Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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 σ(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	μ = 30.53 mm^{-1}
b = 3.9884 (1) Å	T = 100 K
c = 14.3837 (4) Å	0.16 × 0.03 × 0.02 mm

Data collection

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

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017	44 parameters
$wR(F^2)$ = 0.050	$\Delta\rho_{max}$ = 2.46 e Å^{-3}
S = 1.87	$\Delta\rho_{min}$ = −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, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); 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.* C**65**, i60–i62.
Carpenter, J. D. & Hwu, S.-J. (1992). *Acta Cryst.* C**48**, 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. (2008*a*). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008*b*). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2013). E**69**, i17 [doi:10.1107/S1600536813003541]

Barium dierbium(III) tetrasulfide

Adel Mesbah, Wojciech Stojko and James. A Ibers

S1. Comment

Orange needles of $BaEr_2S_4$ 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 $BaLn_2S_4$ family (Ln = rare earth element) no structures have been determined from single-crystal data but that of the closely related compound $BaLu_2S_4$ has (Schurz & Schleid, 2011). Here, from X-ray diffraction single-crystal data we find that $BaEr_2S_4$ crystallizes in the $CaFe_2O_4$ 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 ErS_6 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 $BaLu_2S_4$ (Schurz & Schleid, 2011). As there are no S - S bonds in the structure, formal oxidation states may be assigned as Ba^{2+}, Er^{3+}, and S^{2-}.

S2. Experimental

In an exploration of the quaternary solid-state Ba/Er/U/S system, orange needles of $BaEr_2S_4$ were obtained instead in a two-step reaction. Uranium powder was obtained by hydridization and decomposition of ^{238}U 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 ^{238}U (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-contolled 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 Sb_2S_3. 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 Sb_2S_3 and US_2.

S3. 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.

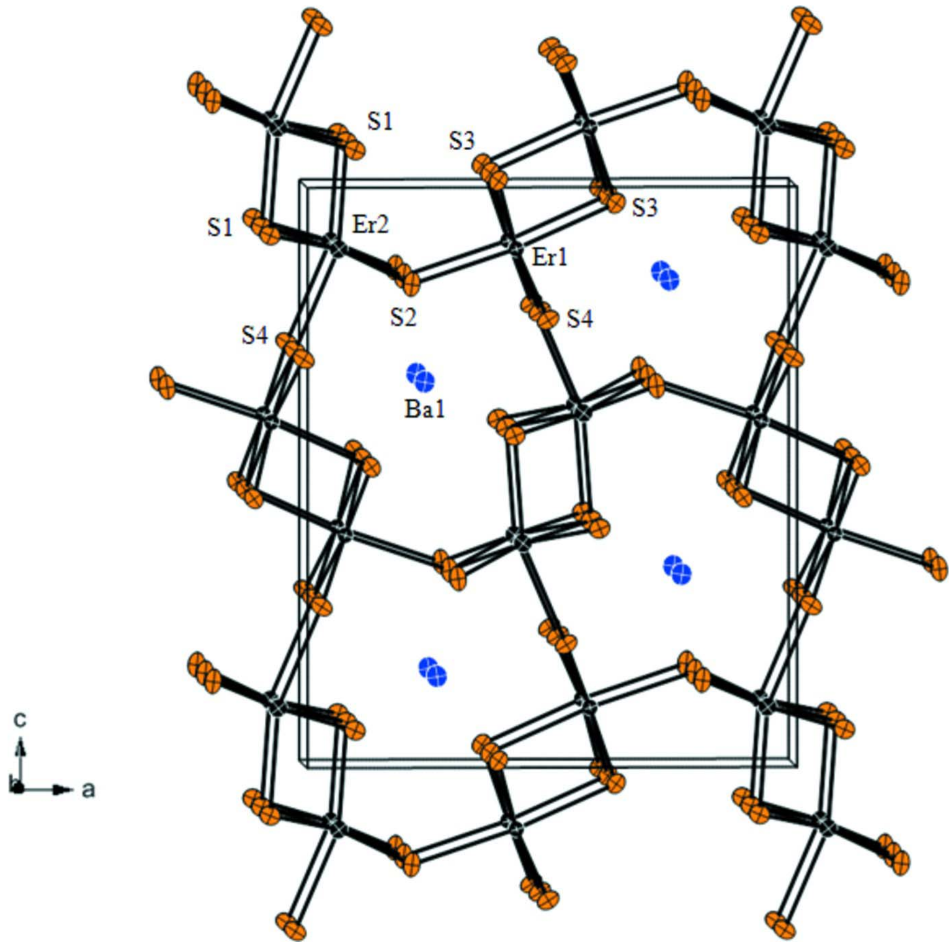

Figure 1

Structure of $BaEr_2S_4$ viewed approximatly 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) Å
$b = 3.9884$ (1) Å
$c = 14.3837$ (4) Å
$V = 696.76$ (3) Å^3
$Z = 4$
$F(000) = 1024$
$D_x = 5.721$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8150 reflections
$\theta = 2.3$–$30.5°$
$\mu = 30.53$ mm^{-1}
$T = 100$ K
Needle, orange
0.16 × 0.03 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: numerical face indexed (Sheldrick, 2008*a*)
$T_{min} = 0.084$, $T_{max} = 0.528$
9866 measured reflections
1207 independent reflections
1196 reflections with $I > 2\sigma(I)$

R_{int} = 0.030
θ_{max} = 30.5°, θ_{min} = 2.2°
h = −17→17
k = −5→5
l = −20→20

Refinement

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

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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) $x, y-1, z$.