inorganic compounds

Barium chromium oxide, Ba$_3$Cr$_2$O$_8$, as grown by the traveling solvent floating-zone technique

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Large single crystals of the incongruently melting compound tribarium dichromium octaoxide, Ba$_3$Cr$_2$O$_8$, were grown by the traveling solvent floating-zone technique for the first time and characterized by X-ray diffraction at room temperature. The structure is composed of CrO$_4^{3-}$ tetrahedra and Ba^{2+} ions. The chromium ions are found in the rare +5 valence state and form double-layered triangular lattices, which are stacked along the c axis with threefold periodicity. All atoms lie on special positions. One Ba, one O and the Cr atoms have site symmetry $3m$, the other Ba atom has site symmetry $\bar{3}m$, and the other O atom has site symmetry m. Magnetic measurements suggest that this material is a spin dimer system with a spin-singlet ground state.

Related literature

For details of the first single-crystal growth of Ba$_3$Cr$_2$O$_8$ (X-ray size crystals), see: Mattausch & Muller-Buschbaum (1972). For a more recent synthesis of Ba$_3$Cr$_2$O$_8$ and some measurements of magnetic properties, see: Nakajima *et al.* (2006). For additional details describing the growth of large single crystals by the traveling solvent floating-zone method and subsequent magnetic characterization measurements, see: Aczel *et al.* (2007).

Experimental

Crystal data

Ba$_3$Cr$_2$O$_8$	Z = 3
M_r = 644.02	Mo $K\alpha$ radiation
Trigonal, $R\bar{3}m$	μ = 16.87 mm^{-1}
a = 5.7450 (2) Å	T = 296 (2) K
c = 21.3883 (10) Å	0.30 × 0.05 × 0.02 mm
V = 611.35 (4) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	9434 measured reflections
Absorption correction: numerical (face correction; *APEX2*; Bruker, 2006)	928 independent reflections
	779 reflections with $I > 2\sigma(I)$
T_{min} = 0.38, T_{max} = 0.77	R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021	19 parameters
$wR(F^2)$ = 0.051	$\Delta\rho_{max}$ = 1.98 e Å^{-3}
S = 1.07	$\Delta\rho_{min}$ = −2.01 e Å^{-3}
928 reflections	

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *GRETEP* (Laugier & Bochu, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2063).

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supplementary materials

Barium chromium oxide, Ba$_3$Cr$_2$O$_8$, as grown by the traveling solvent floating-zone technique

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Comment

The system Ba$_3$Cr$_2$O$_8$ was recently synthesized in polycrystalline form to study its magnetic properties (Nakajima *et al.*, 2006). Susceptibility and high-field magnetization measurements have provided evidence that this material is a new spin dimer system. The interesting magnetic properties observed motivated our growth of large single crystals up to 6 mm *x* 4 mm *x* 1 mm in size. Fig.1 shows the structure of Ba$_3$Cr$_2$O$_8$, which consists of a series of CrO4^{3-} tetrahedra and Ba^{2+} ions.

Smaller single crystals of Ba$_3$Cr$_2$O$_8$ (suitable for *x*-ray work) were previously grown using a flux method (Mattausch and Muller-Buschbaum, 1972), but the magnetic properties of these crystals were never investigated. The authors did solve the crystallographic structure, but the reported *R* values were quite high (> 0.08) and both the isotropic and anisotropic displacement parameters were not presented. It follows that the purpose of this work is to present a more accurate and complete solution of the crystallographic structure of this system. This work also proves that single crystals of materials containing the difficult-to-stabilize Cr^{5+} ion can be grown by the traveling solvent floating zone technique.

