Crystal structure of distrontium oxide diiodide, Sr_2OI_2

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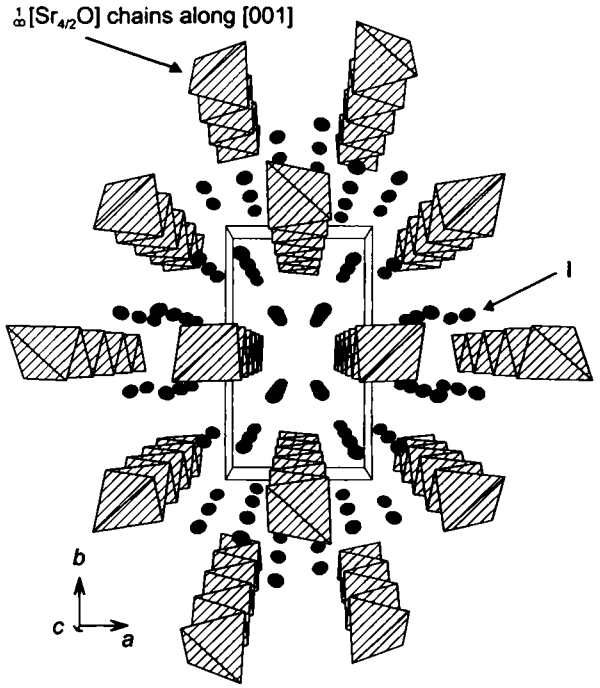

Abstract

I_2OSr_2, orthorhombic, *Ibam* (no. 72), a = 7.412(1) Å, b = 12.955(3) Å, c = 6.475(1) Å, V = 621.8 Å^3, Z = 4, $R_{gt}(F)$ = 0.031, $wR_{ref}(F^2)$ = 0.060, T = 173 K.

Source of material

360 mg Sr, 145 mg NH_4I and 100 mg Na were arc-welded into a stainless-steel ampule which in turn was fused into an evacuated silica tube. The reaction vessel was placed upright in a box furnace, which was heated within six hours to the reaction temperature of 1200 K. The sample was kept at this temperature for 24 hours. Then the furnace was switched off and allowed to cool to room temperature. The reaction product contained Sr, Na, Sr_2N and estimated 5-10 % of the title compound which forms transparent needles and plates.

Discussion

While exploring alkaline earth metal hydrides, we found by serendipity the new compound Sr_2OI_2. The oxygen source is probably the Sr metal which sometimes develops even under protective gas atmosphere superficial coatings with SrO, $Sr(OH)_2$ or $SrCO_3$. Not taking the compounds containing complex anions into account, to our knowledge only compounds crystallizing with the AE_4OX_6 structure type (AE = Ca, Sr or Ba; X = Cl, Br, I) [1-7] have been described in the ternary AE-O-X system. The title compound exhibits [$Sr_{4/2}O$] cationic chains along [001] which are held together by iodide anions located between these chains. The Sr—O distance of 236.94(3) pm compares well to the distances in isolated [Sr_4O] tetrahedra found in Sr_4OCl_6 [2,3] and in Sr_4OI_6 [4] (d(Sr—O) = 233.8 pm – 239.4 pm). Sr_2OI_2 can be regarded as an *anti*-type to compounds of the A_2MX_2 type (A = alkali metal; M = Mn, Co, Zn or tetrelide; X = pentelide or chalcogenide) [8-14] which can be seen as a stuffed variant of the SiS_2 structure.

Table 1. Data collection and handling.

Crystal:	transparent colorless needle, size 0.02 × 0.02 × 0.10 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	269.52 cm^{-1}
Diffractometer, scan mode:	Bruker X8 Apex II & 4K CCD, φ/ω
$2\theta_{max}$:	74.76°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7087, 856
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 709
$N(param)_{refined}$:	17
Programs:	SHELXS-97 [15], SHELXL-97 [16], DIAMOND [17]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I	8*j*	0.14836(3)	0.84922(2)	0	0.0179(2)	0.0128(2)	0.0138(2)	–0.00225(9)	0	0
Sr	8*j*	0.17227(5)	0.59013(3)	0	0.0149(2)	0.0102(2)	0.0097(2)	–0.0033(1)	0	0
O	4*b*	½	0	¼	0.012(2)	0.010(2)	0.010(2)	0	0	0

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