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Barium oxide iodide

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Barium oxide iodide, Ba_4OI_6, has been prepared by a solid-state reaction and shown to be isostructural with both A_4OCl_6, where A is Ba or Sr, and Sr_4OI_6.

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(O–Ba) = 0.008 Å
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.

Comment

Alkaline earth oxide chlorides and oxide bromides, of general formula A_4OX_6 (A = alkaline earth; $X = Cl^-, Br^-$) are known for their luminescence properties, when the alkaline earth site is doped with small amounts of Eu^{2+} or Pb^{2+} (Schipper *et al.*, 1992). We have succeeded in extending this family to the barium oxide iodide compound Ba_4OI_6. Ba_4OI_6 was prepared by a solid-state reaction and is isostructural with Sr_4OCl_6 (Hagemann *et al.*, 1996), Ba_4OCl_6 (Bergerhoff & Goost, 1970) and Sr_4OI_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

BaO and 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 K h^{-1}.

Crystal data

Ba_4OI_6
M_r = 1326.72
Hexagonal, $P6_3mc$
a = 10.838 (4) Å
c = 8.410 (3) Å
V = 855.5 (9) Å^3
Z = 2
D_x = 5.150 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 802 reflections
θ = 4.3–27.8°
μ = 19.87 mm^{-1}
T = 150 (2) K
Block, colourless
0.18 × 0.12 × 0.10 mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer
ω 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_{int} = 0.040
θ_{max} = 28.8°
$h = -14 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -11 \rightarrow 11$
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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −1.20 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = −0.06 (10)

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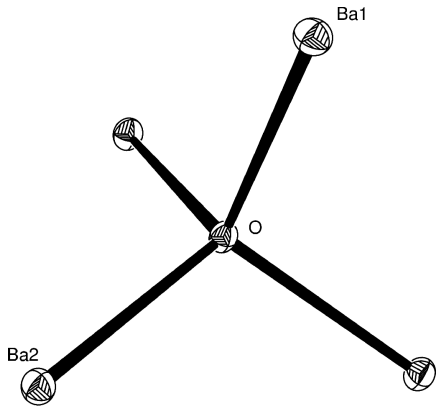

Figure 1
A view showing the tetrahedral coordination around the O atom. Displacement ellipsoids are drawn at the 50% probability level.

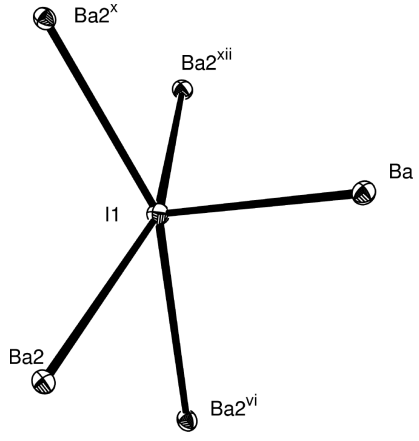

Figure 2
A view showing coordination around atom I1. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (vi) $1-y$, $1+x-y$, z; (x) y, $-x+y$, $\frac{1}{2}+z$; (xii) $1-x$, $1-y$, $\frac{1}{2}+z$.]

Table 1
Selected geometric parameters (Å, °).

Ba1—O^{i}	2.542 (12)	Ba2—I2^{iv}	3.5115 (16)
Ba1—I1^{ii}	3.5848 (17)	Ba2—I1^{v}	3.5560 (15)
Ba1—I2	3.6927 (18)	Ba2—I1	3.6781 (15)
Ba2—O	2.555 (4)	O—Ba1^{iii}	2.542 (12)
Ba2—I2^{iii}	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 *SHELXL*97 (Sheldrick, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 and *WINGX* (Farrugia, 1999); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2001).

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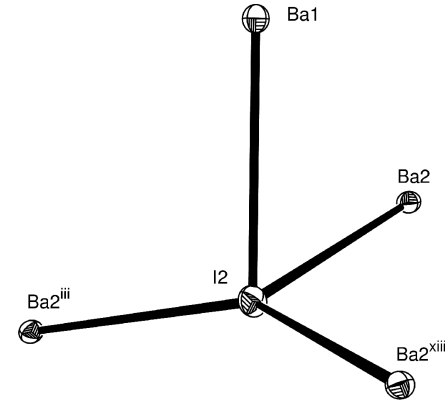

Figure 3
A view showing the coordination around atom I2. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (iii) $x-y$, x, $z-\frac{1}{2}$; (xiii) y, $-x+y$, $z-\frac{1}{2}$.]

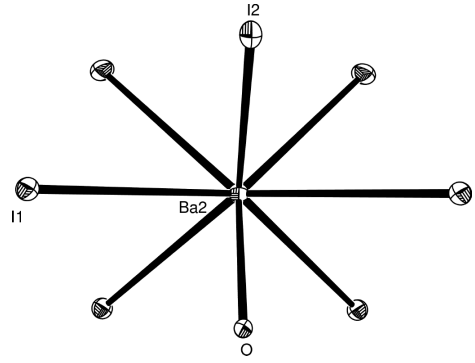

Figure 4
A view showing the coordination around atom Ba2. Displacement ellipsoids are drawn at the 50% probability level.

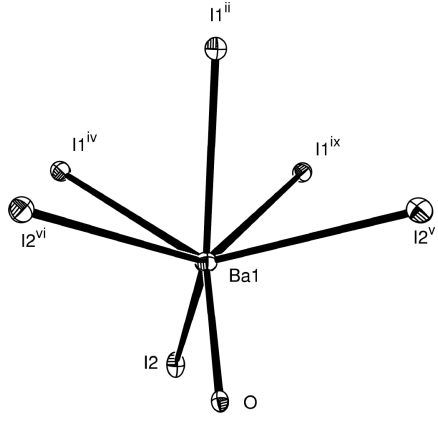

Figure 5
A view showing the coordination around atom Ba1. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (ii) y, $1-x+y$, $z-\frac{1}{2}$; (iv) $1-x$, $1-y$, $z-\frac{1}{2}$; (v) $-x+y$, $1-x$, z; (vi) $1-y$, $1+x-y$, z; (ix) $x-y$, x, $\frac{1}{2}+z$.]

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