Experimental

Large single crystals of the title compound were grown by the traveling solvent floating zone method in an Ar enviroment, using BaCO$_3$ and Cr$_2$O$_3$ as starting materials. The growth rate was fast (both 27 mm/h and 18 mm/h were applied), which was necessary to maintain zone stability. The feed and seed rods were rotating in opposite directions at 20 rpm throughout the growth, and a 3 cm boule of the desired Ba$_3$Cr$_2$O$_8$ phase was obtained on the seed rod. Due to the very fast growth, the as-obtained boule consisted of many well oriented crystalline grains.
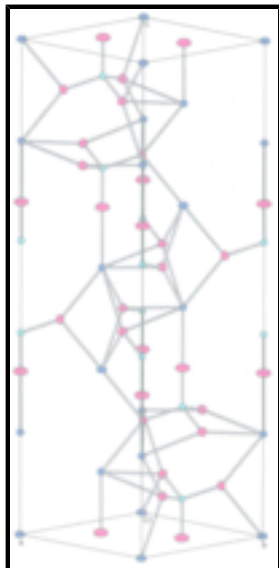
supplementary materials

Figures

Fig. 1. 50% displacement ellipsoid plot of the unit cell. Ba ions are shown in dark blue, Cr ions are shown in blue, and O ions are shown in red.

tribarium dichromium octaoxide

Crystal data

$Ba_3Cr_2O_8$	$Z = 3$
$M_r = 644.02$	$F_{000} = 840$
Trigonal, $R\bar{3}m$	$D_x = 5.248$ Mg m^{-3}
Hall symbol: -R 3 2"	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.7450$ (2) Å	Cell parameters from 2788 reflections
$b = 5.7450$ (2) Å	$\theta = 2.9–42.1°$
$c = 21.3883$ (10) Å	$\mu = 16.87$ mm^{-1}
$\alpha = 90°$	$T = 296$ (2) K
$\beta = 90°$	Rod, blue
$\gamma = 120°$	$0.30 \times 0.05 \times 0.02$ mm
$V = 611.35$ (4) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	928 independent reflections
Radiation source: fine-focus sealed tube	779 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 296(2)$ K	$\theta_{max} = 52.2°$
φ and ω scans	$\theta_{min} = 2.9°$
Absorption correction: numerical (face correction; APEX2; Bruker, 2006)	$h = -8 \rightarrow 12$
$T_{min} = 0.38$, $T_{max} = 0.77$	$k = -12 \rightarrow 10$

9434 measured reflections

$l = -47 \rightarrow 46$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o{}^2) + (0.0269P)^2]$ where $P = (F_o{}^2 + 2F_c{}^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.021$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.051$	$\Delta\rho_{max} = 1.98$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -2.01$ e Å^{-3}
928 reflections	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
19 parameters	Extinction coefficient: 0.0065 (3)
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	y	z	$U_{iso}*/U_{eq}$
Ba1	0.0000	0.0000	0.0000	0.01420 (5)
Ba2	0.0000	0.0000	0.205924 (6)	0.00918 (5)
Cr1	0.0000	0.0000	0.407042 (18)	0.00721 (6)
O1	0.82832 (9)	0.17168 (9)	0.89871 (5)	0.01272 (17)
O2	0.0000	0.0000	0.32872 (9)	0.0273 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.01762 (7)	0.01762 (7)	0.00736 (7)	0.00881 (3)	0.000	0.000
Ba2	0.00956 (5)	0.00956 (5)	0.00841 (6)	0.00478 (3)	0.000	0.000
Cr1	0.00723 (8)	0.00723 (8)	0.00718 (11)	0.00361 (4)	0.000	0.000
O1	0.0143 (3)	0.0143 (3)	0.0137 (4)	0.0102 (3)	0.00047 (14)	−0.00047 (14)
O2	0.0366 (8)	0.0366 (8)	0.0085 (7)	0.0183 (4)	0.000	0.000

Geometric parameters (Å, °)

