

## Barium oxide iodide

Marten G. Barker,† M. Grazia Francesconi and Claire Wilson\*

School of Chemistry, University of Nottingham,  
Nottingham NG7 2RD, England

† Deceased.

Correspondence e-mail:  
claire.wilson@nott.ac.uk

## Key indicators

Single-crystal X-ray study

T = 150 K

Mean  $\sigma(\text{O}-\text{Ba}) = 0.008 \text{ \AA}$ 

R factor = 0.022

wR factor = 0.051

Data-to-parameter ratio = 31.3

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Barium oxide iodide,  $\text{Ba}_4\text{OI}_6$ , has been prepared by a solid-state reaction and shown to be isostructural with both  $\text{A}_4\text{OCl}_6$ , where A is Ba or Sr, and  $\text{Sr}_4\text{OI}_6$ .

Received 13 February 2001

Accepted 20 April 2001

Online 22 May 2001

## Comment

Alkaline earth oxide chlorides and oxide bromides, of general formula  $\text{A}_4\text{OX}_6$  (A = alkaline earth; X =  $\text{Cl}^-$ ,  $\text{Br}^-$ ) are known for their luminescence properties, when the alkaline earth site is doped with small amounts of  $\text{Eu}^{2+}$  or  $\text{Pb}^{2+}$  (Schipper *et al.*, 1992). We have succeeded in extending this family to the barium oxide iodide compound  $\text{Ba}_4\text{OI}_6$ .  $\text{Ba}_4\text{OI}_6$  was prepared by a solid-state reaction and is isostructural with  $\text{Sr}_4\text{OCl}_6$  (Hagemann *et al.*, 1996),  $\text{Ba}_4\text{OCl}_6$  (Bergerhoff & Goost, 1970) and  $\text{Sr}_4\text{OI}_6$  (Barker *et al.*, 2001). The O atom is four-coordinated by Ba cations (see Fig. 1), the iodine is four- and five-coordinated by Ba cations (Figs. 2 and 3) and the Ba is eight-coordinated by one oxygen and seven iodine anions at one site, and seven-coordinated by one oxygen and six iodine anions at the other (Figs. 4 and 5). The overall structure is shown in Fig. 1 of Barker *et al.* (2001).

## Experimental

$\text{BaO}$  and  $\text{BaI}_2$  powders were mixed in stoichiometric proportions and placed in a nickel crucible. The mixture was then heated at 1273 K for 24 h in a silica tube, under flowing nitrogen. The product was cooled to room temperature at a rate of  $1 \text{ K h}^{-1}$ .

## Crystal data

$\text{Ba}_4\text{OI}_6$   
 $M_r = 1326.72$   
 Hexagonal,  $P6_3mc$   
 $a = 10.838 (4) \text{ \AA}$   
 $c = 8.410 (3) \text{ \AA}$   
 $V = 855.5 (9) \text{ \AA}^3$   
 $Z = 2$   
 $D_x = 5.150 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 802 reflections  
 $\theta = 4.3\text{--}27.8^\circ$   
 $\mu = 19.87 \text{ mm}^{-1}$   
 $T = 150 (2) \text{ K}$   
 Block, colourless  
 $0.18 \times 0.12 \times 0.10 \text{ mm}$

## Data collection

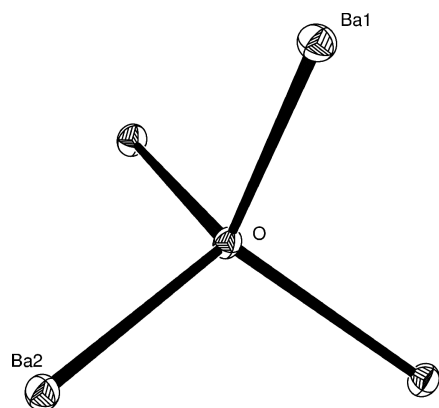
Bruker SMART1000 CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1996)  
 $T_{\min} = 0.077$ ,  $T_{\max} = 0.137$   
 4900 measured reflections  
 842 independent reflections

732 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$   
 $\theta_{\text{max}} = 28.8^\circ$   
 $h = -14 \rightarrow 12$   
 $k = -14 \rightarrow 14$   
 $l = -11 \rightarrow 11$   
 Intensity decay: none

