83.5 (3)
Al5^{xiv}—Al3—Al4^{xii}	154.2 (5)
Cr5—Al3—Al4^{ix}	58.2 (3)
Cr6—Al3—Al4^{ix}	105.2 (4)
Cr4^{xiii}—Al3—Al4^{ix}	141.1 (3)
Cr7—Al3—Al4^{ix}	103.4 (4)
Al5^{xiii}—Al3—Al4^{ix}	154.2 (5)
Al5^{xiv}—Al3—Al4^{ix}	83.5 (3)
Al4^{xii}—Al3—Al4^{ix}	76.6 (5)
Cr5—Cr3—Cr6	157.4 (4)
Cr5^{i}—Cr7—Al3^{i}	58.3 (2)
Al2^{xviii}—Cr7—Al3^{i}	64.46 (17)
Al2^{xix}—Cr7—Al3^{i}	64.46 (17)
Al2^{xvi}—Cr7—Al3^{i}	135.3 (5)
Al3—Cr7—Al3^{i}	82.8 (4)
Cr3—Cr7—Al3^{i}	82.8 (4)
Cr5—Cr7—Al3^{v}	124.25 (17)
Cr5^{v}—Cr7—Al3^{v}	58.3 (2)
Cr5^{i}—Cr7—Al3^{v}	124.25 (17)
Cr5—Cr7—Al1^{v}	58.5 (2)
Cr5^{v}—Cr7—Al1^{v}	58.5 (2)
Cr5^{i}—Cr7—Al1^{v}	106.2 (4)
Al2^{xviii}—Cr7—Al1^{v}	110.2 (3)
Al2^{xix}—Cr7—Al1^{v}	110.2 (3)
Al2^{xvi}—Cr7—Al1^{v}	60.3 (3)
Al3—Cr7—Al1^{v}	108.7 (3)
Cr3—Cr7—Al1^{v}	108.7 (3)
Al3^{i}—Cr7—Al1^{v}	164.4 (4)
Al3^{v}—Cr7—Al1^{v}	108.7 (3)
Cr5—Cr7—Al1^{i}	106.2 (4)
Cr5^{v}—Cr7—Al1^{i}	58.5 (2)
Cr5^{i}—Cr7—Al1^{i}	58.5 (2)
Al2^{xviii}—Cr7—Al1^{i}	60.3 (3)
Al2^{xix}—Cr7—Al1^{i}	110.2 (3)
Al2^{xvi}—Cr7—Al1^{i}	110.2 (3)
Al3—Cr7—Al1^{i}	164.4 (4)
Cr3—Cr7—Al1^{i}	164.4 (4)
Al3^{i}—Cr7—Al1^{i}	108.7 (3)
Al3^{v}—Cr7—Al1^{i}	108.7 (3)
Al1^{v}—Cr7—Al1^{i}	58.2 (4)
Cr5^{xvi}—Al4—Cr5	144.8 (4)
Cr5^{xvi}—Al4—Al1^{v}	86.3 (4)
Cr5—Al4—Al1^{v}	59.0 (3)
Cr5^{xvi}—Al4—Al2^{xx}	62.9 (2)
Cr5—Al4—Al2^{xx}	150.4 (5)
Al1^{v}—Al4—Al2^{xx}	148.8 (4)
Cr5^{xvi}—Al4—Al5^{x}	145.4 (6)
Cr5—Al4—Al5^{x}	60.2 (3)
Al1^{v}—Al4—Al5^{x}	106.3 (3)
Al2^{xx}—Al4—Al5^{x}	102.4 (4)
Cr5^{xvi}—Al4—Al4^{ix}	134.5 (5)
Cr5—Al4—Al4^{ix}	58.3 (4)
Al1^{v}—Al4—Al4^{ix}	103.5 (4)
Al2^{xx}—Al4—Al4^{ix}	95.5 (4)
Al5^{x}—Al4—Al4^{ix}	74.9 (5)
Cr5^{xvi}—Al4—Al4^{xvi}	59.4 (3)
Cr5—Al4—Al4^{xvi}	128.9 (4)
Al1^{v}—Al4—Al4^{xvi}	102.1 (5)