Ba1—O1^{i}	2.7589 (10)	Ba2—Cr1^{xix}	3.51010 (18)
Ba1—O1^{ii}	2.7589 (10)	Ba2—Cr1^{xx}	3.51011 (18)
Ba1—O1^{iii}	2.7589 (10)	Cr1—O2	1.675 (2)
Ba1—O1^{iv}	2.7589 (10)	Cr1—O1^{xxi}	1.7133 (9)
Ba1—O1^{v}	2.7589 (10)	Cr1—O1^{xxii}	1.7133 (9)
Ba1—O1^{vi}	2.7589 (10)	Cr1—O1^{xxiii}	1.7134 (9)
Ba1—O2^{vii}	3.31834 (13)	Cr1—Ba2^{xx}	3.51007 (19)
Ba1—O2^{viii}	3.31834 (13)	Cr1—Ba2^{xxiv}	3.51007 (18)
Ba1—O2^{ix}	3.31834 (13)	Cr1—Ba2^{xix}	3.51010 (18)
Ba1—O2^{x}	3.31834 (13)	Cr1—Ba1^{xxv}	3.6724 (2)
Ba1—O2^{xi}	3.31838 (13)	Cr1—Ba1^{xxvi}	3.6724 (2)
Ba1—O2^{xii}	3.31838 (13)	Cr1—Ba1^{xxvii}	3.6725 (2)
Ba2—O2	2.626 (2)	Cr1—Cr1^{xxiv}	4.5764 (6)
Ba2—O1^{i}	2.8155 (10)	Cr1—Cr1^{xx}	4.5764 (6)
Ba2—O1^{v}	2.8155 (10)	O2—Ba1^{xxvi}	3.31834 (13)
Ba2—O1^{iii}	2.8155 (10)	O2—Ba1^{xxv}	3.31834 (13)
Ba2—O1^{xiii}	2.9268 (2)	O2—Ba1^{xxvii}	3.31837 (13)
Ba2—O1^{xiv}	2.9268 (2)	O1—Cr1^{xxiii}	1.7133 (9)
Ba2—O1^{xv}	2.9268 (2)	O1—Ba1^{xxviii}	2.7589 (10)
Ba2—O1^{xvi}	2.9268 (2)	O1—Ba2^{i}	2.8155 (10)
Ba2—O1^{xvii}	2.9268 (2)	O1—Ba2^{xxix}	2.9268 (2)
Ba2—O1^{xviii}	2.9268 (2)	O1—Ba2^{xxx}	2.9268 (2)
O1^{i}—Ba1—O1^{ii}	180.00 (3)	O1^{xvi}—Ba2—O1^{xviii}	56.85 (4)
O1^{i}—Ba1—O1^{iii}	64.86 (3)	O1^{xvii}—Ba2—O1^{xviii}	116.445 (13)
O1^{ii}—Ba1—O1^{iii}	115.14 (3)	O2—Ba2—Cr1^{xix}	70.902 (7)
O1^{i}—Ba1—O1^{iv}	115.14 (3)	O1^{i}—Ba2—Cr1^{xix}	71.74 (2)
O1^{ii}—Ba1—O1^{iv}	64.86 (3)	O1^{v}—Ba2—Cr1^{xix}	123.145 (7)
O1^{iii}—Ba1—O1^{iv}	180.00 (3)	O1^{iii}—Ba2—Cr1^{xix}	123.145 (7)
O1^{i}—Ba1—O1^{v}	64.86 (3)	O1^{xiii}—Ba2—Cr1^{xix}	87.343 (18)
O1^{ii}—Ba1—O1^{v}	115.14 (3)	O1^{xiv}—Ba2—Cr1^{xix}	87.343 (18)
O1^{iii}—Ba1—O1^{v}	64.86 (3)	O1^{xv}—Ba2—Cr1^{xix}	137.11 (2)
O1^{iv}—Ba1—O1^{v}	115.14 (3)	O1^{xvi}—Ba2—Cr1^{xix}	29.108 (18)
O1^{i}—Ba1—O1^{vi}	115.14 (3)	O1^{xvii}—Ba2—Cr1^{xix}	137.11 (2)
O1^{ii}—Ba1—O1^{vi}	64.86 (3)	O1^{xviii}—Ba2—Cr1^{xix}	29.109 (18)
O1^{iii}—Ba1—O1^{vi}	115.14 (3)	O2—Ba2—Cr1^{xx}	70.900 (7)
O1^{iv}—Ba1—O1^{vi}	64.86 (3)	O1^{i}—Ba2—Cr1^{xx}	123.146 (7)
O1^{v}—Ba1—O1^{vi}	180.00 (3)	O1^{v}—Ba2—Cr1^{xx}	123.146 (7)
O1^{i}—Ba1—O2^{vii}	70.56 (3)	O1^{iii}—Ba2—Cr1^{xx}	71.74 (2)