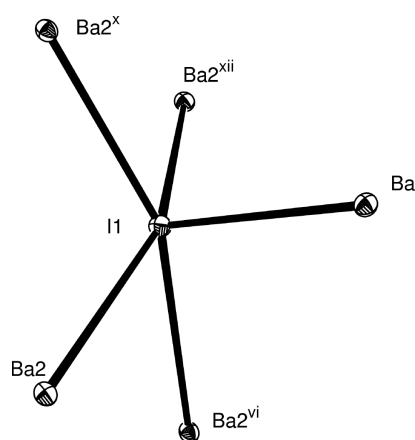
## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.051$   
 $S = 1.09$   
 782 reflections  
 25 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0263P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.82 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.20 \text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983)  
 Flack parameter =  $-0.06 (10)$



**Figure 1**  
A view showing the tetrahedral coordination around the O atom. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
A view showing coordination around atom I1. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (vi)  $1 - y, 1 + x - y, z$ ; (x)  $y, -x + y, \frac{1}{2} + z$ ; (xii)  $1 - x, 1 - y, \frac{1}{2} + z$ .]

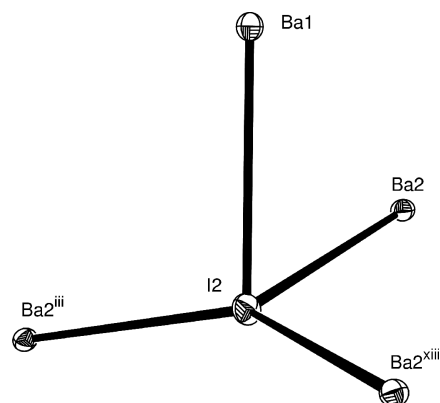
**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ba1—O <sup>i</sup>	2.542 (12)	Ba2—I2 <sup>iv</sup>	3.5115 (16)
Ba1—I1 <sup>ii</sup>	3.5848 (17)	Ba2—I1 <sup>v</sup>	3.5560 (15)
Ba1—I2	3.6927 (18)	Ba2—I1	3.6781 (15)
Ba2—O	2.555 (4)	O—Ba1 <sup>iii</sup>	2.542 (12)
Ba2—I2 <sup>iii</sup>	3.467 (2)		

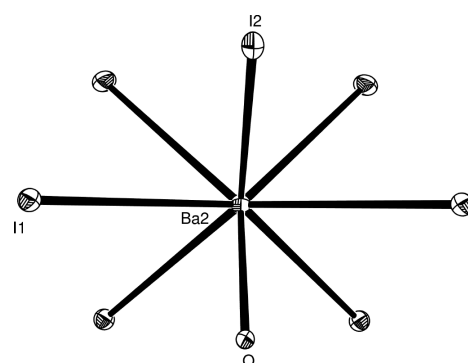
Symmetry codes: (i)  $x, y, z - 1$ ; (ii)  $y, 1 - x + y, z - \frac{1}{2}$ ; (iii)  $x, y, 1 + z$ ; (iv)  $y, -x + y, \frac{1}{2} + z$ ; (v)  $1 - x, 1 - y, z - \frac{1}{2}$ .

The origin was fixed by application of a floating origin restraint which effectively fixes the centre of gravity of the structure in the polar-axis direction. This leads to smaller correlations than fixing a single atom in structures with no dominant heavy atom (Flack & Schwarzenbach, 1988).

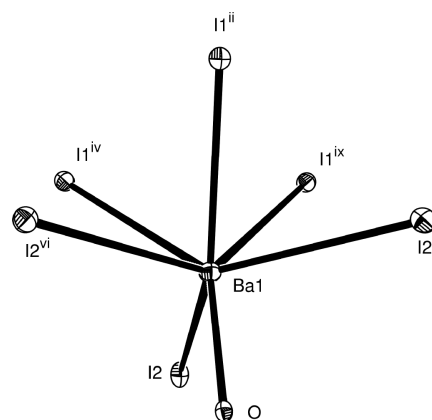
Data collection: *SMART* Bruker, 1998; cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* and *SHELXL97* (Sheldrick, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* and *WINGX* (Farrugia, 1999); molecular graphics: *ORTEP-3* (Farrugia, 1997);



**Figure 3**  
A view showing the coordination around atom I2. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (iii)  $x - y, x, z - \frac{1}{2}$ ; (xiii)  $y, -x + y, z - \frac{1}{2}$ .]



