

Barium dierbium(III) tetrasulfide

Adel Mesbah, Wojciech Stojko and James. A Ibers*

Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3113, USA

Correspondence e-mail: ibers@chem.northwestern.edu

Received 31 January 2013; accepted 4 February 2013

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{Er-S}) = 0.001$ Å; R factor = 0.017; wR factor = 0.050; data-to-parameter ratio = 27.4.

Barium dierbium(III) tetrasulfide, BaEr_2S_4 , crystallizes with four formula units in the orthorhombic space group $Pnma$ in the CaFe_2O_4 structure type. The asymmetric unit contains two Er, one Ba, and four S atoms, each with $.m$. site symmetry. The structure consists of channels formed by corner- and edge-sharing ErS_6 octahedra in which Ba atoms reside. The resultant coordination of Ba is that of a bicapped trigonal prism.

Related literature

The unit-cell parameters of BaEr_2S_4 , which crystallizes in the CaFe_2O_4 structure type (Decker & Kasper, 1957), were previously determined from X-ray powder diffraction data (Patrie *et al.*, 1964). For related structures, see: Bugaris & Ibers (2009); Narducci *et al.* (2000); Carpenter & Hwu (1992); Flahaut *et al.* (1965); Schurz & Schleid (2011). For synthetic details, see: Bugaris & Ibers (2008); Haneveld & Jellinek (1969). For standardization of structural data, see: Gelato & Parthé (1987).

Experimental

Crystal data

BaEr_2S_4	$V = 696.76$ (3) Å ³
$M_r = 600.10$	$Z = 4$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
$a = 12.1455$ (3) Å	$\mu = 30.53$ mm ⁻¹
$b = 3.9884$ (1) Å	$T = 100$ K
$c = 14.3837$ (4) Å	$0.16 \times 0.03 \times 0.02$ mm

Data collection

Bruker APEXII CCD diffractometer	9866 measured reflections
Absorption correction: numerical face indexed (Sheldrick, 2008a)	1207 independent reflections
$T_{\min} = 0.084$, $T_{\max} = 0.528$	1196 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$	44 parameters
$wR(F^2) = 0.050$	$\Delta\rho_{\text{max}} = 2.46$ e Å ⁻³
$S = 1.87$	$\Delta\rho_{\text{min}} = -2.58$ e Å ⁻³
1207 reflections	

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008b); molecular graphics: *CrystalMaker* (Palmer, 2012); software used to prepare material for publication: *SHELXL97*.

The research was kindly supported at Northwestern University by the US Department of Energy, Basic Energy Sciences, Chemical Sciences, Biosciences, and Geosciences Division and Division of Materials Science and Engineering Grant ER-15522. Use was made of the IMSERC X-ray Facility at Northwestern University, supported by the International Institute of Nanotechnology (IIN).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2222).

References

- Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bugaris, D. E. & Ibers, J. A. (2008). *J. Solid State Chem.* **181**, 3189–3193.
- Bugaris, D. E. & Ibers, J. A. (2009). *Acta Cryst.* **C65**, i60–i62.
- Carpenter, J. D. & Hwu, S.-J. (1992). *Acta Cryst.* **C48**, 1164–1167.
- Decker, B. F. & Kasper, J. S. (1957). *Acta Cryst.* **10**, 332–337.
- Flahaut, J., Guittard, M., Patrie, M., Pardo, M. P., Golabi, S. M. & Domange, L. (1965). *Acta Cryst.* **19**, 14–19.
- Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
- Haneveld, A. J. K. & Jellinek, F. (1969). *J. Less Common Met.* **18**, 123–129.
- Narducci, A. A., Yang, Y., Digman, M. A., Sipes, A. B. & Ibers, J. A. (2000). *J. Alloys Compd.* **303–304**, 432–439.
- Palmer, D. (2012). *CrystalMaker Software*. CrystalMaker Software Ltd, Oxfordshire, England.
- Patrie, M., Golabi, S. M., Flahaut, J. & Domange, L. (1964). *C. R. Hebd. Seances Acad. Sci.* **259**, 4039–4042.
- Schurz, C. M. & Schleid, T. (2011). *Crystals*, **1**, 78–86.
- Sheldrick, G. M. (2008a). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008b). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2013). E69, i17 [doi:10.1107/S1600536813003541]

