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Redetermination of the crystal structure of yttrium chromium tetraboride, $YCrB_4$, from single-crystal X-ray diffraction data

Makoto Tokuda,[a]* Kunio Yubuta,[b] Toetsu Shishido[c] and Kazumasa Sugiyama[c]

[a]Institute of Industrial Nano Materials, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan, [b]Department of Applied Quantum Physics and Nuclear Engineering, Kyushu University, Fukuoka 819-0395, Japan, and [c]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan. *Correspondence e-mail: tokuda@nech.kumamoto-u.ac.jp

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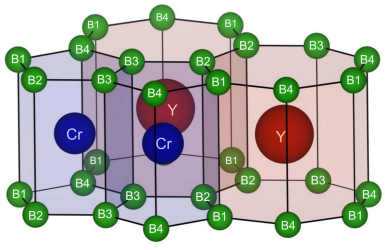
The structural parameters of yttrium chromium tetraboride $YCrB_4$ were refined based on single-crystal X-ray diffraction data. $YCrB_4$ is orthorhombic, having a space group of type *Pbam* (No. 55) and with lattice parameters of a = 5.9425 (2), b = 11.4831 (4), c = 3.4643 (1) Å. The Y and Cr atoms are located at Wyckoff 4*h* sites (x, y, 0) and B atoms at the Wyckoff 4*g* sites (x, y, 1/2). The first structural investigation of $YCrB_4$ was performed using a single crystalline sample [Kuz'ma, (1970). *Kristallografiya*. **15**, 372–374]. The present study successfully refined all the positional and atomic displacement parameters of the Y, Cr, and B atoms.

1. Chemical context

The investigation of AlB_2-type-analogous intermetallic compounds (RB_2, MB_2, RMB_4, and R_2MB_6; R = rare-earth, M = aluminium or transition metal) has been pursued using various experimental and theoretical methods. Recently, hydrogenated monolayer boron sheets (borophene) have attracted attention because of their topological Dirac nodal loops, with the AlB_2-type-analogous compounds expected to be the parent materials (Cuong *et al.*, 2020; Niibe *et al.*, 2021; Tateishi *et al.*, 2022). $YCrB_4$ is a parent material candidate for the synthesis of (5-7)-α-borophene sheets (*i.e.*, boron networks with five- and seven-membered rings), for which detailed structural data are currently required (Zhang *et al.*, 2022, 2023). $YCrB_4$ is a promising semiconductor material with good thermoelectric properties and a good power factor of 6.0 μW cm^{-1} K^{-2} at 500 K (Simonson & Poon, 2010; Flipo *et al.*, 2021). The $YCrB_4$ compound is also expected to be a super-hard material (Akopov *et al.*, 2018) and a narrow bandgap semiconductor (Medvedeva *et al.*, 2002). A theoretically calculated Debye temperature θ_D for $YCrB_4$ of 965 K was given by Candan *et al.* (2019). Notably, Kuz'ma (1970) conducted the first structural analysis of $YCrB_4$.



2. Structural commentary

The AlB_2-type-analogous compounds are composed of borophene layers stacked with other metal atomic layers. The boron network is composed of six-membered rings (honeycomb layer), with R or M atoms located at the center of a hexagonal prism formed by twelve boron atoms (Fig. 1*a*). $YCrB_4$ exhibits an ordered and rearranged crystal structure derived from the AlB_2-type structure of YB_2 or CrB_2 (Kuz'ma, 1970). The six-membered rings are rearranged into five- and seven-membered rings [(5-7)-α-borophene layer]

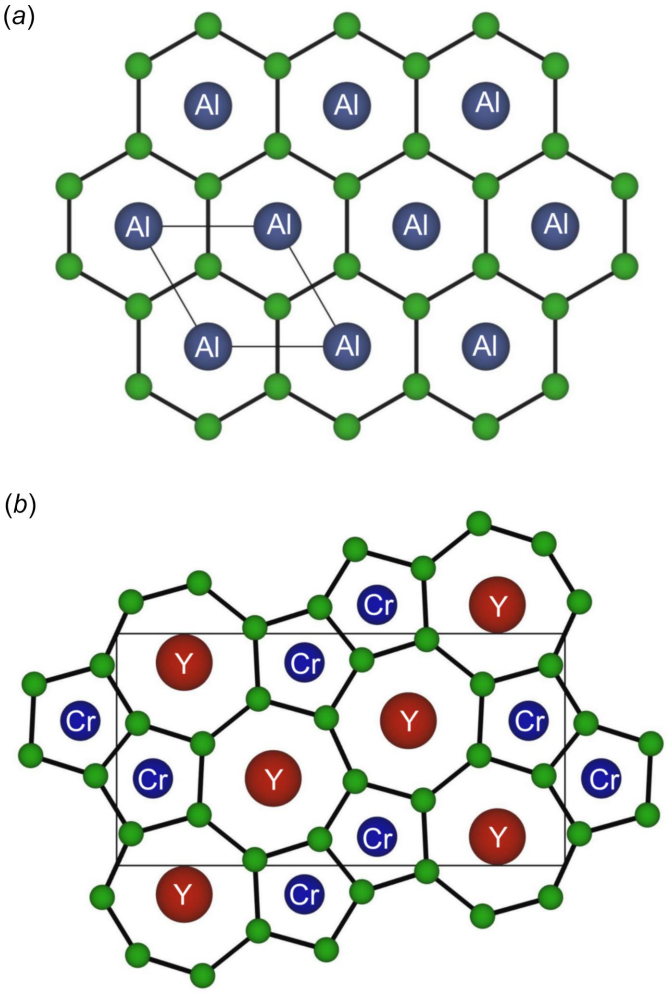


Figure 1
Crystal structure of boron-metal-layered compounds. Honeycomb borophene layer in AlB_2 (*b*) and (5–7)-α-borophene layer in $YCrB_4$ (*a*) viewed along the *c*-axis and illustrated using *VESTA* (Momma & Izumi, 2011).