**Figure 4**  
A view showing the coordination around atom Ba2. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 5**  
A view showing the coordination around atom Ba1. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (ii)  $y, 1 - x + y, z - \frac{1}{2}$ ; (iv)  $1 - x, 1 - y, z - \frac{1}{2}$ ; (v)  $-x + y, 1 - x, z$ ; (vi)  $1 - y, 1 + x - y, z$ ; (ix)  $x - y, x, \frac{1}{2} + z$ .]

software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2001).

We wish to thank the EPSRC for support.

**References**

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Barker, M. G., Francesconi, M. G., Shutt, T. H. & Wilson C. (2001). *Acta Cryst.* **E57**, i44–45.
- Bergerhoff, G. & Goost, L. (1970). *Acta Cryst.* **B26**, 19–23.
- Bruker (1996). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1998). *SMART Area-Detector Software Package*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2000). *SAINT Frame Integration Software*. Version 6.02a. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Flack, H. D. & Schwarzenbach, D. (1988). *Acta Cryst.* **A44**, 499–506.
- Hagemann, H., Kubel, F. & Bill, H. (1996). *Eur. J. Solid State Inorg. Chem.* **33**, 1101–1109.
- Schipper, W. J., Vroon, Z. A. E. P., Blasse, G. & Schleid, T. (1992). *Chem. Mater.* **4**, 688–692.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2001). *PLATON*. University of Utrecht, The Netherlands.

## supporting information

*Acta Cryst.* (2001). E57, i41–i43 [https://doi.org/10.1107/S1600536801006614]

## Barium oxide iodide

Marten G. Barker, M. Grazia Francesconi and Claire Wilson

(I)

*Crystal data*

Ba <sub>4</sub> OI <sub>6</sub>	$D_x = 5.150 \text{ Mg m}^{-3}$
$M_r = 1326.72$	Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$
Hexagonal, $P6_3mc$	Cell parameters from 802 reflections
$a = 10.838 (4) \text{ \AA}$	$\theta = 4.3\text{--}27.8^\circ$
$c = 8.410 (3) \text{ \AA}$	$\mu = 19.87 \text{ mm}^{-1}$
$V = 855.5 (9) \text{ \AA}^3$	$T = 150 \text{ K}$
$Z = 2$	Block, colourless
$F(000) = 1100$	$0.18 \times 0.12 \times 0.10 \text{ mm}$

*Data collection*

Bruker SMART1000 CCD area-detector diffractometer	4900 measured reflections
Radiation source: fine-focus sealed tube	842 independent reflections
Graphite monochromator	732 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.040$
Absorption correction: multi-scan (SADABS; Bruker, 1996)	$\theta_{\text{max}} = 28.8^\circ$ , $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.077$ , $T_{\text{max}} = 0.137$	$h = -14 \rightarrow 12$
	$k = -14 \rightarrow 14$
	$l = -11 \rightarrow 11$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0263P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.022$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.051$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.82 \text{ e \AA}^{-3}$
782 reflections	$\Delta\rho_{\text{min}} = -1.20 \text{ e \AA}^{-3}$
25 parameters	Absolute structure: Flack (1983)
1 restraint	Absolute structure parameter: $-0.06 (10)$
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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba1	0.3333	0.6667	0.02342 (13)	0.0133 (2)
Ba2	0.20359 (3)	0.40719 (6)	0.62927 (8)	0.01196 (14)
I1	0.53228 (3)	0.46772 (3)	0.82627 (8)	0.01280 (15)
I2	0.13667 (3)	0.27334 (6)	0.01355 (8)	0.01651 (16)
O	0.3333	0.6667	0.7212 (15)	0.010 (2)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0142 (3)	0.0142 (3)	0.0113 (5)	0.00711 (15)	0.000	0.000
Ba2	0.0109 (2)	0.0100 (3)	0.0147 (3)	0.00499 (14)	-0.00039 (13)	-0.0008 (3)
I1	0.0127 (2)	0.0127 (2)	0.0130 (3)	0.0064 (3)	-0.00047 (14)	0.00047 (14)
I2	0.0126 (2)	0.0184 (3)	0.0204 (3)	0.00919 (17)	0.00145 (15)	0.0029 (3)
O	0.008 (3)	0.008 (3)	0.013 (6)	0.0041 (16)	0.000	0.000