O1^{ii}—Ba1—O2^{vii}	109.44 (3)	O1^{xiii}—Ba2—Cr1^{xx}	29.109 (18)
O1^{iii}—Ba1—O2^{vii}	70.56 (3)	O1^{xiv}—Ba2—Cr1^{xx}	137.11 (2)
O1^{iv}—Ba1—O2^{vii}	109.44 (3)	O1^{xv}—Ba2—Cr1^{xx}	29.109 (18)
O1^{v}—Ba1—O2^{vii}	126.55 (4)	O1^{xvi}—Ba2—Cr1^{xx}	87.343 (18)
O1^{vi}—Ba1—O2^{vii}	53.45 (4)	O1^{xvii}—Ba2—Cr1^{xx}	87.343 (18)
O1^{i}—Ba1—O2^{viii}	70.56 (3)	O1^{xviii}—Ba2—Cr1^{xx}	137.11 (2)
O1^{ii}—Ba1—O2^{viii}	109.44 (3)	Cr1^{xix}—Ba2—Cr1^{xx}	109.841 (7)
O1^{iii}—Ba1—O2^{viii}	126.55 (4)	O2—Cr1—O1^{xxi}	110.14 (4)
O1^{iv}—Ba1—O2^{viii}	53.45 (4)	O2—Cr1—O1^{xxii}	110.14 (4)
O1^{v}—Ba1—O2^{viii}	70.56 (3)	O1^{xxi}—Cr1—O1^{xxii}	108.80 (4)
O1^{vi}—Ba1—O2^{viii}	109.44 (3)	O2—Cr1—O1^{xxiii}	110.14 (4)
O2^{vii}—Ba1—O2^{viii}	119.913 (4)	O1^{xxi}—Cr1—O1^{xxiii}	108.79 (4)
O1^{i}—Ba1—O2^{ix}	109.44 (3)	O1^{xxii}—Cr1—O1^{xxiii}	108.79 (4)
O1^{ii}—Ba1—O2^{ix}	70.56 (3)	O2—Cr1—Ba2^{xx}	109.099 (7)
O1^{iii}—Ba1—O2^{ix}	53.45 (4)	O1^{xxi}—Cr1—Ba2^{xx}	56.202 (7)
O1^{iv}—Ba1—O2^{ix}	126.55 (4)	O1^{xxii}—Cr1—Ba2^{xx}	140.76 (4)
O1^{v}—Ba1—O2^{ix}	109.44 (3)	O1^{xxiii}—Cr1—Ba2^{xx}	56.204 (7)
O1^{vi}—Ba1—O2^{ix}	70.56 (3)	O2—Cr1—Ba2^{xxiv}	109.099 (7)
O2^{vii}—Ba1—O2^{ix}	60.087 (4)	O1^{xxi}—Cr1—Ba2^{xxiv}	140.76 (4)
O2^{viii}—Ba1—O2^{ix}	180.00 (7)	O1^{xxii}—Cr1—Ba2^{xxiv}	56.202 (7)
O1^{i}—Ba1—O2^{x}	109.44 (3)	O1^{xxiii}—Cr1—Ba2^{xxiv}	56.204 (7)
O1^{ii}—Ba1—O2^{x}	70.56 (3)	Ba2^{xx}—Cr1—Ba2^{xxiv}	109.842 (7)
O1^{iii}—Ba1—O2^{x}	109.44 (3)	O2—Cr1—Ba2^{xix}	109.098 (7)
O1^{iv}—Ba1—O2^{x}	70.56 (3)	O1^{xxi}—Cr1—Ba2^{xix}	56.205 (7)
O1^{v}—Ba1—O2^{x}	53.45 (4)	O1^{xxii}—Cr1—Ba2^{xix}	56.205 (7)
O1^{vi}—Ba1—O2^{x}	126.55 (4)	O1^{xxiii}—Cr1—Ba2^{xix}	140.76 (4)
O2^{vii}—Ba1—O2^{x}	180.00 (7)	Ba2^{xx}—Cr1—Ba2^{xix}	109.841 (7)
O2^{viii}—Ba1—O2^{x}	60.087 (4)	Ba2^{xxiv}—Cr1—Ba2^{xix}	109.841 (7)
O2^{ix}—Ba1—O2^{x}	119.913 (4)	O2—Cr1—Ba1^{xxv}	64.579 (6)
O1^{i}—Ba1—O2^{xi}	126.55 (4)	O1^{xxi}—Cr1—Ba1^{xxv}	124.876 (11)
O1^{ii}—Ba1—O2^{xi}	53.45 (4)	O1^{xxii}—Cr1—Ba1^{xxv}	45.56 (4)
O1^{iii}—Ba1—O2^{xi}	70.56 (3)	O1^{xxiii}—Cr1—Ba1^{xxv}	124.874 (11)
O1^{iv}—Ba1—O2^{xi}	109.44 (3)	Ba2^{xx}—Cr1—Ba1^{xxv}	173.677 (12)
O1^{v}—Ba1—O2^{xi}	70.56 (3)	Ba2^{xxiv}—Cr1—Ba1^{xxv}	73.364 (2)
O1^{vi}—Ba1—O2^{xi}	109.44 (3)	Ba2^{xix}—Cr1—Ba1^{xxv}	73.365 (2)
O2^{vii}—Ba1—O2^{xi}	119.912 (4)	O2—Cr1—Ba1^{xxvi}	64.579 (6)
O2^{viii}—Ba1—O2^{xi}	119.912 (4)	O1^{xxi}—Cr1—Ba1^{xxvi}	45.56 (4)
O2^{ix}—Ba1—O2^{xi}	60.088 (4)	O1^{xxii}—Cr1—Ba1^{xxvi}	124.876 (11)
O2^{x}—Ba1—O2^{xi}	60.088 (4)	O1^{xxiii}—Cr1—Ba1^{xxvi}	124.874 (11)
O1^{i}—Ba1—O2^{xii}	53.45 (4)	Ba2^{xx}—Cr1—Ba1^{xxvi}	73.364 (2)
O1^{ii}—Ba1—O2^{xii}	126.55 (4)	Ba2^{xxiv}—Cr1—Ba1^{xxvi}	173.677 (12)