Barium dierbium(III) tetrasulfide

Adel Mesbah, Wojciech Stojko and James. A Ibers

Comment

Orange needles of BaEr₂S₄ were obtained in a solid-state reaction. The compound was synthesized previously (Patrie *et al.*, 1964), and its unit cell parameters were determined from X-powder diffraction data. In the BaLn₂S₄ family (Ln = rare earth element) no structures have been determined from single-crystal data but that of the closely related compound BaLu₂S₄ has (Schurz & Schleid, 2011). Here, from X-ray diffraction single-crystal data we find that BaEr₂S₄ crystallizes in the CaFe₂O₄ structure type (Decker & Kasper, 1957) with four formula units in space group *Pnma* of the orthorhombic system. In the asymmetric unit there are two Er, one Ba, and four S atoms, each with site symmetry *m*. A projection of the structure down [010] is shown in Figure 1. The structure consists of ErS₆ octahedra that form dimers by edge-sharing. Four such dimers form an infinite channel by corner-sharing in the (010) plane. Each channel is filled by one Ba atom. Each Er1 atom is octahedrally coordinated to one S2, three S3, and two S4 atoms; each Er2 atom is coordinated to three S1, two S2, and one S4 atom. The interatomic Er - S distances at 2.6706 (10) to 2.7376 (7) Å compare favorably to those of 2.672 (4) to 2.720 (4) Å in the structure of BaLu₂S₄ (Schurz & Schleid, 2011). As there are no S - S bonds in the structure, formal oxidation states may be assigned as Ba²⁺, Er³⁺, and S²⁻.

Experimental

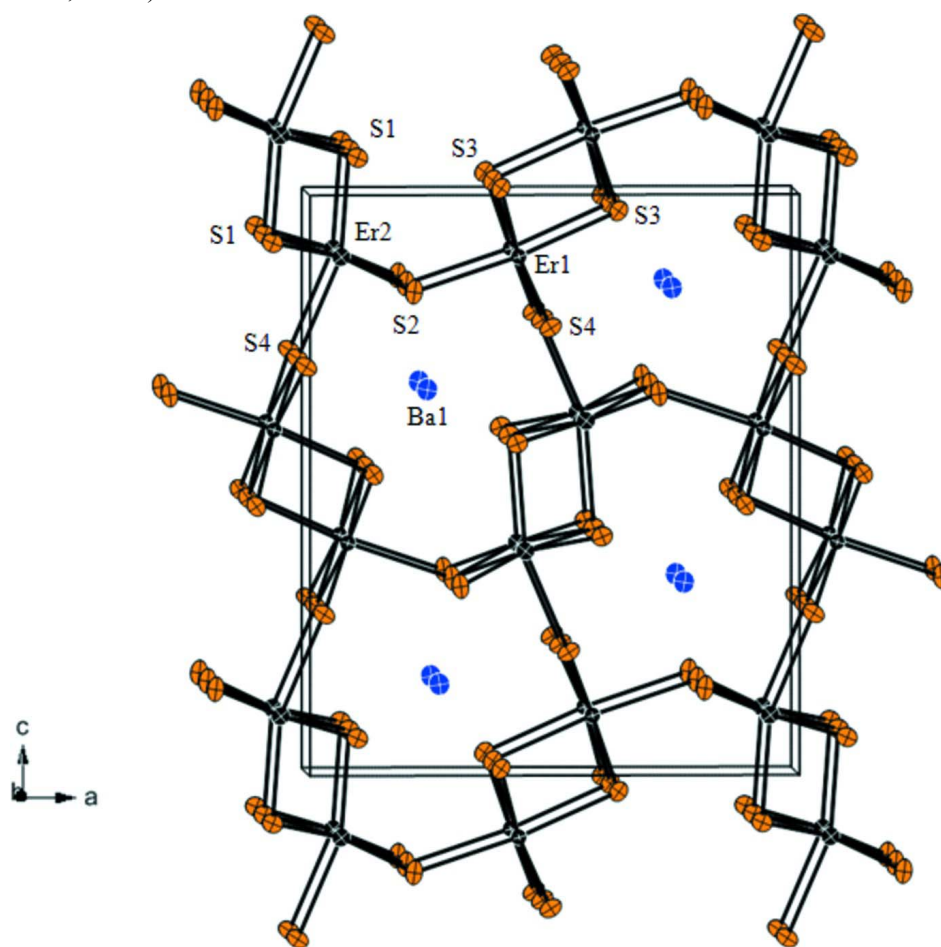
In an exploration of the quaternary solid-state Ba/Er/U/S system, orange needles of BaEr₂S₄ were obtained instead in a two-step reaction. Uranium powder was obtained by hydridization and decomposition of ²³⁸U turnings (Oak Ridge National Laboratory) (Bugaris & Ibers, 2008; Haneveld & Jellinek, 1969). The other reactants were used as obtained. In the first step, a mixture consisting of powdered ²³⁸U (20.9 mg, 0.088 mmol), Er (14.0 mg, 0.084 mmol), BaS (42.7 mg, 0.252 mmol), and S (8.0 mg, 0.25 mmol) was loaded into a carbon-coated fused-silica tube under an Ar atmosphere in a glove box. The tube was evacuated to 10⁻⁴ Torr, and flame sealed. It was placed in computer-controlled furnace, heated to 1273 K in 48 h, held there for 8 d, then cooled to 293 K at 3 K/h. In the second step, the resultant black powder was ground and mixed thoroughly with 50 mg of Sb₂S₃. This mixture was re-loaded into a carbon-coated fused-silica tube, evacuated, sealed, and then placed in a computer-controlled furnace. The tube was heated to 1273 K in 24 h, held there for 4 d, then cooled to 293 K at 2 K/h. Orange needles were obtained in about 50 wt% yield. Analysis of these orange crystals on an EDX-equipped Hitachi S-3400 SEM showed the presence of Ba, Er, and S in the approximate ratio 1:2:4 but no U. The other products were black crystals of Sb₂S₃ and US₂.