due to the ordering of Cr and Y (Fig. 1*b*). These (5-7)-α-borophene layers are accumulated along the *c* axis in an $\alpha\alpha$ stacking sequence with the metal atomic layers. The Cr and Y atoms are located at the centers of the CrB_{10} pentagonal and YB_{14} heptagonal prisms, respectively (Fig. 2). With different arrangements of the MB_{10} pentagonal prism and RB_{14} heptagonal prism, three distinct structural types have been reported for the AlB_2-type-analogous compounds: (5-7)-α-type ($YCrB_4$-type: Rogl, 1978; Sobczak & Rogl, 1979), (5-7)-β-type ($ThMoB_4$-type: Rogl & Nowotny 1974; Veremchuk *et al.*, 2008), and (5-6-7)-γ-type (Y_2ReB_6-type: Kuz'ma & Svarichevskaya, 1972; Okada *et al.*, 2006).

The Cr—B and Y—B interatomic distances are in the range of 2.2677 (15)–2.3254 (10) and 2.6177 (16)–2.7478 (14) Å, respectively (Table 1), which are close to the sums of the respective Goldschmidt radii (r_B = 0.97 Å, r_{Cr} = 1.36 Å, and r_Y = 1.81 Å; Brandes & Brook, 1992). The interplanar Cr—Cr distance is 2.3745 (4) Å, indicating a strong correlation between the Cr atoms. The intra- and interplanar Y—Y distances are 3.7446 (3)–3.7653 (5) and 3.46425 (12) Å, respectively (the latter simply corresponding to the *c*-axis length). The interplanar Y—Y distance is much smaller than the sum of radii of the Y atoms. A short intraplanar *R*—*R* distance can be observed in various *R*–*M*–B systems with layered structures (Higashi *et al.*, 1988; Tokuda *et al.*, 2022). The B—B interatomic distances within the pentagons and heptagons in $YCrB_4$ are in the ranges 1.724 (4)–1.828 (2) and 1.741 (3)–1.832 (2) Å, respectively, similar to the average B—B covalent bonding distances of 1.77 Å in α-rhombohedral boron (Donohue, 1974).

Table 1
Selected bond lengths (Å) in $YCrB_4$.

CrB_{10} Pentagonal prism		*Five-membered ring*	
Cr—B3×2	2.2677 (15)	B3–B3^{viii}	1.724 (4)
Cr—B3×2	2.2723 (9)	B2^{i}–B3^{viii}	1.741 (4)
Cr—B1×2	2.2962 (11)	B3–B4	1.742 (2)
Cr—B2×2	2.3081 (16)	B1^{i}–B2^{i}	1.807 (2)
Cr—B4×6	2.3254 (10)	B1^{i}–B4	1.828 (2)
YB_{14} Heptagonal prism		*Seven-membered ring*	
Y—B3×2	2.6177 (16)	B2^{v}–B3^{i}	1.741 (3)
Y—B4×2	2.6582 (11)	B3^{i}–B4^{i}	1.742 (2)
Y—B2×2	2.6959 (15)	B2–B2^{v}	1.788 (4)
Y—B1×2	2.7003 (12)	B1–B2	1.807 (2)
Y—B2×6	2.7241 (11)	B1^{i}–B4	1.828 (2)
Y—B1×2	2.7350 (13)	B1–B4	1.832 (2)
Y—B4×6	2.7478 (14)	B1^{i}–B4^{i}	1.832 (2)
Interplanar atomic distances			
Cr^{i}—Cr^{x}	2.3745 (4)	Y^{i}—Y	3.7446 (3)
Y^{i}—Cr^{iii}	3.0517 (4)	Y^{i}—Y^{ix}	3.7446 (3)
Y^{i}—Cr^{ix}	3.0760 (3)	Y^{i}—Y^{ii}	3.7653 (5)
Y^{i}—Cr	3.0789 (3)		
Y^{i}—Cr^{i}	3.0803 (4)		

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z$; (iii) $1-x, 1-y, -z$; (v) $1-x, 1-y, 1-z$; (viii) $1-x, -y, 1-z$; (ix) $1+x, y, z$; (x) $-x+\frac{1}{2}, y-\frac{1}{2}, -z$]

A covalently bonded boron network in boride compounds plays an important role for thermal conductivity and mechanical and lattice dynamical properties. The Debye temperature θ_D was used to characterize these physical properties. Previous studies on intermetallic boride compounds have also proposed that the bulk θ_D is associated with the rigidity of the boron network (Korsukova *et al.*, 1987; Levchenko *et al.*, 2006; Singh *et al.*, 2010). Using the isotropic