Cr5—Cr3—Cr4$^{\text{xiii}}$	139.3 (5)	Al2$^{\text{xx}}$—Al4—Al4$^{\text{xvi}}$	67.6 (4)
Cr6—Cr3—Cr4$^{\text{xiii}}$	63.3 (3)	Al5$^{\text{x}}$—Al4—Al4$^{\text{xvi}}$	86.1 (5)
Cr5—Cr3—Cr7	59.4 (3)	Al4$^{\text{ix}}$—Al4—Al4$^{\text{xvi}}$	151.5 (6)
Cr6—Cr3—Cr7	143.2 (4)	Cr5$^{\text{xvi}}$—Al4—Cr6$^{\text{ii}}$	106.6 (5)
Cr4$^{\text{xiii}}$—Cr3—Cr7	79.9 (4)	Cr5—Al4—Cr6$^{\text{ii}}$	61.8 (2)
Cr5—Cr3—Al5$^{\text{xiii}}$	123.2 (3)	Al1$^{\text{v}}$—Al4—Cr6$^{\text{ii}}$	58.4 (3)
Cr6—Cr3—Al5$^{\text{xiii}}$	64.1 (3)	Al2$^{\text{xx}}$—Al4—Cr6$^{\text{ii}}$	132.5 (4)
Cr4$^{\text{xiii}}$—Cr3—Al5$^{\text{xiii}}$	57.8 (3)	Al5$^{\text{x}}$—Al4—Cr6$^{\text{ii}}$	58.5 (3)
Cr7—Cr3—Al5$^{\text{xiii}}$	97.1 (3)	Al4$^{\text{ix}}$—Al4—Cr6$^{\text{ii}}$	116.5 (5)
Cr5—Cr3—Al5$^{\text{xiv}}$	123.2 (3)	Al4$^{\text{xvi}}$—Al4—Cr6$^{\text{ii}}$	68.0 (3)
Cr6—Cr3—Al5$^{\text{xiv}}$	64.1 (3)	Cr5$^{\text{xvi}}$—Al4—Al3$^{\text{xvi}}$	56.6 (3)
Cr4$^{\text{xiii}}$—Cr3—Al5$^{\text{xiv}}$	57.8 (3)	Cr5—Al4—Al3$^{\text{xvi}}$	118.0 (5)
Cr7—Cr3—Al5$^{\text{xiv}}$	97.1 (3)	Al1$^{\text{v}}$—Al4—Al3$^{\text{xvi}}$	97.2 (4)
Al5$^{\text{xiii}}$—Cr3—Al5$^{\text{xiv}}$	109.5 (6)	Al2$^{\text{xx}}$—Al4—Al3$^{\text{xvi}}$	62.7 (3)
Cr5—Cr3—Al4$^{\text{xii}}$	58.2 (3)	Al5$^{\text{x}}$—Al4—Al3$^{\text{xvi}}$	147.5 (5)
Cr6—Cr3—Al4$^{\text{xii}}$	105.2 (4)	Al4$^{\text{ix}}$—Al4—Al3$^{\text{xvi}}$	78.0 (4)
Cr4$^{\text{xiii}}$—Cr3—Al4$^{\text{xii}}$	141.1 (3)	Al4$^{\text{xvi}}$—Al4—Al3$^{\text{xvi}}$	110.9 (4)
Cr7—Cr3—Al4$^{\text{xii}}$	103.4 (4)	Cr6$^{\text{ii}}$—Al4—Al3$^{\text{xvi}}$	153.0 (5)
Al5$^{\text{xiii}}$—Cr3—Al4$^{\text{xii}}$	83.5 (3)	Cr5$^{\text{xvi}}$—Al4—Al2$^{\text{xvi}}$	99.8 (4)
