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Strontium oxide iodide

Marten G. Barker,† M. Grazia Francesconi, Thomas H. Shutt and Claire Wilson*

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

† Deceased.

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

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Strontium oxide iodide, Sr_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 Ba_4OI_6.

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(Sr–O) = 0.01 Å
R factor = 0.030
wR factor = 0.055
Data-to-parameter ratio = 28.8

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). This family has now been extended to the strontium oxide iodide compounds Sr_4OI_6. Sr_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 Ba_4OI_6 (Barker *et al.*, 2001). The oxygen is four-coordinated by Sr cations, the iodine is four- and five-coordinated by Sr cations, and the Sr 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 (Fig. 1). shows the overall structure and figures for the isostructural Ba_4OI_6 given in Barker *et al.* (2001) show the coordination at each of these sites.

Experimental

SrO and SrI_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}.

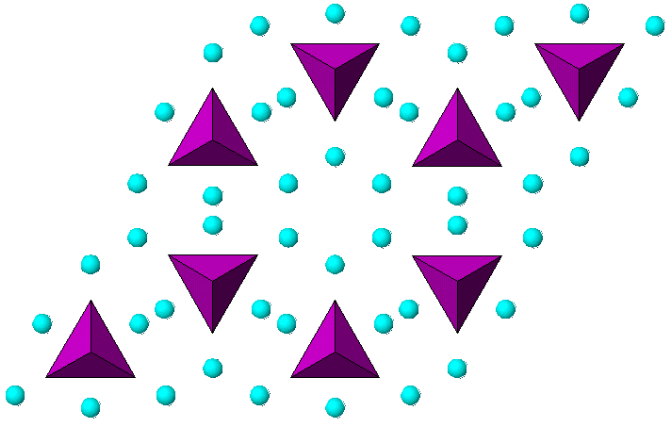

Figure 1
[001] projection of the Sr_4OI_6 structure showing the I^- anions (blue) and the O–Sr tetrahedra.

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Crystal data

Sr_4OI_6	Mo $K\alpha$ radiation
M_r = 1127.88	Cell parameters from 841 reflections
Hexagonal, $P6_3mc$	θ = 5.9–27.6°
a = 10.747 (1) Å	μ = 25.21 mm^{-1}
c = 7.8678 (9) Å	T = 150 (2) K
V = 787.0 (3) Å^3	Block, colourless
Z = 2	0.05 × 0.04 × 0.04 mm
D_x = 4.760 Mg m^{-3}	

Data collection

Bruker SMART1000 CCD area-detector diffractometer	586 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.054
Absorption correction: multi-scan (*SADABS*; Bruker, 1996)	θ_{max} = 27.6°
T_{min} = 0.272, T_{max} = 0.365	$h = -13 \rightarrow 6$
3527 measured reflections	$k = -10 \rightarrow 4$
776 independent reflections	$l = -9 \rightarrow 10$
	Intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0206P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.055	$\Delta\rho_{max}$ = 1.27 e Å^{-3}
S = 0.94	$\Delta\rho_{min}$ = −0.99 e Å^{-3}
721 reflections	Absolute structure: Flack (1983)
25 parameters	Flack parameter = 0.064 (18)

Table 1
Selected bond lengths (Å).

Sr1—O	2.37 (2)	Sr2—I1^{iv}	3.3947 (18)
Sr1—I1^{i}	3.366 (2)	Sr2—I2^{v}	3.5567 (19)
Sr1—I2^{ii}	3.830 (2)	Sr2—I1^{vi}	3.5967 (17)
Sr2—O	2.393 (6)	O—Sr2^{iv}	2.393 (6)
Sr2—I2^{iii}	3.392 (2)	O—Sr2^{vii}	2.393 (6)

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

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: *ATOMS* (Dowty, 1998) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2001).

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