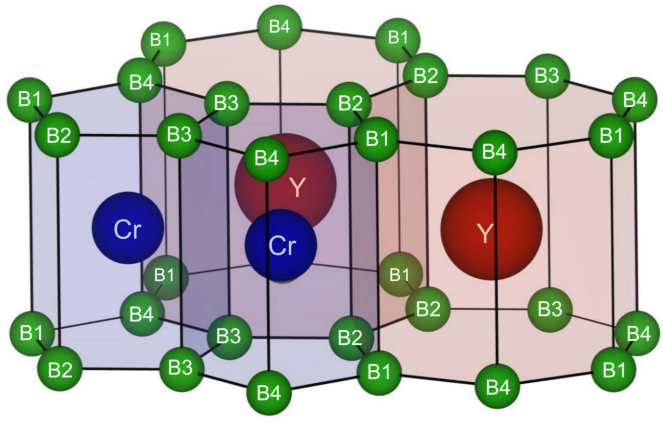


Figure 2
Cr and Y atoms settle in the center of the pentagonal CrB_{10} and heptagonal YB_{14} prisms, respectively.

Table 2
Atomic coordinates and anisotropic displacement parameters (10^3 Å^2) for $YCrB_4$.

The Y and Cr atoms lie on the Wyckoff sites 4*h* (*x*, *y*, 0), and the B atoms occupy the 4*g* (*x*, *y*, 1/2) site. The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11} + \cdots + 2hka^*b^*U_{12}]$. U_{iso} is defined as a third of the trace of the orthogonalized U_{ij} tensor. $U_{12} = U_{23} = 0$.

Atom	*x*	*y*	U_{11}	U_{22}	U_{33}	U_{12}	U_{iso}
Y	0.12446 (2)	0.15077 (2)	0.00298 (4)	0.00275 (4)	0.00284 (4)	0.00027 (4)	0.00285 (3)
Cr	0.12421 (4)	0.41902 (2)	0.00262 (6)	0.00241 (6)	0.00297 (6)	0.00007 (6)	0.00267 (3)
B1	0.2818 (3)	0.31614 (15)	0.0045 (5)	0.0035 (4)	0.0047 (5)	0.0007 (4)	0.0042 (2)
B2	0.3630 (4)	0.46779 (13)	0.0037 (6)	0.0035 (4)	0.0053 (5)	0.0001 (5)	0.0042 (2)
B3	0.3869 (4)	0.04697 (12)	0.0029 (5)	0.0034 (4)	0.0043 (4)	−0.0001 (5)	0.0036 (2)
B4	0.4746 (3)	0.19170 (13)	0.0041 (5)	0.0028 (5)	0.0054 (5)	−0.0001 (4)	0.0041 (2)

atomic displacement parameter U_{iso} and Debye approximation (Willis & Pryor, 1975), the θ_D were derived using the following equation: $<U_{iso}^2> = (3h^2\ T)\ /(4\pi^2\ m\ k_B\ \theta_D^2)$, where *h* is Planck's constant, *m* is the mass of the atom, and k_B is the Boltzmann constant. The mean square $<U_{iso}^2>$ for B atoms was calculated using the average U_{iso} for the boron sites. The anisotropic displacement parameters (ADPs) for each atom are listed in Table 2, with no significant anisotropy being observed in the ADPs of any atom (Fig. 3). The estimated θ_D for Y, Cr, and B were 413 (2), 524 (3), and 996 (25) K, respectively. Candan *et al.* (2019) studied the lattice-dynamical properties of $YCrB_4$ using density functional theory and gave a calculated θ_D of 965 K that corresponds well with our estimated θ_D for the B atoms. This result indicates that the bulk θ_D of the AlB_2-type-analogous compounds can be estimated from the ADPs for the B atom.

3. Synthesis and crystallization

The starting materials were Y (99.9%), Cr (99.95%), and B (99.5%). They were weighed in an atomic ratio Y:Cr:B = 1:1:4. The mixture was melted in an argon-arc melting furnace (ACM-01, Diavac). The product was then turned over and remelted three times to improve its chemical homogeneity. Homogeneous $YCrB_4$ crystals were obtained.

4. Refinement details

Refinement was conducted using a space group of type *Pbam*, as reported by Kuz'ma, 1970. A correction for isotropic extinction was applied during the least-squares refinement. Final refinements were performed with inclusion of anisotropic ADPs to each atom. The final refinement results are listed in Table 3. The refinement was successful, with the *R* factor converging without any problems and no noticeable residuals.

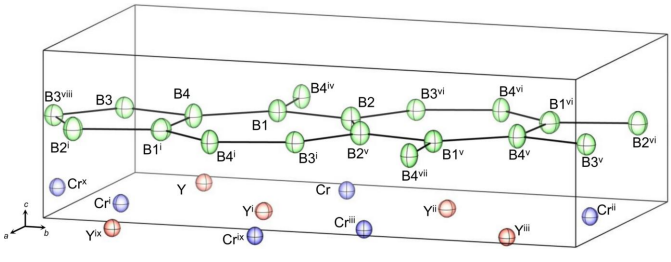


Figure 3
Displacement ellipsoids of each atom in $YCrB_4$. Displacement ellipsoids are drawn at the 99% probability level. [Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, z$; (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z$; (iii) $1 - x, 1 - y, -z$; (iv) $x - \frac{1}{2}, -y + \frac{1}{2}, z$; (v) $1 - x, 1 - y, 1 - z$; (vi) $-x + \frac{1}{2}, y + \frac{1}{2}, 1 - z$; (vii) $-x + \frac{3}{2}, y + \frac{1}{2}, 1 - z$; (viii) $1 - x, -y, 1 - z$; (ix) $1 + x, y, z$; (x) $-x + \frac{1}{2}, y - \frac{1}{2}, -z$].