Al5$^{\text{xiv}}$—Cr3—Al4$^{\text{xii}}$	154.2 (5)	Cr5—Al4—Al2$^{\text{xvi}}$	58.0 (2)
Cr5—Cr3—Al4$^{\text{ix}}$	58.2 (3)	Al1$^{\text{v}}$—Al4—Al2$^{\text{xvi}}$	56.9 (3)
Cr6—Cr3—Al4$^{\text{ix}}$	105.2 (4)	Al2$^{\text{xx}}$—Al4—Al2$^{\text{xvi}}$	120.5 (4)
Cr4$^{\text{xiii}}$—Cr3—Al4$^{\text{ix}}$	141.1 (3)	Al5$^{\text{x}}$—Al4—Al2$^{\text{xvi}}$	114.1 (4)
Cr7—Cr3—Al4$^{\text{ix}}$	103.4 (4)	Al4$^{\text{ix}}$—Al4—Al2$^{\text{xvi}}$	55.1 (2)
Al5$^{\text{xiii}}$—Cr3—Al4$^{\text{ix}}$	154.2 (5)	Al4$^{\text{xvi}}$—Al4—Al2$^{\text{xvi}}$	153.3 (5)
Al5$^{\text{xiv}}$—Cr3—Al4$^{\text{ix}}$	83.5 (3)	Cr6$^{\text{ii}}$—Al4—Al2$^{\text{xvi}}$	106.8 (3)
Al4$^{\text{xii}}$—Cr3—Al4$^{\text{ix}}$	76.6 (5)	Al3$^{\text{xvi}}$—Al4—Al2$^{\text{xvi}}$	61.3 (4)
Al5—Cr4—Al5$^{\text{v}}$	118.81 (14)	Cr4—Al5—Cr6$^{\text{xxi}}$	152.4 (6)
Al5—Cr4—Al5$^{\text{i}}$	118.81 (14)	Cr4—Al5—Cr1	60.2 (4)
Al5$^{\text{v}}$—Cr4—Al5$^{\text{i}}$	118.81 (14)	Cr6$^{\text{xxi}}$—Al5—Cr1	147.5 (5)
Al5—Cr4—Cr1	60.7 (4)	Cr4—Al5—Al1	60.2 (4)
Al5$^{\text{v}}$—Cr4—Cr1	112.2 (3)	Cr6$^{\text{xxi}}$—Al5—Al1	147.5 (5)
Al5$^{\text{i}}$—Cr4—Cr1	112.2 (3)	Cr4—Al5—Cr5$^{\text{xix}}$	145.1 (6)
Al5—Cr4—Al1	60.7 (4)	Cr6$^{\text{xxi}}$—Al5—Cr5$^{\text{xix}}$	62.5 (3)
Al5$^{\text{v}}$—Cr4—Al1	112.2 (3)	Cr1—Al5—Cr5$^{\text{xix}}$	84.9 (5)
Al5$^{\text{i}}$—Cr4—Al1	112.2 (3)	Al1—Al5—Cr5$^{\text{xix}}$	84.9 (5)
Al5—Cr4—Al1$^{\text{i}}$	112.2 (3)	Cr4—Al5—Al4$^{\text{xxii}}$	125.1 (3)
Al5$^{\text{v}}$—Cr4—Al1$^{\text{i}}$	112.2 (3)	Cr6$^{\text{xxi}}$—Al5—Al4$^{\text{xxii}}$	61.6 (3)
Al5$^{\text{i}}$—Cr4—Al1$^{\text{i}}$	60.7 (4)	Al1—Al5—Al4$^{\text{xxii}}$	102.9 (4)
Cr1—Cr4—Al1$^{\text{i}}$	60.5 (4)	Cr5$^{\text{xix}}$—Al5—Al4$^{\text{xxii}}$	59.1 (3)