Refinement

The structure was standardized by means of the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak in the difference electron density map (2.46 e. Å⁻³) was 0.47 Å from atom Er1 and the deepest hole (-2.58 e. Å⁻³) was 0.20 Å from atom Ba1.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008b); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008b); molecular graphics: *CrystalMaker* (Palmer, 2012); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008b).


Figure 1

Structure of BaEr_2S_4 viewed approximately down $[010]$. Displacement ellipsoids are drawn at 95% probability level.

Barium dierbium(III) tetrasulfide
Crystal data

BaEr_2S_4

$M_r = 600.10$

Orthorhombic, *Pnma*

Hall symbol: $-P\ 2ac\ 2n$

$a = 12.1455\ (3)\ \text{\AA}$

$b = 3.9884\ (1)\ \text{\AA}$

$c = 14.3837\ (4)\ \text{\AA}$

$V = 696.76\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1024$

$D_x = 5.721\ \text{Mg m}^{-3}$

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

Cell parameters from 8150 reflections

$\theta = 2.3\text{--}30.5^\circ$

$\mu = 30.53\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Needle, orange

$0.16 \times 0.03 \times 0.02\ \text{mm}$

Data collection

Bruker APEXII CCD diffractometer	9866 measured reflections
Radiation source: fine-focus sealed tube	1207 independent reflections
Graphite monochromator	1196 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.030$
Absorption correction: numerical face indexed (Sheldrick, 2008a)	$\theta_{\text{max}} = 30.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.084$, $T_{\text{max}} = 0.528$	$h = -17 \rightarrow 17$
	$k = -5 \rightarrow 5$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$1/[s^2(F_o^2) + (0.0192F_o^2)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.017$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$wR(F^2) = 0.050$	$\Delta\rho_{\text{max}} = 2.46 \text{ e } \text{\AA}^{-3}$
$S = 1.87$	$\Delta\rho_{\text{min}} = -2.58 \text{ e } \text{\AA}^{-3}$
1207 reflections	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008a), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
44 parameters	Extinction coefficient: 0.00257 (16)
0 restraints	
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Er1	0.079448 (16)	0.2500	0.398817 (12)	0.00349 (8)
Er2	0.566211 (16)	0.2500	0.608465 (12)	0.00444 (8)
Ba1	0.24191 (2)	0.2500	0.662667 (18)	0.00705 (9)
S1	0.08229 (8)	0.2500	0.07671 (7)	0.00485 (18)
S2	0.29294 (9)	0.2500	0.33808 (7)	0.00537 (18)
S3	0.37564 (8)	0.2500	0.02341 (7)	0.00449 (18)
S4	0.47727 (8)	0.2500	0.78311 (7)	0.00490 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.00359 (11)	0.00300 (12)	0.00388 (11)	0.000	0.00010 (5)	0.000
Er2	0.00495 (12)	0.00349 (12)	0.00487 (11)	0.000	-0.00020 (5)	0.000
Ba1	0.00595 (14)	0.00835 (14)	0.00683 (13)	0.000	0.00015 (8)	0.000
S1	0.0057 (4)	0.0040 (4)	0.0049 (4)	0.000	-0.0004 (3)	0.000
S2	0.0037 (4)	0.0044 (4)	0.0080 (4)	0.000	-0.0006 (3)	0.000
S3	0.0046 (4)	0.0037 (4)	0.0052 (4)	0.000	0.0009 (3)	0.000
S4	0.0061 (4)	0.0039 (4)	0.0047 (4)	0.000	0.0015 (3)	0.000

Geometric parameters (\AA , $^\circ$)

Er1—S4 ⁱ	2.6872 (6)	Ba1—S4	3.3426 (11)
Er1—S4 ⁱⁱ	2.6872 (6)	Ba1—Er2 ^x	3.9231 (3)
Er1—S3 ⁱⁱⁱ	2.7164 (10)	Ba1—Ba1 ^{xi}	3.9884 (1)
Er1—S3 ^{iv}	2.7360 (7)	Ba1—Ba1 ^{xii}	3.9884
Er1—S3 ^v	2.7360 (7)	S1—Er2 ⁱⁱⁱ	2.6706 (10)
Er1—S2	2.7362 (11)	S1—Er2 ⁱ	2.7273 (7)