Funding information

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References

Akopov, K., Yin, H., Roh, I., Pangilinan, L. E. & Kaner, R. B. (2018). *Chem. Mater.* **30**, 6494–6502.
Brandes, E. A. & Brook, G. B. (1992). *Smithells Metals Reference Book*, pp. 4–41. Oxford, London: Butterworth-Heinemann Ltd.

Table 3
Experimental details.

Crystal data	
Chemical formula	$YCrB_4$
M_r	184.15
Crystal system, space group	Orthorhombic, *Pbam*
Temperature (K)	294
a, *b*, *c* (Å)	5.9425 (2), 11.4831 (4), 3.46425 (12)
V (Å^3)	236.40 (1)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	28.57
Crystal size (mm)	0.05 × 0.03 × 0.03
Data collection	
Diffractometer	XtaLAB Synergy, HyPix
Absorption correction	Numerical (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.367, 0.655
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13376, 1074, 865
R_{int}	0.036
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.992
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.015, 0.029, 1.11
No. of reflections	1074
No. of parameters	38
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.71

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), and *VESTA* (Momma & Izumi, 2011).

Candan, A., Surucu, G. & Gencer, A. (2019). *Phys. Scr.* **94**, 125710.
Cuong, N. T., Tateishi, I., Cameau, M., Niibe, M., Umezawa, N., Slater, B., Yubuta, K., Kondo, T., Ogata, M., Okada, S. & Matsuda, I. (2020). *Phys. Rev. B*, **101**, 195412.
Donohue, J. (1974). *The Structures of the Elements.* New York: Wiley.
Flipo, S., Rosner, H., Bobnar, M., Kvashnina, K. O., Leithe-Jasper, A. & Gumeniuk, R. (2021). *Phys. Rev. B*, **103**, 195121.
Higashi, I., Shishido, T., Takei, H. & Kobayashi, T. (1988). *J. Less-Common Met.* **139**, 211–220.
Korsukova, M. M., Lundström, T., Tergenius, L.-E. & Gurin, V. N. (1987). *Solid State Commun.* **63**, 187–189.
Kuz'ma, Y. B. (1970). *Kristallografiya*, **15**, 372–374.
Kuz'ma, Yu. B. & Svarichevskaya, S. I. (1972). *Kristallografiya*, **17**, 569–571.
Levchenko, G., Lyashchenko, A., Baumer, V., Evdokimova, A., Filippov, V., Paderno, Y. & Shitsevalova, N. (2006). *J. Solid State Chem.* **179**, 2949–2953.
Medvedeva, N. I., Medvedeva, Y. E. & Ivanovskii, A. L. (2002). *Dokl. Phys. Chem.* **383**, 75–77.
Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
Niibe, M., Cameau, M., Cuong, N. T., Sunday, O. I., Zhang, X., Tsujikawa, Y., Okada, S., Yubuta, K., Kondo, T. & Matsuda, I. (2021). *Phys. Rev. Mater.* **5**, 084007.
Okada, S., Shishido, T., Mori, T., Kudou, K., Iizumi, K., Lundström, T. & Nakajima, K. (2006). *J. Alloys Compd.* **408–412**, 547–550.
Rigaku OD (2021). *CrysAlis PRO*. Rigaku Corporation, Oxford, UK.
Rogl, P. (1978). *Mater. Res. Bull.* **13**, 519–523.
Rogl, P. & Nowotny, H. (1974). *Monatshefte f?r Chemie*, **105**, 1082–1098.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Simonson, J. & Poon, S. (2010). *J. Alloys Compd.* **504**, 265–272.
Singh, Y., Martin, C., Bud'ko, S. L., Ellern, A., Prozorov, R. & Johnston, D. C. (2010). *Phys. Rev. B*, **82**, 144532.
Sobczak, R. & Rogl, P. (1979). *J. Solid State Chem.* **27**, 343–348.
Tateishi, I., Zhang, X. & Matsuda, I. (2022). *Molecules*, **27**, 1808.
Tokuda, M., Yubuta, K., Shishido, T. & Sugiyama, K. (2022). *Acta Cryst.* E**78**, 76–79.
Veremchuk, I., Mori, T., Prots, Yu., Schnelle, W., Leithe-Jasper, A., Kohout, M. & Grin, Yu. (2008). *J. Solid State Chem.* **181**, 1983–1991.
Willis, B. T. M. & Pryor, A. W. (1975). *Thermal vibrations in crystallography*. London: Cambridge University Press.
Zhang, X., Hikichi, M., Iimori, T., Tsujikawa, Y., Yuan, M., Horio, M., Yubuta, K., Komori, F., Miyauchi, M., Kondo, T. & Matsuda, I. (2023). *Molecules*, **28**, 2985.
Zhang, X., Tsujikawa, Y., Tateishi, I., Niibe, M., Wada, T., Horio, M., Hikichi, M., Ando, Y., Yubuta, K., Kondo, T. & Matsuda, I. (2022). *J. Phys. Chem. C*, **126**, 12802–12808.

supporting information

Acta Cryst. (2023). E**79**, 1072-1075 [https://doi.org/10.1107/S2056989023008952]

Redetermination of the crystal structure of yttrium chromium tetraboride, $YCrB_4$, from single-crystal X-ray diffraction data

Makoto Tokuda, Kunio Yubuta, Toetsu Shishido and Kazumasa Sugiyama

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011).