O1^{iii}—Ba1—O2^{xii}	109.44 (3)	Ba2^{xix}—Cr1—Ba1^{xxvi}	73.365 (2)
O1^{iv}—Ba1—O2^{xii}	70.56 (3)	Ba1^{xxv}—Cr1—Ba1^{xxvi}	102.921 (7)
O1^{v}—Ba1—O2^{xii}	109.44 (3)	O2—Cr1—Ba1^{xxvii}	64.579 (6)
O1^{vi}—Ba1—O2^{xii}	70.56 (3)	O1^{xxi}—Cr1—Ba1^{xxvii}	124.873 (11)
O2^{vii}—Ba1—O2^{xii}	60.088 (4)	O1^{xxii}—Cr1—Ba1^{xxvii}	124.873 (11)
O2^{viii}—Ba1—O2^{xii}	60.088 (4)	O1^{xxiii}—Cr1—Ba1^{xxvii}	45.56 (4)
O2^{ix}—Ba1—O2^{xii}	119.912 (4)	Ba2^{xx}—Cr1—Ba1^{xxvii}	73.365 (2)
O2^{x}—Ba1—O2^{xii}	119.912 (4)	Ba2^{xxiv}—Cr1—Ba1^{xxvii}	73.365 (2)
O2^{xi}—Ba1—O2^{xii}	180.00 (7)	Ba2^{xix}—Cr1—Ba1^{xxvii}	173.678 (12)
O2—Ba2—O1^{i}	142.65 (2)	Ba1^{xxv}—Cr1—Ba1^{xxvii}	102.920 (7)
O2—Ba2—O1^{v}	142.64 (2)	Ba1^{xxvi}—Cr1—Ba1^{xxvii}	102.920 (7)
O1^{i}—Ba2—O1^{v}	63.40 (3)	O2—Cr1—Cr1^{xxiv}	46.451 (7)
O2—Ba2—O1^{iii}	142.64 (2)	O1^{xxi}—Cr1—Cr1^{xxiv}	156.59 (4)
O1^{i}—Ba2—O1^{iii}	63.40 (3)	O1^{xxii}—Cr1—Cr1^{xxiv}	84.09 (3)
O1^{v}—Ba2—O1^{iii}	63.40 (3)	O1^{xxiii}—Cr1—Cr1^{xxiv}	84.09 (3)
O2—Ba2—O1^{xiii}	78.99 (2)	Ba2^{xx}—Cr1—Cr1^{xxiv}	124.602 (5)
O1^{i}—Ba2—O1^{xiii}	99.33 (2)	Ba2^{xxiv}—Cr1—Cr1^{xxiv}	62.648 (3)
O1^{v}—Ba2—O1^{xiii}	131.476 (10)	Ba2^{xix}—Cr1—Cr1^{xxiv}	124.602 (5)
O1^{iii}—Ba2—O1^{xiii}	68.34 (4)	Ba1^{xxv}—Cr1—Cr1^{xxiv}	51.460 (3)
O2—Ba2—O1^{xiv}	78.99 (2)	Ba1^{xxvi}—Cr1—Cr1^{xxiv}	111.030 (13)
O1^{i}—Ba2—O1^{xiv}	99.33 (2)	Ba1^{xxvii}—Cr1—Cr1^{xxiv}	51.460 (3)
O1^{v}—Ba2—O1^{xiv}	68.34 (4)	O2—Cr1—Cr1^{xx}	46.451 (7)
O1^{iii}—Ba2—O1^{xiv}	131.476 (10)	O1^{xxi}—Cr1—Cr1^{xx}	84.09 (3)
O1^{xiii}—Ba2—O1^{xiv}	157.90 (4)	O1^{xxii}—Cr1—Cr1^{xx}	156.59 (4)
O2—Ba2—O1^{xv}	78.99 (2)	O1^{xxiii}—Cr1—Cr1^{xx}	84.09 (3)
O1^{i}—Ba2—O1^{xv}	131.476 (10)	Ba2^{xx}—Cr1—Cr1^{xx}	62.648 (3)
O1^{v}—Ba2—O1^{xv}	99.33 (2)	Ba2^{xxiv}—Cr1—Cr1^{xx}	124.602 (5)
O1^{iii}—Ba2—O1^{xv}	68.34 (4)	Ba2^{xix}—Cr1—Cr1^{xx}	124.602 (5)
O1^{xiii}—Ba2—O1^{xv}	56.85 (4)	Ba1^{xxv}—Cr1—Cr1^{xx}	111.030 (13)
O1^{xiv}—Ba2—O1^{xv}	116.445 (13)	Ba1^{xxvi}—Cr1—Cr1^{xx}	51.460 (3)
O2—Ba2—O1^{xvi}	78.99 (2)	Ba1^{xxvii}—Cr1—Cr1^{xx}	51.460 (4)
O1^{i}—Ba2—O1^{xvi}	68.34 (4)	Cr1^{xxiv}—Cr1—Cr1^{xx}	77.758 (11)
O1^{v}—Ba2—O1^{xvi}	131.476 (10)	Cr1—O2—Ba2	180.0
O1^{iii}—Ba2—O1^{xvi}	99.33 (2)	Cr1—O2—Ba1^{xxvi}	88.29 (4)
O1^{xiii}—Ba2—O1^{xvi}	60.73 (4)	Ba2—O2—Ba1^{xxvi}	91.71 (4)
O1^{xiv}—Ba2—O1^{xvi}	116.445 (13)	Cr1—O2—Ba1^{xxv}	88.29 (4)
O1^{xv}—Ba2—O1^{xvi}	116.445 (13)	Ba2—O2—Ba1^{xxv}	91.71 (4)
O2—Ba2—O1^{xvii}	78.99 (2)	Ba1^{xxvi}—O2—Ba1^{xxv}	119.913 (4)
O1^{i}—Ba2—O1^{xvii}	131.475 (10)	Cr1—O2—Ba1^{xxvii}	88.29 (4)
O1^{v}—Ba2—O1^{xvii}	68.34 (4)	Ba2—O2—Ba1^{xxvii}	91.71 (4)
O1^{iii}—Ba2—O1^{xvii}	99.33 (2)	Ba1^{xxvi}—O2—Ba1^{xxvii}	119.912 (4)

