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Dineodymium tritelluride, Nd_2Te_3

Ismail Ijjaali and James A. Ibers*

Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3113, USA
Correspondence e-mail: ibers@chem.northwestern.edu

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From a single-crystal study, Nd_2Te_3 is found to be isostructural with Gd_2Te_3, crystallizing in the U_2S_3 structure type. Each of the two non-equivalent Nd atoms is surrounded by seven Te atoms, with the polyhedra best described as a seven-octahedron and a monocapped trigonal prism. All atoms lie on mirror planes.

Comment

Although the structures of NdTe (Iandelli, 1955), $NdTe_{1.8}$ (Wang *et al.*, 1966), $NdTe_2$ (Yarembash *et al.*, 1965), Nd_2Te_5 (Pardo & Flahaut, 1967) and $NdTe_3$ (Norling & Steinfink, 1966) are known from single-crystal studies, it is surprising that the work presented here is the first single-crystal study of Nd_2Te_3. In fact, in the Ln_2Te_3 family (Ln is a rare earth element), there are only two other single-crystal studies, namely Gd_2Te_3 (Swinnea *et al.*, 1987), with the U_2S_3 structure type (Zachariasen, 1949), and Er_2Te_3 (Stöwe, 1998), with the Sc_2S_3 structure type (Dismukes & White, 1964). In the latter structure, the two independent Er atoms are octahedrally coordinated, sharing edges in the three directions of the orthorhombic structure.

Nd_2Te_3 crystallizes in the U_2S_3 structure type. In this structure (Fig. 1), there are two non-equivalent Nd atoms, each located at a site with *m* symmetry. Atom Nd1 is coordinated by seven Te atoms in a seven-octahedron, with Nd—Te distances in the range 3.1496 (4)–3.2287 (5) Å. These octahedra are interconnected along the *b* axis by the edge-sharing of two equatorial Te atoms (Te1 and Te3).

Atom Nd2 is coordinated by seven Te atoms in a monocapped trigonal prism, with Nd—Te distances in the range 3.2099 (4)–3.2732 (5) Å. There is a second capping Te2 atom at a distance of 3.6768 (5) Å, which is too long for the first coordination sphere. The height of the prism corresponds to the length of the *b* axis.

The $Nd2Te_7$ trigonal prisms share triangular faces along the *b* axis. For comparison, the Nd—Te distances are in the range 3.1247 (5)–3.2980 (5) Å in $NdCu_{0.37}Te_2$ (Huang *et al.*, 2000). In Gd_2Te_3 (Swinnea *et al.*, 1987), the Gd—Te distances are in the range 3.104 (1)–3.205 (3) Å for Gd1 and 3.169 (2)–3.240 (3) Å for Gd2.

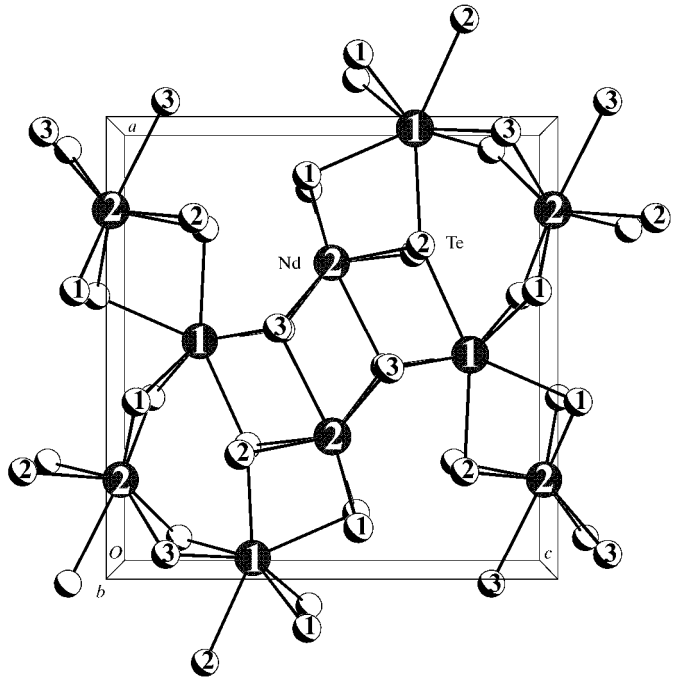

Figure 1
A view of the structure of Nd_2Te_3 along [010].

Experimental

Flat black needles of Nd_2Te_3 were obtained accidentally, in about 10% yield, from the reaction of Nd (0.0696 g; Alfa, 99.9%), Mn (0.0265 g; Alfa, 99.9%) and Te (0.1539 g; Aldrich, 99.8%) in a fused-silica tube, with KBr (200 mg; Alfa, 99%) added to promote crystal growth. The materials were mixed and sealed in the tube, which was then evacuated to 10^{-4} Torr (1 Torr = 133.322 Pa). The tube was heated to 1153 K at a rate of 0.3 K min^{-1}, kept at 1153 K for 4 d and then cooled to 873 K at a rate of 0.04 K min^{-1}; the furnace was then turned off. The reaction mixture was washed free of bromide salts with water, and then dried with acetone. Semi-quantitative energy dispersive spectroscopy (EDS) verified the presence of Nd and Te in the ratio 2:3 but provided no evidence for the presence of Mn or K.

Crystal data

Nd_2Te_3
M_r = 671.28
Orthorhombic, *Pnma*
a = 12.1856 (5) Å
b = 4.3869 (2) Å
c = 11.8687 (5) Å
V = 634.47 (5) $Å^3$
Z = 4
D_x = 7.028 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5792 reflections
θ = 2.4–29.0°
μ = 29.56 mm^{-1}
T = 153 (2) K
Flat needle, black
0.19 × 0.04 × 0.02 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
0.3° ω scans
Absorption correction: numerical (*XPREP* in *SHELXTL*; Sheldrick, 2000)
T_{min} = 0.118, T_{max} = 0.588
7307 measured reflections
904 independent reflections
886 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 29°
$h = -16 \rightarrow 16$
$k = -5 \rightarrow 5$
$l = -15 \rightarrow 15$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.046$
$S = 1.41$
904 reflections
32 parameters
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.47$ e Å^{-3}
$\Delta\rho_{min} = -2.38$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2000)
Extinction coefficient: 0.0095 (3)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* in *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1384). Services for accessing these data are described at the back of the journal.

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