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Ba1—O <sup>i</sup>	2.542 (12)	Ba2—I1 <sup>v</sup>	3.6781 (15)
Ba1—I1 <sup>ii</sup>	3.5848 (17)	Ba2—I1	3.6781 (15)
Ba1—I1 <sup>iii</sup>	3.5848 (17)	Ba2—Ba1 <sup>ix</sup>	4.113 (2)
Ba1—I1 <sup>iv</sup>	3.5848 (17)	Ba2—Ba2 <sup>vi</sup>	4.218 (2)
Ba1—I2 <sup>v</sup>	3.6927 (18)	Ba2—Ba2 <sup>v</sup>	4.218 (2)
Ba1—I2 <sup>vi</sup>	3.6927 (18)	I1—Ba2 <sup>x</sup>	3.5560 (15)
Ba1—I2	3.6927 (18)	I1—Ba2 <sup>xii</sup>	3.5560 (15)
Ba1—Ba2 <sup>vii</sup>	4.113 (2)	I1—Ba1 <sup>xii</sup>	3.5848 (17)
Ba1—Ba2 <sup>i</sup>	4.113 (2)	I1—Ba2 <sup>vi</sup>	3.6781 (15)
Ba1—Ba2 <sup>viii</sup>	4.113 (2)	I2—Ba2 <sup>i</sup>	3.467 (2)
Ba2—O	2.555 (4)	I2—Ba2 <sup>iii</sup>	3.5115 (16)
Ba2—I2 <sup>ix</sup>	3.467 (2)	I2—Ba2 <sup>xiii</sup>	3.5115 (16)
Ba2—I2 <sup>x</sup>	3.5115 (16)	O—Ba1 <sup>ix</sup>	2.542 (12)
Ba2—I2 <sup>xi</sup>	3.5115 (16)	O—Ba2 <sup>v</sup>	2.555 (4)
Ba2—I1 <sup>iii</sup>	3.5560 (15)	O—Ba2 <sup>vi</sup>	2.555 (4)
Ba2—I1 <sup>iv</sup>	3.5560 (15)		
O <sup>i</sup> —Ba1—I1 <sup>ii</sup>	135.27 (3)	I2 <sup>ix</sup> —Ba2—I1 <sup>v</sup>	68.66 (2)
O <sup>i</sup> —Ba1—I1 <sup>iii</sup>	135.27 (3)	I2 <sup>x</sup> —Ba2—I1 <sup>v</sup>	142.459 (19)
I1 <sup>ii</sup> —Ba1—I1 <sup>iii</sup>	75.10 (4)	I2 <sup>xi</sup> —Ba2—I1 <sup>v</sup>	71.35 (2)
O <sup>i</sup> —Ba1—I1 <sup>iv</sup>	135.27 (3)	I1 <sup>iii</sup> —Ba2—I1 <sup>v</sup>	74.43 (4)
I1 <sup>ii</sup> —Ba1—I1 <sup>iv</sup>	75.10 (4)	I1 <sup>iv</sup> —Ba2—I1 <sup>v</sup>	144.294 (19)
I1 <sup>iii</sup> —Ba1—I1 <sup>iv</sup>	75.10 (4)	O—Ba2—I1	73.53 (11)