Yttrium chromium tetraboride

Crystal data

$YCrB_4$
M_r = 184.15
Orthorhombic, *Pbam*
a = 5.9425 (2) Å
b = 11.4831 (4) Å
c = 3.46425 (12) Å
V = 236.40 (1) Å^3
Z = 4
F(000) = 332
D_x = 5.174 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6090 reflections
θ = 3.5–44.9°
μ = 28.57 mm^{-1}
T = 294 K
Block, metallic
0.05 × 0.03 × 0.03 mm

Data collection

XtaLAB Synergy, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: numerical (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.367, T_{max} = 0.655
13376 measured reflections
1074 independent reflections
865 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 44.9°, θ_{min} = 3.6°
h = −11→11
k = −22→22
l = −6→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.029
S = 1.11
1074 reflections
38 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0074P)^2 + 0.1807P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.020
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Extinction correction: *SHELXL* (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0111 (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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Y	0.12446 (2)	0.15077 (2)	0.000000	0.00285 (3)
Cr	0.12421 (4)	0.41902 (2)	0.000000	0.00267 (3)
B1	0.2818 (3)	0.31614 (15)	0.500000	0.0042 (2)
B2	0.3630 (4)	0.46779 (13)	0.500000	0.0042 (2)
B3	0.3869 (4)	0.04697 (12)	0.500000	0.0036 (2)
B4	0.4746 (3)	0.19170 (13)	0.500000	0.0041 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Y	0.00298 (4)	0.00275 (4)	0.00284 (4)	0.00027 (4)	0.000	0.000
Cr	0.00262 (6)	0.00241 (6)	0.00297 (6)	0.00007 (6)	0.000	0.000
B1	0.0045 (5)	0.0035 (4)	0.0047 (5)	0.0007 (4)	0.000	0.000
B2	0.0037 (6)	0.0035 (4)	0.0053 (5)	0.0001 (5)	0.000	0.000
B3	0.0029 (5)	0.0034 (4)	0.0043 (4)	0.0000 (5)	0.000	0.000
B4	0.0041 (5)	0.0028 (5)	0.0054 (5)	−0.0001 (4)	0.000	0.000

Geometric parameters (Å, º)

Y—B3	2.6177 (16)	Cr—B3^{vii}	2.2723 (9)
Y—B3^{i}	2.6177 (16)	Cr—B1^{i}	2.2962 (11)
Y—B4^{ii}	2.6582 (11)	Cr—B1	2.2962 (11)
Y—B4^{iii}	2.6582 (11)	Cr—B2^{i}	2.3081 (16)
Y—B2^{iii}	2.6959 (15)	Cr—B2	2.3081 (16)
Y—B2^{ii}	2.6959 (15)	Cr—B4^{iii}	2.3254 (10)
Y—B1^{iii}	2.7003 (12)	Cr—B4^{ii}	2.3254 (10)
Y—B1^{ii}	2.7003 (12)	Cr—Cr^{viii}	2.3745 (4)
Y—B2^{iv}	2.7241 (11)	B1—B2	1.807 (2)
Y—B2^{v}	2.7241 (11)	B1—B4^{ii}	1.828 (2)
Y—B1	2.7350 (13)	B1—B4	1.832 (2)
Y—B1^{i}	2.7350 (13)	B2—B3^{vi}	1.741 (4)
Cr—B3^{iii}	2.2677 (15)	B2—B2^{ix}	1.789 (5)
Cr—B3^{ii}	2.2677 (15)	B3—B3^{x}	1.724 (4)
Cr—B3^{vi}	2.2723 (9)	B3—B4	1.742 (2)
B3—Y—B3^{i}	82.86 (6)	B2—B1—Cr^{xi}	67.24 (6)
B3—Y—B4^{ii}	94.49 (3)	B4^{ii}—B1—Cr^{xi}	67.55 (5)
B3^{i}—Y—B4^{ii}	160.16 (5)	B4—B1—Cr^{xi}	131.03 (3)
B3—Y—B4^{iii}	160.16 (5)	Cr—B1—Cr^{xi}	97.93 (6)