Er1—Ba1	4.2774 (3)	S1—Er2 ⁱⁱ	2.7273 (7)
Er2—S1 ^{vi}	2.6706 (10)	S1—Ba1 ⁱⁱ	3.1725 (8)
Er2—S1 ^v	2.7274 (7)	S1—Ba1 ⁱ	3.1725 (8)
Er2—S1 ^{iv}	2.7274 (7)	S2—Er2 ^{vii}	2.7376 (7)
Er2—S4	2.7345 (9)	S2—Er2 ^{viii}	2.7376 (7)
Er2—S2 ^{vii}	2.7376 (7)	S2—Ba1 ⁱ	3.2437 (9)
Er2—S2 ^{viii}	2.7376 (7)	S2—Ba1 ⁱⁱ	3.2437 (9)
Er2—Ba1 ^{ix}	3.9231 (3)	S3—Er1 ^{vi}	2.7163 (10)
Er2—Ba1	4.0153 (3)	S3—Er1 ⁱ	2.7360 (7)
Ba1—S3 ^v	3.1666 (8)	S3—Er1 ⁱⁱ	2.7360 (7)
Ba1—S3 ^{iv}	3.1666 (8)	S3—Ba1 ⁱⁱ	3.1666 (8)
Ba1—S1 ^{iv}	3.1725 (8)	S3—Ba1 ⁱ	3.1666 (8)
Ba1—S1 ^v	3.1725 (8)	S4—Er1 ^{iv}	2.6873 (6)
Ba1—S2 ^{iv}	3.2438 (9)	S4—Er1 ^v	2.6873 (6)
Ba1—S2 ^v	3.2438 (9)	S4—Ba1 ^{ix}	3.3074 (11)
Ba1—S4 ^x	3.3074 (11)		
S4 ⁱ —Er1—S4 ⁱⁱ	95.82 (3)	S3 ^{iv} —Ba1—Er2 ^x	106.592 (19)
S4 ⁱ —Er1—S3 ⁱⁱⁱ	91.23 (3)	S1 ^{iv} —Ba1—Er2 ^x	133.879 (16)
S4 ⁱⁱ —Er1—S3 ⁱⁱⁱ	91.23 (3)	S1 ^v —Ba1—Er2 ^x	133.879 (16)
S4 ⁱ —Er1—S3 ^{iv}	176.07 (3)	S2 ^{iv} —Ba1—Er2 ^x	43.642 (15)
S4 ⁱⁱ —Er1—S3 ^{iv}	85.17 (2)	S2 ^v —Ba1—Er2 ^x	43.642 (15)
S3 ⁱⁱⁱ —Er1—S3 ^{iv}	84.95 (3)	S4 ^x —Ba1—Er2 ^x	43.408 (16)
S4 ⁱ —Er1—S3 ^v	85.17 (2)	S4—Ba1—Er2 ^x	91.735 (18)
S4 ⁱⁱ —Er1—S3 ^v	176.07 (3)	S3 ^v —Ba1—Ba1 ^{xi}	129.032 (11)
S3 ⁱⁱⁱ —Er1—S3 ^v	84.95 (3)	S3 ^{iv} —Ba1—Ba1 ^{xi}	50.967 (11)
S3 ^{iv} —Er1—S3 ^v	93.58 (3)	S1 ^{iv} —Ba1—Ba1 ^{xi}	51.054 (12)