Al1—Cr4—Al1$^{\text{i}}$	60.5 (4)	Cr4—Al5—Al4$^{\text{xix}}$	125.1 (3)
Al5—Cr4—Al1$^{\text{v}}$	112.2 (3)	Cr6$^{\text{xxi}}$—Al5—Al4$^{\text{xix}}$	61.6 (3)
Al5$^{\text{v}}$—Cr4—Al1$^{\text{v}}$	60.7 (4)	Cr1—Al5—Al4$^{\text{xix}}$	102.9 (4)
Al5$^{\text{i}}$—Cr4—Al1$^{\text{v}}$	112.2 (3)	Al1—Al5—Al4$^{\text{xix}}$	102.9 (4)
Cr1—Cr4—Al1$^{\text{v}}$	60.5 (4)	Cr5$^{\text{xix}}$—Al5—Al4$^{\text{xix}}$	59.1 (3)
Al1—Cr4—Al1$^{\text{v}}$	60.5 (4)	Al4$^{\text{xxii}}$—Al5—Al4$^{\text{xix}}$	109.2 (5)
Al1$^{\text{i}}$—Cr4—Al1$^{\text{v}}$	60.5 (4)	Cr4—Al5—Al3$^{\text{iii}}$	59.1 (3)
Al5—Cr4—Al3$^{\text{iii}}$	63.1 (2)	Cr6$^{\text{xxi}}$—Al5—Al3$^{\text{iii}}$	101.0 (4)

Al5^{v}—Cr4—Al3^{iii}	134.0 (6)
Al5^{i}—Cr4—Al3^{iii}	63.1 (2)
Cr1—Cr4—Al3^{iii}	107.2 (3)
Al1—Cr4—Al3^{iii}	107.2 (3)
Al1^{i}—Cr4—Al3^{iii}	107.2 (3)
Al1^{v}—Cr4—Al3^{iii}	165.2 (4)
Al5—Cr4—Al3^{xvii}	134.0 (6)
Al5^{v}—Cr4—Al3^{xvii}	63.1 (2)
Al5^{i}—Cr4—Al3^{xvii}	63.1 (2)
Cr1—Cr4—Al3^{xvii}	165.2 (4)
Al1—Cr4—Al3^{xvii}	165.2 (4)
Al1^{i}—Cr4—Al3^{xvii}	107.2 (3)
Al1^{v}—Cr4—Al3^{xvii}	107.2 (3)
Al3^{iii}—Cr4—Al3^{xvii}	83.6 (4)
Al5—Cr4—Al3^{ii}	63.1 (2)
Al5^{v}—Cr4—Al3^{ii}	63.1 (2)
Al5^{i}—Cr4—Al3^{ii}	134.0 (6)
Cr1—Cr4—Al3^{ii}	107.2 (3)
Al1—Cr4—Al3^{ii}	107.2 (3)
Al1^{i}—Cr4—Al3^{ii}	165.2 (4)
Al1^{v}—Cr4—Al3^{ii}	107.2 (3)
Al3^{iii}—Cr4—Al3^{ii}	83.6 (4)
Al3^{xvii}—Cr4—Al3^{ii}	83.6 (4)
Al5—Cr4—Cr6^{iii}	63.93 (12)
Al5^{v}—Cr4—Cr6^{iii}	168.5 (6)
Al5^{i}—Cr4—Cr6^{iii}	63.93 (12)
Cr1—Cr4—Cr6^{iii}	58.27 (18)
Al1—Cr4—Cr6^{iii}	58.27 (18)
Al1^{i}—Cr4—Cr6^{iii}	58.27 (18)
Al1^{v}—Cr4—Cr6^{iii}	107.8 (4)
Al3^{iii}—Cr4—Cr6^{iii}	57.5 (3)
Al3^{xvii}—Cr4—Cr6^{iii}	124.18 (16)
Al3^{ii}—Cr4—Cr6^{iii}	124.18 (16)
Al5—Cr4—Cr6^{ii}	63.93 (12)