B3^{i}—Y—B4^{iii}	94.49 (3)	B2—B1—Y^{xii}	70.31 (7)
B4^{ii}—Y—B4^{iii}	81.33 (4)	B4^{ii}—B1—Y^{xii}	139.48 (3)
B3—Y—B2^{iii}	122.58 (4)	B4—B1—Y^{xii}	68.78 (5)
B3^{i}—Y—B2^{iii}	71.84 (4)	Cr—B1—Y^{xii}	135.97 (7)
B4^{ii}—Y—B2^{iii}	124.69 (6)	Cr^{xi}—B1—Y^{xii}	75.60 (2)
B4^{iii}—Y—B2^{iii}	74.45 (4)	B2—B1—Y^{xiii}	70.31 (7)
B3—Y—B2^{ii}	71.84 (4)	B4^{ii}—B1—Y^{xiii}	139.48 (3)
B3^{i}—Y—B2^{ii}	122.58 (4)	B4—B1—Y^{xiii}	68.78 (5)
B4^{ii}—Y—B2^{ii}	74.45 (4)	Cr—B1—Y^{xiii}	75.60 (2)
B4^{iii}—Y—B2^{ii}	124.69 (5)	Cr^{xi}—B1—Y^{xiii}	135.97 (7)
B2^{iii}—Y—B2^{ii}	79.96 (5)	Y^{xii}—B1—Y^{xiii}	79.80 (4)
B3—Y—B1^{iii}	159.68 (5)	B2—B1—Y^{xi}	139.50 (3)
B3^{i}—Y—B1^{iii}	95.10 (4)	B4^{ii}—B1—Y^{xi}	67.94 (6)
B4^{ii}—Y—B1^{iii}	93.99 (4)	B4—B1—Y^{xi}	70.86 (5)
B4^{iii}—Y—B1^{iii}	39.96 (4)	Cr—B1—Y^{xi}	134.07 (6)
B2^{iii}—Y—B1^{iii}	39.13 (5)	Cr^{xi}—B1—Y^{xi}	74.94 (2)
B2^{ii}—Y—B1^{iii}	92.78 (5)	Y^{xii}—B1—Y^{xi}	87.09 (2)
B3—Y—B1^{ii}	95.10 (4)	Y^{xiii}—B1—Y^{xi}	139.62 (6)
B3^{i}—Y—B1^{ii}	159.68 (5)	B2—B1—Y	139.50 (3)
B4^{ii}—Y—B1^{ii}	39.96 (4)	B4^{ii}—B1—Y	67.94 (6)
B4^{iii}—Y—B1^{ii}	93.99 (4)	B4—B1—Y	70.86 (5)
B2^{iii}—Y—B1^{ii}	92.78 (5)	Cr—B1—Y	74.94 (2)
B2^{ii}—Y—B1^{ii}	39.13 (5)	Cr^{xi}—B1—Y	134.07 (6)
B1^{iii}—Y—B1^{ii}	79.80 (4)	Y^{xii}—B1—Y	139.62 (6)
B3—Y—B2^{iv}	93.05 (4)	Y^{xiii}—B1—Y	87.09 (2)
B3^{i}—Y—B2^{iv}	37.98 (7)	Y^{xi}—B1—Y	78.59 (4)
B4^{ii}—Y—B2^{iv}	161.52 (6)	B3^{vi}—B2—B2^{ix}	124.09 (14)
B4^{iii}—Y—B2^{iv}	96.88 (3)	B3^{vi}—B2—B1	105.99 (17)
B2^{iii}—Y—B2^{iv}	38.53 (9)	B2^{ix}—B2—B1	129.92 (17)
B2^{ii}—Y—B2^{iv}	92.00 (3)	B3^{vi}—B2—Cr	66.58 (9)
B1^{iii}—Y—B2^{iv}	73.82 (5)	B2^{ix}—B2—Cr	131.30 (4)
B1^{ii}—Y—B2^{iv}	122.48 (5)	B1—B2—Cr	66.55 (6)
B3—Y—B2^{v}	37.98 (7)	B3^{vi}—B2—Cr^{xi}	66.58 (9)
B3^{i}—Y—B2^{v}	93.05 (4)	B2^{ix}—B2—Cr^{xi}	131.30 (4)
B4^{ii}—Y—B2^{v}	96.88 (3)	B1—B2—Cr^{xi}	66.55 (6)
B4^{iii}—Y—B2^{v}	161.52 (6)	Cr—B2—Cr^{xi}	97.26 (9)
B2^{iii}—Y—B2^{v}	92.00 (3)	B3^{vi}—B2—Y^{xii}	139.05 (5)
B2^{ii}—Y—B2^{v}	38.53 (9)	B2^{ix}—B2—Y^{xii}	71.58 (9)
B1^{iii}—Y—B2^{v}	122.48 (5)	B1—B2—Y^{xii}	70.56 (6)
B1^{ii}—Y—B2^{v}	73.82 (5)	Cr—B2—Y^{xii}	135.56 (6)
B2^{iv}—Y—B2^{v}	78.97 (4)	Cr^{xi}—B2—Y^{xii}	75.50 (2)
B3—Y—B1	72.15 (4)	B3^{vi}—B2—Y^{xiii}	139.05 (5)
B3^{i}—Y—B1	122.11 (5)	B2^{ix}—B2—Y^{xiii}	71.58 (9)
B4^{ii}—Y—B1	39.59 (4)	B1—B2—Y^{xiii}	70.56 (6)
B4^{iii}—Y—B1	93.14 (3)	Cr—B2—Y^{xiii}	75.50 (2)
B2^{iii}—Y—B1	162.65 (5)	Cr^{xi}—B2—Y^{xiii}	135.56 (6)
B2^{ii}—Y—B1	98.09 (3)	Y^{xii}—B2—Y^{xiii}	79.95 (5)
B1^{iii}—Y—B1	124.49 (3)	B3^{vi}—B2—Y^{vi}	67.70 (5)

