The sesquitelluride Sc_2Te_3

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Scandium sesquitelluride, Sc_2Te_3, was obtained as a side product by reacting the elements Sc, Ni and Te at 1073 K in an evacuated silica tube. This is the third modification of Sc_2Te_3, which crystallizes in the orthorhombic space group *Fddd* and adopts the Sc_2S_3 structure type [Dismukes & White (1964). *Inorg. Chem.* **3**, 1220–1228]. The structure consists of edge-sharing (slightly distorted) $ScTe_6$ octahedra and may be regarded as a defect variant of the NaCl type.

Comment

Recently, we reported the crystal structure of Yb_2Se_3, which crystallizes in the Sc_2S_3 structure type (Assoud & Kleinke, 2003). The chalcogenides Ln_2Q_3 (Ln = lanthanide, Q = chalcogen) adopt different structure types depending on the radius of the lanthanide. The large lanthanide chalcogenides prefer the defect variant of the Th_3P_4 type (Mauricot *et al.*, 1995), whereas the smaller ones crystallize in the α-Al_2O_3 (El Fadli *et al.*, 1994) and Sc_2S_3 types (Dismukes & White, 1965; Flahaut *et al.*, 1965).

In the system Sc–Te, several binaries have been synthesized and their crystal structures characterized, *viz.* ScTe, $Sc_{2/3}Te$ (Men'kov *et al.*, 1961), Sc_2Te_3, $Sc_{2.3}Te_3$ (White & Dismukes, 1965), Sc_2Te (Maggard & Corbett, 1997), Sc_9Te_2 (Maggard & Corbett, 2000) and Sc_8Te_3 (Maggard & Corbett, 1998). The first modification of Sc_2Te_3 was reported, on the basis of X-ray powder diffraction data (Men'kov *et al.*, 1959), to exhibit the γ-Al_2O_3 structure type. The second, rhombohedral modification was found by reacting the mixture of elements at the same reaction temperature (1325 K) but using chemical transport reactions. This modification was described as comprising alternating regions of NaCl and NiAs structure types (White & Dismukes, 1965).

Our single-crystal structure study on Sc_2Te_3 shows a third modification, which adopts the Sc_2S_3 type (Dismukes & White, 1964). This seems to be the low-temperature form, as we have routinely observed it at reaction temperatures below 1100 K, regardless of whether nickel was present in the reaction mixture or not. This structure is a distorted deficient variant of the NaCl type, forming a 12-fold supercell ($a = 2^{1/2}a$, $b = 2b$, $c = 3 \times 2^{1/2}c$). A detailed description of the Sc_2S_3 type and its relation to NaCl was given by Dismukes & White (1964). The distortion can be seen in, for example, the shifts of the Te atoms from the ideal position with $x = 0.375$ to $x = 0.37907$ (2) (Te1) and $x = 0.375092$ (12) (Te2). The Sc—Te bond lengths vary slightly around 2.91 Å (Table 1), and the Te—Sc—Te angles deviate up to $2°$ from the ideal octahedral angles.

Experimental

Sc_2Te_3 was obtained from a reaction of elemental scandium, nickel and tellurium in the ratio 1:4:7. The mixture was heated at 1073 K

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over a period of 3 d, annealed at 923 K for 5 d, and then cooled slowly (5 K h^{-1}) to room temperature. The X-ray powder diagram obtained from the ground sample (utilizing the INEL powder diffractometer with position-sensitive detector) revealed the presence of Sc_2Te_3, NiTe and $NiTe_2$. Sc_2Te_3 crystallized in the form of black block-shaped crystals.

Crystal data

Sc_2Te_3	Mo $K\alpha$ radiation
$M_r = 472.72$	Cell parameters from 4570
Orthorhombic, $Fddd$	reflections
$a = 8.2223\ (6)$ Å	$\theta = 3.2–30.0°$
$b = 11.6292\ (9)$ Å	$\mu = 16.73$ mm^{-1}
$c = 24.6085\ (18)$ Å	$T = 298\ (2)$ K
$V = 2353.0\ (3)$ Å^3	Block, black
$Z = 16$	$0.02 \times 0.02 \times 0.01$ mm
$D_x = 5.338$ Mg m^{-3}	

Data collection

Bruker SMART APEX CCD diffractometer	858 independent reflections
	672 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.030$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 30.0°$
	$h = -11 \rightarrow 11$
$T_{min} = 0.70$, $T_{max} = 0.90$	$k = -16 \rightarrow 16$
4570 measured reflections	$l = -34 \rightarrow 33$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.031$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.089$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.41$	$\Delta\rho_{max} = 1.27$ e Å^{-3}
858 reflections	$\Delta\rho_{min} = -2.84$ e Å^{-3}
26 parameters	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.00165 (5)

Table 1
Selected bond distances (Å).

Sc1—Te1	2.9047 (4)	Sc2—Te2^{iii}	2.8960 (4)
Sc1—Te2^i	2.9091 (2)	Sc2—Te1^i	2.9075 (2)
Sc1—Te2^{ii}	2.9275 (4)	Sc2—Te2	2.9084 (4)

Symmetry codes: (i) $-x+\frac{1}{2}, -y, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{4}, -y+\frac{1}{4}, z-\frac{1}{2}$; (iii) $-x+\frac{3}{4}, y, -z+\frac{3}{4}$.

The highest peak is located 0.06 Å from Sc1 and the deepest hole 0.66 Å from Te1.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; method used to solve structure: coordinates taken from the isotypic Sc_2S_3 compound (Dismukes & White, 1964); program(s) used to refine structure: *SHELXL97*
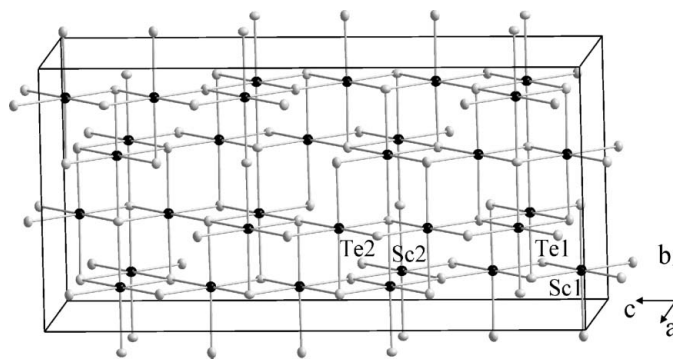

Figure 1
The crystal structure of Sc_2Te_3, with anisotropic displacement ellipsoids drawn at the 90% probability level.

(Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff, 1999); software used to prepare material for publication: *SHELXL97*.

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