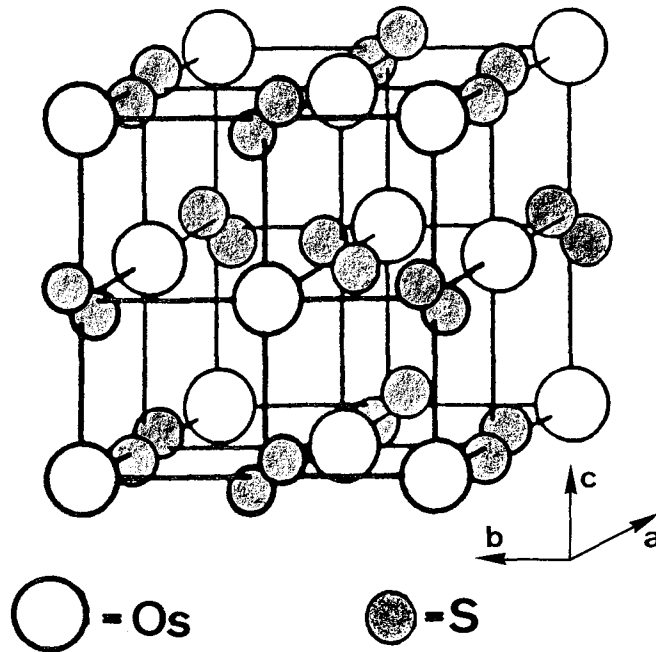


Crystal structure refinement of osmium(II) disulfide, OsS_2

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(Received November 14, 1991, transferred to database ICSD January 2, 1992)



Source of material: see ref. 3.

The M-S distance in OsS_2 (2.3510(5) Å) resembles that of RuS_2 (2.3520(3) Å). The S-S bond length (2.2160(12) Å) is remarkably longer than those of all known pyrite-type sulfides.

Cubic, Pa3 (no 205), $a = 5.6194(7)$ Å, $V = 177.4$ Å³, $Z = 4$, $R = 0.016$.

Table 1. Parameters used for the X-ray data collection

Diffractometer type:	Enraf-Nonius CAD4	Number of unique reflections:	313
Wave length:	Mo K _α radiation (0.7107 Å)	Criterion for unobserved reflections:	$I_0 < 2\sigma(I_0)$
Crystal characteristics:	black sphere, 0.1 mm in diameter	Number of refined parameters:	7
Temperature of measurement:	293 K	Scan mode:	ω -2 θ
$2\theta_{\max}$:	100°	μ :	736.8 cm ⁻¹
		Structure solution program used:	SDP

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	x	y	z	U_{11}/U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Os	0.0	0.0	0.0	0.00205(3)	0.00205(3)	0.00205(3)	-0.00004(2)	-0.00004(2)	-0.00004(2)
S	0.38616(6)	0.38616(6)	0.38616(6)	0.00288(6)	0.00288(6)	0.00288(6)	0.0001(1)	0.0001(1)	0.0001(1)

Further details of the structure determination (e.g. structure factors) have been deposited within the relevant database and can be accessed as Collection No. 300224 or ordered from the Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen.

References:

1. Meisel, K.: Über die Gitterkonstante des OsS₂. Z. Anorg. Allg. Chem. **219** (1934) 141–142.
2. Sutarno, Knopp, O., Reid, K.I.G.: Chalcogenides of the transition elements. V. Crystal structures of the disulfides and ditelluride of ruthenium and osmium. Can. J. Chem. **45** (1967) 1391–1400.
3. Müller, B., Lutz, H.D.: Single crystal raman studies of pyrite-type RuS₂, RuSe₂, OsS₂, OsSe₂, PtP₂, and PtAs₂. Phys. Chem. Minerals **17** (1991) 716–719.