O <sup>i</sup> —Ba1—I2 <sup>v</sup>	88.71 (2)	I2 <sup>ix</sup> —Ba2—I1	68.66 (2)
I1 <sup>ii</sup> —Ba1—I2 <sup>v</sup>	70.379 (15)	I2 <sup>x</sup> —Ba2—I1	71.35 (2)
I1 <sup>iii</sup> —Ba1—I2 <sup>v</sup>	70.379 (16)	I2 <sup>xi</sup> —Ba2—I1	142.459 (19)
I1 <sup>iv</sup> —Ba1—I2 <sup>v</sup>	136.01 (4)	I1 <sup>iii</sup> —Ba2—I1	144.29 (2)
O <sup>i</sup> —Ba1—I2 <sup>vi</sup>	88.71 (2)	I1 <sup>iv</sup> —Ba2—I1	74.43 (4)
I1 <sup>ii</sup> —Ba1—I2 <sup>vi</sup>	70.379 (16)	I1 <sup>v</sup> —Ba2—I1	123.13 (4)
I1 <sup>iii</sup> —Ba1—I2 <sup>vi</sup>	136.01 (4)	O—Ba2—Ba1 <sup>ix</sup>	36.1 (3)
I1 <sup>iv</sup> —Ba1—I2 <sup>vi</sup>	70.379 (16)	I2 <sup>ix</sup> —Ba2—Ba1 <sup>ix</sup>	57.55 (4)
I2 <sup>v</sup> —Ba1—I2 <sup>vi</sup>	119.950 (2)	I2 <sup>x</sup> —Ba2—Ba1 <sup>ix</sup>	130.653 (17)
O <sup>i</sup> —Ba1—I2	88.71 (2)	I2 <sup>xi</sup> —Ba2—Ba1 <sup>ix</sup>	130.653 (17)
I1 <sup>ii</sup> —Ba1—I2	136.01 (4)	I1 <sup>iii</sup> —Ba2—Ba1 <sup>ix</sup>	112.46 (4)
I1 <sup>iii</sup> —Ba1—I2	70.379 (16)	I1 <sup>iv</sup> —Ba2—Ba1 <sup>ix</sup>	112.46 (4)
I1 <sup>iv</sup> —Ba1—I2	70.379 (16)	I1 <sup>v</sup> —Ba2—Ba1 <sup>ix</sup>	62.97 (2)
I2 <sup>v</sup> —Ba1—I2	119.950 (2)	I1—Ba2—Ba1 <sup>ix</sup>	62.97 (2)
I2 <sup>vi</sup> —Ba1—I2	119.950 (2)	O—Ba2—Ba2 <sup>vi</sup>	34.36 (12)
O <sup>i</sup> —Ba1—Ba2 <sup>vii</sup>	36.31 (2)	I2 <sup>ix</sup> —Ba2—Ba2 <sup>vi</sup>	108.287 (17)
I1 <sup>ii</sup> —Ba1—Ba2 <sup>vii</sup>	111.36 (4)	I2 <sup>x</sup> —Ba2—Ba2 <sup>vi</sup>	108.049 (12)
I1 <sup>iii</sup> —Ba1—Ba2 <sup>vii</sup>	111.36 (4)	I2 <sup>xi</sup> —Ba2—Ba2 <sup>vi</sup>	160.488 (17)
I1 <sup>iv</sup> —Ba1—Ba2 <sup>vii</sup>	171.58 (2)	I1 <sup>iii</sup> —Ba2—Ba2 <sup>vi</sup>	91.216 (11)
I2 <sup>v</sup> —Ba1—Ba2 <sup>vii</sup>	52.41 (3)	I1 <sup>iv</sup> —Ba2—Ba2 <sup>vi</sup>	53.62 (2)
I2 <sup>vi</sup> —Ba1—Ba2 <sup>vii</sup>	106.13 (2)	I1 <sup>v</sup> —Ba2—Ba2 <sup>vi</sup>	107.812 (11)
I2—Ba1—Ba2 <sup>vii</sup>	106.13 (2)	I1—Ba2—Ba2 <sup>vi</sup>	55.009 (12)
O <sup>i</sup> —Ba1—Ba2 <sup>i</sup>	36.31 (2)	Ba1 <sup>ix</sup> —Ba2—Ba2 <sup>vi</sup>	59.152 (19)
I1 <sup>ii</sup> —Ba1—Ba2 <sup>i</sup>	171.58 (2)	O—Ba2—Ba2 <sup>v</sup>	34.36 (12)
I1 <sup>iii</sup> —Ba1—Ba2 <sup>i</sup>	111.36 (4)	I2 <sup>ix</sup> —Ba2—Ba2 <sup>v</sup>	108.287 (17)
I1 <sup>iv</sup> —Ba1—Ba2 <sup>i</sup>	111.36 (4)	I2 <sup>x</sup> —Ba2—Ba2 <sup>v</sup>	160.488 (17)
I2 <sup>v</sup> —Ba1—Ba2 <sup>i</sup>	106.13 (2)	I2 <sup>xi</sup> —Ba2—Ba2 <sup>v</sup>	108.049 (12)