Al5^{v}—Cr4—Cr6^{ii}	63.93 (12)
Al5^{i}—Cr4—Cr6^{ii}	168.5 (6)
Cr1—Cr4—Cr6^{ii}	58.27 (18)
Al1—Cr4—Cr6^{ii}	58.27 (18)
Al1^{i}—Cr4—Cr6^{ii}	107.8 (4)
Al1^{v}—Cr4—Cr6^{ii}	58.27 (18)
Al3^{iii}—Cr4—Cr6^{ii}	124.18 (16)
Al3^{xvii}—Cr4—Cr6^{ii}	124.18 (16)
Al3^{ii}—Cr4—Cr6^{ii}	57.5 (3)
Cr6^{iii}—Cr4—Cr6^{ii}	111.1 (2)
Cr1—Al5—Al3^{iii}	103.8 (4)
Al1—Al5—Al3^{iii}	103.8 (4)
Cr5^{xix}—Al5—Al3^{iii}	138.3 (3)
Al4^{xxii}—Al5—Al3^{iii}	149.3 (6)
Al4^{xix}—Al5—Al3^{iii}	79.2 (3)
Cr4—Al5—Al3^{ii}	59.1 (3)
Cr6^{xxi}—Al5—Al3^{ii}	101.0 (4)
Cr1—Al5—Al3^{ii}	103.8 (4)
Al1—Al5—Al3^{ii}	103.8 (4)
Cr5^{xix}—Al5—Al3^{ii}	138.3 (3)
Al4^{xxii}—Al5—Al3^{ii}	79.2 (3)
Al4^{xix}—Al5—Al3^{ii}	149.3 (6)
Al3^{iii}—Al5—Al3^{ii}	79.9 (6)
Cr4—Al5—Cr6^{ii}	60.5 (3)
Cr6^{xxi}—Al5—Cr6^{ii}	126.6 (2)
Cr1—Al5—Cr6^{ii}	57.0 (2)
Al1—Al5—Cr6^{ii}	57.0 (2)
Cr5^{xix}—Al5—Cr6^{ii}	101.9 (3)
Al4^{xxii}—Al5—Cr6^{ii}	66.8 (2)
Al4^{xix}—Al5—Cr6^{ii}	155.4 (6)
Al3^{iii}—Al5—Cr6^{ii}	117.2 (4)
Al3^{ii}—Al5—Cr6^{ii}	55.4 (2)
Cr4—Al5—Cr6^{iii}	60.5 (3)
Cr6^{xxi}—Al5—Cr6^{iii}	126.6 (2)
Cr1—Al5—Cr6^{iii}	57.0 (2)
Al1—Al5—Cr6^{iii}	57.0 (2)
Cr5^{xix}—Al5—Cr6^{iii}	101.9 (3)
Al4^{xxii}—Al5—Cr6^{iii}	155.4 (6)
Al4^{xix}—Al5—Cr6^{iii}	66.8 (2)
Al3^{iii}—Al5—Cr6^{iii}	55.4 (2)
Al3^{ii}—Al5—Cr6^{iii}	117.2 (4)
Cr6^{ii}—Al5—Cr6^{iii}	106.1 (4)
Cr4—Al5—Al2^{xxi}	97.0 (4)
Cr6^{xxi}—Al5—Al2^{xxi}	55.3 (3)
Cr1—Al5—Al2^{xxi}	157.2 (5)
Al1—Al5—Al2^{xxi}	157.2 (5)
Cr5^{xix}—Al5—Al2^{xxi}	117.9 (4)
Al4^{xxii}—Al5—Al2^{xxi}	90.1 (4)
Al4^{xix}—Al5—Al2^{xxi}	90.1 (4)
Al3^{iii}—Al5—Al2^{xxi}	59.8 (3)
Al3^{ii}—Al5—Al2^{xxi}	59.8 (3)
Cr6^{ii}—Al5—Al2^{xxi}	113.8 (3)
Cr6^{iii}—Al5—Al2^{xxi}	113.8 (3)

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