B1^{ii}—Y—B1	75.75 (3)	B2^{ix}—B2—Y^{vi}	69.88 (7)
B2^{iv}—Y—B1	158.26 (6)	B1—B2—Y^{vi}	138.64 (4)
B2^{v}—Y—B1	97.09 (4)	Cr—B2—Y^{vi}	132.94 (8)
B3—Y—B1^{i}	122.11 (5)	Cr^{xi}—B2—Y^{vi}	74.15 (3)
B3^{i}—Y—B1^{i}	72.15 (4)	Y^{xii}—B2—Y^{vi}	88.01 (3)
B4^{ii}—Y—B1^{i}	93.14 (3)	Y^{xiii}—B2—Y^{vi}	141.47 (9)
B4^{iii}—Y—B1^{i}	39.59 (4)	B3^{vi}—B2—Y^{vii}	67.70 (5)
B2^{iii}—Y—B1^{i}	98.09 (3)	B2^{ix}—B2—Y^{vii}	69.88 (7)
B2^{ii}—Y—B1^{i}	162.65 (5)	B1—B2—Y^{vii}	138.64 (4)
B1^{iii}—Y—B1^{i}	75.75 (3)	Cr—B2—Y^{vii}	74.15 (3)
B1^{ii}—Y—B1^{i}	124.49 (3)	Cr^{xi}—B2—Y^{vii}	132.94 (8)
B2^{iv}—Y—B1^{i}	97.09 (4)	Y^{xii}—B2—Y^{vii}	141.47 (9)
B2^{v}—Y—B1^{i}	158.26 (6)	Y^{xiii}—B2—Y^{vii}	88.01 (3)
B1—Y—B1^{i}	78.59 (4)	Y^{vi}—B2—Y^{vii}	78.97 (4)
B3^{iii}—Cr—B3^{ii}	99.61 (9)	B3^{x}—B3—B2^{v}	109.78 (13)
B3^{iii}—Cr—B3^{vi}	116.93 (3)	B3^{x}—B3—B4	111.32 (18)
B3^{ii}—Cr—B3^{vi}	44.63 (10)	B2^{v}—B3—B4	138.90 (18)
B3^{iii}—Cr—B3^{vii}	44.63 (10)	B3^{x}—B3—Cr^{xii}	67.83 (9)
B3^{ii}—Cr—B3^{vii}	116.93 (3)	B2^{v}—B3—Cr^{xii}	128.34 (4)
B3^{vi}—Cr—B3^{vii}	99.33 (5)	B4—B3—Cr^{xii}	69.48 (6)
B3^{iii}—Cr—B1^{i}	76.47 (5)	B3^{x}—B3—Cr^{xiii}	67.83 (9)
B3^{ii}—Cr—B1^{i}	156.70 (6)	B2^{v}—B3—Cr^{xiii}	128.34 (4)
B3^{vi}—Cr—B1^{i}	156.85 (7)	B4—B3—Cr^{xiii}	69.48 (6)
B3^{vii}—Cr—B1^{i}	76.67 (5)	Cr^{xii}—B3—Cr^{xiii}	99.61 (9)
B3^{iii}—Cr—B1	156.70 (6)	B3^{x}—B3—Cr^{iv}	67.54 (6)
B3^{ii}—Cr—B1	76.47 (5)	B2^{v}—B3—Cr^{iv}	68.75 (5)
B3^{vi}—Cr—B1	76.67 (5)	B4—B3—Cr^{iv}	128.73 (4)
B3^{vii}—Cr—B1	156.85 (7)	Cr^{xii}—B3—Cr^{iv}	135.37 (10)
B1^{i}—Cr—B1	97.94 (6)	Cr^{xiii}—B3—Cr^{iv}	63.07 (3)
B3^{iii}—Cr—B2^{i}	76.55 (4)	B3^{x}—B3—Cr^{v}	67.54 (6)
B3^{ii}—Cr—B2^{i}	156.04 (5)	B2^{v}—B3—Cr^{v}	68.75 (5)
B3^{vi}—Cr—B2^{i}	115.66 (5)	B4—B3—Cr^{v}	128.73 (4)
B3^{vii}—Cr—B2^{i}	44.67 (8)	Cr^{xii}—B3—Cr^{v}	63.07 (3)
B1^{i}—Cr—B2^{i}	46.21 (5)	Cr^{xiii}—B3—Cr^{v}	135.37 (10)
B1—Cr—B2^{i}	116.12 (6)	Cr^{iv}—B3—Cr^{v}	99.33 (5)
B3^{iii}—Cr—B2	156.04 (5)	B3^{x}—B3—Y	138.55 (3)
B3^{ii}—Cr—B2	76.55 (4)	B2^{v}—B3—Y	74.33 (10)
B3^{vi}—Cr—B2	44.67 (8)	B4—B3—Y	75.16 (6)
B3^{vii}—Cr—B2	115.66 (5)	Cr^{xii}—B3—Y	142.90 (6)
B1^{i}—Cr—B2	116.12 (6)	Cr^{xiii}—B3—Y	77.682 (19)
B1—Cr—B2	46.22 (5)	Cr^{iv}—B3—Y	76.87 (3)
B2^{i}—Cr—B2	97.26 (9)	Cr^{v}—B3—Y	141.41 (10)
B3^{iii}—Cr—B4^{iii}	44.55 (5)	B3^{x}—B3—Y^{xi}	138.55 (3)
B3^{ii}—Cr—B4^{iii}	115.17 (6)	B2^{v}—B3—Y^{xi}	74.33 (10)
B3^{vi}—Cr—B4^{iii}	155.54 (7)	B4—B3—Y^{xi}	75.15 (6)
B3^{vii}—Cr—B4^{iii}	76.98 (5)	Cr^{xii}—B3—Y^{xi}	77.682 (19)
B1^{i}—Cr—B4^{iii}	46.59 (5)	Cr^{xiii}—B3—Y^{xi}	142.89 (6)
B1—Cr—B4^{iii}	115.88 (4)	Cr^{iv}—B3—Y^{xi}	141.41 (10)