S4 ⁱ —Er1—S2	92.59 (3)	S1 ^v —Ba1—Ba1 ^{xi}	128.946 (12)
S4 ⁱⁱ —Er1—S2	92.59 (3)	S2 ^{iv} —Ba1—Ba1 ^{xi}	52.064 (12)
S3 ⁱⁱⁱ —Er1—S2	174.30 (3)	S2 ^v —Ba1—Ba1 ^{xi}	127.936 (12)
S3 ^{iv} —Er1—S2	91.16 (3)	S4 ^x —Ba1—Ba1 ^{xi}	90.0
S3 ^v —Er1—S2	91.16 (3)	S4—Ba1—Ba1 ^{xi}	90.0
S4 ⁱ —Er1—Ba1	131.894 (15)	Er2 ^x —Ba1—Ba1 ^{xi}	90.0
S4 ⁱⁱ —Er1—Ba1	131.894 (15)	S3 ^v —Ba1—Ba1 ^{xii}	50.967 (11)
S3 ⁱⁱⁱ —Er1—Ba1	93.15 (2)	S3 ^{iv} —Ba1—Ba1 ^{xii}	129.032 (11)
S3 ^{iv} —Er1—Ba1	47.693 (15)	S1 ^{iv} —Ba1—Ba1 ^{xii}	128.946 (12)
S3 ^v —Er1—Ba1	47.693 (15)	S1 ^v —Ba1—Ba1 ^{xii}	51.054 (12)
S2—Er1—Ba1	81.15 (2)	S2 ^{iv} —Ba1—Ba1 ^{xii}	127.936 (12)
S1 ^{vi} —Er2—S1 ^v	83.18 (3)	S2 ^v —Ba1—Ba1 ^{xii}	52.064 (12)
S1 ^{vi} —Er2—S1 ^{iv}	83.18 (3)	S4 ^x —Ba1—Ba1 ^{xii}	90.0
S1 ^v —Er2—S1 ^{iv}	93.97 (3)	S4—Ba1—Ba1 ^{xii}	90.0
S1 ^{vi} —Er2—S4	160.92 (3)	Er2 ^x —Ba1—Ba1 ^{xii}	90.0
S1 ^v —Er2—S4	83.84 (3)	Ba1 ^{xi} —Ba1—Ba1 ^{xii}	180.0
S1 ^{iv} —Er2—S4	83.84 (3)	S3 ^v —Ba1—Er2	108.630 (19)
S1 ^{vi} —Er2—S2 ^{vii}	103.56 (3)	S3 ^{iv} —Ba1—Er2	108.630 (19)
S1 ^v —Er2—S2 ^{vii}	173.17 (3)	S1 ^{iv} —Ba1—Er2	42.616 (14)
S1 ^{iv} —Er2—S2 ^{vii}	85.85 (2)	S1 ^v —Ba1—Er2	42.616 (14)
S4—Er2—S2 ^{vii}	89.36 (3)	S2 ^{iv} —Ba1—Er2	106.201 (19)
S1 ^{vi} —Er2—S2 ^{viii}	103.56 (3)	S2 ^v —Ba1—Er2	106.201 (19)