I2 <sup>vi</sup> —Ba1—Ba2 <sup>i</sup>	106.13 (2)	I1 <sup>iii</sup> —Ba2—Ba2 <sup>v</sup>	53.62 (2)
I2—Ba1—Ba2 <sup>i</sup>	52.41 (3)	I1 <sup>iv</sup> —Ba2—Ba2 <sup>v</sup>	91.216 (11)
Ba2 <sup>vii</sup> —Ba1—Ba2 <sup>i</sup>	61.70 (4)	I1 <sup>v</sup> —Ba2—Ba2 <sup>v</sup>	55.009 (12)
O <sup>i</sup> —Ba1—Ba2 <sup>viii</sup>	36.31 (2)	I1—Ba2—Ba2 <sup>v</sup>	107.812 (11)
I1 <sup>ii</sup> —Ba1—Ba2 <sup>viii</sup>	111.36 (4)	Ba1 <sup>ix</sup> —Ba2—Ba2 <sup>v</sup>	59.152 (19)
I1 <sup>iii</sup> —Ba1—Ba2 <sup>viii</sup>	171.58 (2)	Ba2 <sup>vi</sup> —Ba2—Ba2 <sup>v</sup>	60.0
I1 <sup>iv</sup> —Ba1—Ba2 <sup>viii</sup>	111.36 (4)	Ba2 <sup>x</sup> —I1—Ba2 <sup>xii</sup>	72.76 (4)
I2 <sup>v</sup> —Ba1—Ba2 <sup>viii</sup>	106.13 (2)	Ba2 <sup>x</sup> —I1—Ba1 <sup>xii</sup>	104.53 (4)
I2 <sup>vi</sup> —Ba1—Ba2 <sup>viii</sup>	52.41 (3)	Ba2 <sup>xii</sup> —I1—Ba1 <sup>xii</sup>	104.53 (4)
I2—Ba1—Ba2 <sup>viii</sup>	106.13 (2)	Ba2 <sup>x</sup> —I1—Ba2 <sup>vi</sup>	156.07 (2)
Ba2 <sup>vii</sup> —Ba1—Ba2 <sup>viii</sup>	61.70 (4)	Ba2 <sup>xii</sup> —I1—Ba2 <sup>vi</sup>	103.52 (3)
Ba2 <sup>i</sup> —Ba1—Ba2 <sup>viii</sup>	61.70 (4)	Ba1 <sup>xii</sup> —I1—Ba2 <sup>vi</sup>	99.29 (4)
O—Ba2—I2 <sup>ix</sup>	93.6 (3)	Ba2 <sup>x</sup> —I1—Ba2	103.52 (3)
O—Ba2—I2 <sup>x</sup>	140.63 (2)	Ba2 <sup>xii</sup> —I1—Ba2	156.07 (2)
I2 <sup>ix</sup> —Ba2—I2 <sup>x</sup>	89.79 (3)	Ba1 <sup>xii</sup> —I1—Ba2	99.29 (4)
O—Ba2—I2 <sup>xi</sup>	140.63 (2)	Ba2 <sup>vi</sup> —I1—Ba2	69.98 (2)
I2 <sup>ix</sup> —Ba2—I2 <sup>xi</sup>	89.79 (3)	Ba2 <sup>i</sup> —I2—Ba2 <sup>iii</sup>	109.018 (17)
I2 <sup>x</sup> —Ba2—I2 <sup>xi</sup>	78.50 (2)	Ba2 <sup>i</sup> —I2—Ba2 <sup>xiii</sup>	109.018 (17)
O—Ba2—I1 <sup>iii</sup>	84.4 (2)	Ba2 <sup>iii</sup> —I2—Ba2 <sup>xiii</sup>	140.98 (3)
I2 <sup>ix</sup> —Ba2—I1 <sup>iii</sup>	141.96 (2)	Ba2 <sup>i</sup> —I2—Ba1	70.05 (3)
I2 <sup>x</sup> —Ba2—I1 <sup>iii</sup>	115.40 (4)	Ba2 <sup>iii</sup> —I2—Ba1	100.378 (13)

$I2^{xi}-Ba2-I1^{iii}$	69.600 (17)	$Ba2^{xiii}-I2-Ba1$	100.378 (13)
$O-Ba2-I1^{iv}$	84.4 (2)	$Ba1^{ix}-O-Ba2^v$	107.6 (3)
$I2^{ix}-Ba2-I1^{iv}$	141.96 (2)	$Ba1^{ix}-O-Ba2$	107.6 (3)
$I2^x-Ba2-I1^{iv}$	69.600 (17)	$Ba2^v-O-Ba2$	111.3 (2)
$I2^{xi}-Ba2-I1^{iv}$	115.40 (4)	$Ba1^{ix}-O-Ba2^{vi}$	107.6 (3)
$I1^{iii}-Ba2-I1^{iv}$	75.81 (4)	$Ba2^v-O-Ba2^{vi}$	111.3 (2)
$O-Ba2-I1^v$	73.53 (11)	$Ba2-O-Ba2^{vi}$	111.3 (2)

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