B2^{i}—Cr—B4^{iii}	78.97 (5)	Cr^{v}—B3—Y^{xi}	76.87 (3)
B2—Cr—B4^{iii}	157.93 (6)	Y—B3—Y^{xi}	82.86 (6)
B3^{iii}—Cr—B4^{ii}	115.17 (6)	B3—B4—B1^{xiii}	104.59 (12)
B3^{ii}—Cr—B4^{ii}	44.55 (5)	B3—B4—B1	123.87 (12)
B3^{vi}—Cr—B4^{ii}	76.98 (5)	B1^{xiii}—B4—B1	131.54 (10)
B3^{vii}—Cr—B4^{ii}	155.54 (7)	B3—B4—Cr^{xiii}	65.97 (6)
B1^{i}—Cr—B4^{ii}	115.88 (4)	B1^{xiii}—B4—Cr^{xiii}	65.87 (5)
B1—Cr—B4^{ii}	46.59 (5)	B1—B4—Cr^{xiii}	131.74 (3)
B2^{i}—Cr—B4^{ii}	157.93 (6)	B3—B4—Cr^{xii}	65.97 (6)
B2—Cr—B4^{ii}	78.97 (5)	B1^{xiii}—B4—Cr^{xii}	65.87 (5)
B4^{iii}—Cr—B4^{ii}	96.30 (6)	B1—B4—Cr^{xii}	131.74 (3)
B3^{iii}—Cr—Cr^{viii}	58.56 (3)	Cr^{xiii}—B4—Cr^{xii}	96.30 (6)
B3^{ii}—Cr—Cr^{viii}	58.56 (3)	B3—B4—Y^{xii}	138.56 (3)
B3^{vi}—Cr—Cr^{viii}	58.37 (4)	B1^{xiii}—B4—Y^{xii}	72.47 (6)
B3^{vii}—Cr—Cr^{viii}	58.37 (4)	B1—B4—Y^{xii}	71.26 (5)
B1^{i}—Cr—Cr^{viii}	131.03 (3)	Cr^{xiii}—B4—Y^{xii}	136.83 (7)
B1—Cr—Cr^{viii}	131.03 (3)	Cr^{xii}—B4—Y^{xii}	76.03 (2)
B2^{i}—Cr—Cr^{viii}	101.08 (4)	B3—B4—Y^{xiii}	138.56 (3)
B2—Cr—Cr^{viii}	101.08 (4)	B1^{xiii}—B4—Y^{xiii}	72.47 (6)
B4^{iii}—Cr—Cr^{viii}	100.98 (4)	B1—B4—Y^{xiii}	71.26 (5)
B4^{ii}—Cr—Cr^{viii}	100.98 (4)	Cr^{xiii}—B4—Y^{xiii}	76.03 (2)
B3^{iii}—Cr—Y^{vii}	98.87 (4)	Cr^{xii}—B4—Y^{xiii}	136.83 (7)
B3^{ii}—Cr—Y^{vii}	98.87 (4)	Y^{xii}—B4—Y^{xiii}	81.33 (4)
B3^{vi}—Cr—Y^{vii}	56.65 (4)	B3—B4—Y^{xi}	67.06 (7)
B3^{vii}—Cr—Y^{vii}	56.65 (4)	B1^{xiii}—B4—Y^{xi}	138.40 (4)
B1^{i}—Cr—Y^{vii}	104.42 (4)	B1—B4—Y^{xi}	70.11 (5)
B1—Cr—Y^{vii}	104.42 (4)	Cr^{xiii}—B4—Y^{xi}	131.73 (6)
B2^{i}—Cr—Y^{vii}	59.17 (4)	Cr^{xii}—B4—Y^{xi}	74.13 (2)
B2—Cr—Y^{vii}	59.17 (4)	Y^{xii}—B4—Y^{xi}	87.67 (2)
B4^{iii}—Cr—Y^{vii}	131.60 (3)	Y^{xiii}—B4—Y^{xi}	141.34 (6)
B4^{ii}—Cr—Y^{vii}	131.60 (3)	B3—B4—Y	67.06 (7)
Cr^{viii}—Cr—Y^{vii}	67.744 (10)	B1^{xiii}—B4—Y	138.40 (4)
B2—B1—B4^{ii}	108.31 (12)	B1—B4—Y	70.11 (5)
B2—B1—B4	125.79 (12)	Cr^{xiii}—B4—Y	74.13 (2)
B4^{ii}—B1—B4	125.90 (10)	Cr^{xii}—B4—Y	131.73 (6)
B2—B1—Cr	67.24 (6)	Y^{xii}—B4—Y	141.34 (6)
B4^{ii}—B1—Cr	67.55 (5)	Y^{xiii}—B4—Y	87.67 (2)
B4—B1—Cr	131.03 (3)	Y^{xi}—B4—Y	78.16 (4)

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