S1 ^v —Er2—S2 ^{viii}	85.85 (2)	S4 ^x —Ba1—Er2	177.557 (18)
S1 ^{iv} —Er2—S2 ^{viii}	173.17 (3)	S4—Ba1—Er2	42.413 (17)
S4—Er2—S2 ^{viii}	89.36 (3)	Er2 ^x —Ba1—Er2	134.149 (8)
S2 ^{vii} —Er2—S2 ^{viii}	93.51 (3)	Ba1 ^{xi} —Ba1—Er2	90.0
S1 ^{vi} —Er2—Ba1 ^{ix}	142.85 (2)	Ba1 ^{xii} —Ba1—Er2	90.0
S1 ^v —Er2—Ba1 ^{ix}	120.02 (2)	Er2 ⁱⁱⁱ —S1—Er2 ⁱ	96.82 (3)
S1 ^{iv} —Er2—Ba1 ^{ix}	120.02 (2)	Er2 ⁱⁱⁱ —S1—Er2 ⁱⁱ	96.82 (3)
S4—Er2—Ba1 ^{ix}	56.22 (2)	Er2 ⁱ —S1—Er2 ⁱⁱ	93.97 (3)
S2 ^{vii} —Er2—Ba1 ^{ix}	54.861 (19)	Er2 ⁱⁱⁱ —S1—Ba1 ⁱⁱ	115.97 (3)
S2 ^{viii} —Er2—Ba1 ^{ix}	54.861 (19)	Er2 ⁱ —S1—Ba1 ⁱⁱ	147.08 (4)
S1 ^{vi} —Er2—Ba1	105.39 (2)	Er2 ⁱⁱ —S1—Ba1 ⁱⁱ	85.422 (12)
S1 ^v —Er2—Ba1	51.961 (18)	Er2 ⁱⁱⁱ —S1—Ba1 ⁱ	115.97 (3)
S1 ^{iv} —Er2—Ba1	51.961 (18)	Er2 ⁱ —S1—Ba1 ⁱ	85.422 (12)
S4—Er2—Ba1	55.53 (2)	Er2 ⁱⁱ —S1—Ba1 ⁱ	147.08 (4)
S2 ^{vii} —Er2—Ba1	123.95 (2)	Ba1 ⁱⁱ —S1—Ba1 ⁱ	77.89 (2)
S2 ^{viii} —Er2—Ba1	123.95 (2)	Er1—S2—Er2 ^{vii}	120.17 (3)
Ba1 ^{ix} —Er2—Ba1	111.755 (5)	Er1—S2—Er2 ^{viii}	120.17 (3)
S3 ^v —Ba1—S3 ^{iv}	78.06 (2)	Er2 ^{vii} —S2—Er2 ^{viii}	93.51 (3)
S3 ^v —Ba1—S1 ^{iv}	116.92 (2)	Er1—S2—Ba1 ⁱ	97.16 (3)
S3 ^{iv} —Ba1—S1 ^{iv}	70.19 (2)	Er2 ^{vii} —S2—Ba1 ⁱ	138.40 (4)
S3 ^v —Ba1—S1 ^v	70.19 (2)	Er2 ^{viii} —S2—Ba1 ⁱ	81.498 (14)
S3 ^{iv} —Ba1—S1 ^v	116.92 (2)	Er1—S2—Ba1 ⁱⁱ	97.16 (3)
S1 ^{iv} —Ba1—S1 ^v	77.89 (2)	Er2 ^{vii} —S2—Ba1 ⁱⁱ	81.498 (14)
S3 ^v —Ba1—S2 ^{iv}	145.12 (3)	Er2 ^{viii} —S2—Ba1 ⁱⁱ	138.40 (4)
S3 ^{iv} —Ba1—S2 ^{iv}	92.639 (19)	Ba1 ⁱ —S2—Ba1 ⁱⁱ	75.87 (2)