O1^{xiii}—Ba2—O1^{xvii}	116.445 (13)	Ba1^{xxv}—O2—Ba1^{xxvii}	119.912 (4)
O1^{xiv}—Ba2—O1^{xvii}	56.85 (4)	Cr1^{xxiii}—O1—Ba1^{xxviii}	108.12 (5)
O1^{xv}—Ba2—O1^{xvii}	60.73 (4)	Cr1^{xxiii}—O1—Ba2^{i}	147.49 (5)
O1^{xvi}—Ba2—O1^{xvii}	157.90 (4)	Ba1^{xxviii}—O1—Ba2^{i}	104.39 (3)
O2—Ba2—O1^{xviii}	78.99 (2)	Cr1^{xxiii}—O1—Ba2^{xxix}	94.688 (19)
O1^{i}—Ba2—O1^{xviii}	68.34 (4)	Ba1^{xxviii}—O1—Ba2^{xxix}	98.010 (19)
O1^{v}—Ba2—O1^{xviii}	99.33 (2)	Ba2^{i}—O1—Ba2^{xxix}	80.67 (2)
O1^{iii}—Ba2—O1^{xviii}	131.476 (10)	Cr1^{xxiii}—O1—Ba2^{xxx}	94.688 (19)
O1^{xiii}—Ba2—O1^{xviii}	116.445 (13)	Ba1^{xxviii}—O1—Ba2^{xxx}	98.009 (19)
O1^{xiv}—Ba2—O1^{xviii}	60.73 (4)	Ba2^{i}—O1—Ba2^{xxx}	80.67 (2)
O1^{xv}—Ba2—O1^{xviii}	157.90 (4)	Ba2^{xxix}—O1—Ba2^{xxx}	157.90 (4)

Symmetry codes: (i) −x+1, −y, −z+1; (ii) x−1, y, z−1; (iii) y, −x+y+1, −z+1; (iv) −y, x−y−1, z−1; (v) x−y−1, x−1, −z+1; (vi) −x+y+1, −x+1, z−1; (vii) −x+2/3, −y+1/3, −z+1/3; (viii) −x−1/3, −y−2/3, −z+1/3; (ix) x+1/3, y+2/3, z−1/3; (x) x−2/3, y−1/3, z−1/3; (xi) −x−1/3, −y+1/3, −z+1/3; (xii) x+1/3, y−1/3, z−1/3; (xiii) x−1/3, y+1/3, z−2/3; (xiv) x−4/3, y−2/3, z−2/3; (xv) −x+y+2/3, −x+4/3, z−2/3; (xvi) −y+2/3, x−y−2/3, z−2/3; (xvii) −y−1/3, x−y−2/3, z−2/3; (xviii) −x+y+2/3, −x+1/3, z−2/3; (xix) −x+1/3, −y−1/3, −z+2/3; (xx) −x+1/3, −y+2/3, −z+2/3; (xxi) x−y−1/3, x−2/3, −z+4/3; (xxii) y−1/3, −x+y+1/3, −z+4/3; (xxiii) −x+2/3, −y+1/3, −z+4/3; (xxiv) −x−2/3, −y−1/3, −z+2/3; (xxv) x−1/3, y−2/3, z+1/3; (xxvi) x+2/3, y+1/3, z+1/3; (xxvii) x−1/3, y+1/3, z+1/3; (xxviii) x+1, y, z+1; (xxix) x+1/3, y−1/3, z+2/3; (xxx) x+4/3, y+2/3, z+2/3.

Fig. 1