S1 ^{iv} —Ba1—S2 ^{iv}	90.26 (2)	Er1 ^{vi} —S3—Er1 ⁱ	95.05 (3)
S1 ^v —Ba1—S2 ^{iv}	141.02 (3)	Er1 ^{vi} —S3—Er1 ⁱⁱ	95.05 (3)
S3 ^v —Ba1—S2 ^v	92.639 (19)	Er1 ⁱ —S3—Er1 ⁱⁱ	93.58 (3)
S3 ^{iv} —Ba1—S2 ^v	145.12 (3)	Er1 ^{vi} —S3—Ba1 ⁱⁱ	98.65 (3)
S1 ^{iv} —Ba1—S2 ^v	141.02 (3)	Er1 ⁱ —S3—Ba1 ⁱⁱ	164.41 (4)
S1 ^v —Ba1—S2 ^v	90.26 (2)	Er1 ⁱⁱ —S3—Ba1 ⁱⁱ	92.590 (8)
S2 ^{iv} —Ba1—S2 ^v	75.87 (2)	Er1 ^{vi} —S3—Ba1 ⁱ	98.65 (3)
S3 ^v —Ba1—S4 ^x	73.20 (2)	Er1 ⁱ —S3—Ba1 ⁱ	92.590 (8)
S3 ^{iv} —Ba1—S4 ^x	73.20 (2)	Er1 ⁱⁱ —S3—Ba1 ⁱ	164.41 (4)
S1 ^{iv} —Ba1—S4 ^x	138.242 (15)	Ba1 ⁱⁱ —S3—Ba1 ⁱ	78.07 (2)
S1 ^v —Ba1—S4 ^x	138.242 (15)	Er1 ^{iv} —S4—Er1 ^v	95.82 (3)
S2 ^{iv} —Ba1—S4 ^x	71.93 (2)	Er1 ^{iv} —S4—Er2	132.085 (15)
S2 ^v —Ba1—S4 ^x	71.93 (2)	Er1 ^v —S4—Er2	132.085 (15)
S3 ^v —Ba1—S4	135.514 (16)	Er1 ^{iv} —S4—Ba1 ^{ix}	95.91 (3)
S3 ^{iv} —Ba1—S4	135.514 (16)	Er1 ^v —S4—Ba1 ^{ix}	95.91 (3)
S1 ^{iv} —Ba1—S4	68.06 (2)	Er2—S4—Ba1 ^{ix}	80.37 (3)
S1 ^v —Ba1—S4	68.06 (2)	Er1 ^{iv} —S4—Ba1	95.84 (3)
S2 ^{iv} —Ba1—S4	73.05 (2)	Er1 ^v —S4—Ba1	95.84 (3)
S2 ^v —Ba1—S4	73.05 (2)	Er2—S4—Ba1	82.05 (3)
S4 ^x —Ba1—S4	135.144 (10)	Ba1 ^{ix} —S4—Ba1	162.42 (3)
S3 ^v —Ba1—Er2 ^x	106.592 (19)		

Symmetry codes: (i) $-x+1/2, -y, z-1/2$; (ii) $-x+1/2, -y+1, z-1/2$; (iii) $x-1/2, y, -z+1/2$; (iv) $-x+1/2, -y+1, z+1/2$; (v) $-x+1/2, -y, z+1/2$; (vi) $x+1/2, y, -z+1/2$; (vii) $-x+1, -y+1, -z+1$; (viii) $-x+1, -y, -z+1$; (ix) $x+1/2, y, -z+3/2$; (x) $x-1/2, y, -z+3/2$; (xi) $x, y+1, z$; (xii) $x, y-1, z$.