

Nickel vanadium tellurium oxide,
 $\text{NiV}_2\text{Te}_2\text{O}_{10}$

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Single crystals of nickel(II) divanadium(V) ditellurium(IV) decaoxide, $\text{NiV}_2\text{Te}_2\text{O}_{10}$, were synthesized *via* a transport reaction in sealed evacuated silica tubes. The compound crystallizes in the triclinic system (space group $P\bar{1}$). The Ni atoms are positioned in the $1c$ position on the inversion centre, while the V and Te atoms are in general positions $2i$. The crystal structure is layered, the building units within a (010) layer being distorted VO_6 octahedra and NiO_6 octahedra. The metal–oxide layers are connected by distorted TeO_4E square pyramids (E being the $5s^2$ lone electron pair of Te^{IV}) to form the framework. The structure contains corner-sharing NiO_6 octahedra, corner- and edge-sharing TeO_4E square pyramids, and corner- and edge-sharing VO_6 octahedra. $\text{NiV}_2\text{Te}_2\text{O}_{10}$ is the first oxide containing all of the cations Ni^{II} , V^{V} and Te^{IV} .

Comment

The crystal chemistry of transition metal tellurates has proved to be rich, and a number of compounds with various crystal structures have previously been described, for example, NiTe_2O_5 (Platte & Trömel, 1981), $\text{Ni}_2\text{Te}_3\text{O}_8$ (Feger *et al.*, 1999), $\text{V}_4\text{Te}_4\text{O}_{18}$ (Xiao *et al.*, 2003) and MnV_2TeO_7 (Feger & Kolis, 1998). The latter is a good example of a framework compound where the stereochemically active lone pairs on Te^{IV} are located in voids in the structure.

The synthesis and crystal structure of the new compound $\text{NiV}_2\text{Te}_2\text{O}_{10}$ is a result of an ongoing investigation of oxide and oxohalide compounds containing transition metal cations as well as p -element cations with stereochemically active lone electron pairs, such as Te^{IV} , Se^{IV} , Sb^{III} and Bi^{III} . The present compound is to the best of our knowledge the first oxide to contain all three of the cations Ni^{II} , V^{V} and Te^{IV} . The stereochemically active lone electron pairs occupy space similar to that taken by an oxygen ion in the crystal structure. This means that the lone electron pairs open up the crystal structure, very often leading to a low-dimensional arrangement of the transition metal cations in such compounds.

$\text{NiV}_2\text{Te}_2\text{O}_{10}$ crystallizes in the centrosymmetric triclinic space group $P\bar{1}$. The V^{V} atoms are surrounded by six O atoms,

forming a very distorted octahedron with one $\text{V1}=\text{O4}$ vanadyl double bond of 1.643 (4) Å and one long $\text{V1}-\text{O5}^{\text{vii}}$ bond [symmetry code: (vii) $-x, -y + 1, -z + 1$] of 2.332 (4) Å (Fig. 1). As a consequence, the V atom is located above the equatorial plane of the octahedron. Bond valence sum analysis (Brown & Altermatt, 1985) confirms this choice, with the calculated valence (V^{V} , the bond valence parameter $R_o = 1.803$) equal to 5.04. The VO_6 octahedra are connected *via* $\text{O5}\cdots\text{O5}^{\text{vii}}$ and $\text{O1}\cdots\text{O1}^{\text{vi}}$ edge sharing [symmetry code: (vi) $-x + 1, -y + 1, -z + 1$] to form chains along [100]. The Ni^{II} ions are in a regular octahedral environment. The centrosymmetric NiO_6 octahedra are not connected to one another but bridge the chains by corner sharing to four different distorted VO_6 octahedra to form metal–oxide layers parallel to (010) (Fig. 2). The Te^{IV} ion has one-sided TeO_4 coordination owing to the presence of the $5s^2$ stereochemically active lone

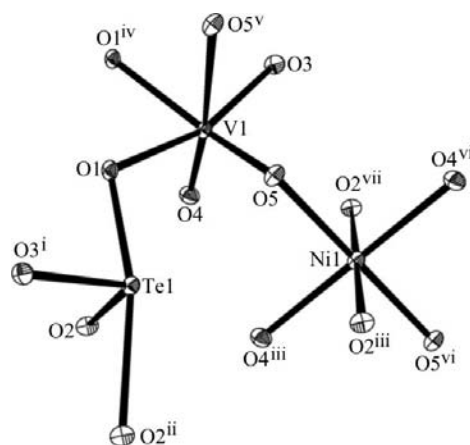


Figure 1

A displacement ellipsoid diagram showing the coordination around the three cations. Atomic displacement parameters are given at the 50% probability level. [Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 2, -z$; (iii) $x - 1, y, z$; (iv) $-x + 1, -y + 1, -z + 1$; (v) $-x, -y + 1, -z + 1$; (vi) $-x, -y + 1, -z$; (vii) $-x + 1, -y + 1, -z$.]

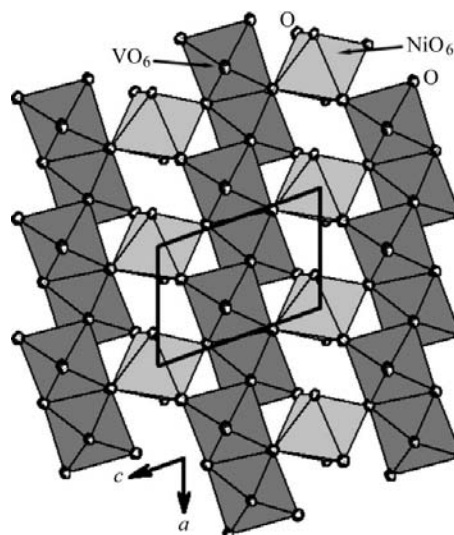


Figure 2

A metal–oxide slab $[\text{NiV}_2\text{O}_{10}]^{8-}$ parallel to (010). Atomic displacement parameters are given at the 50% probability level.

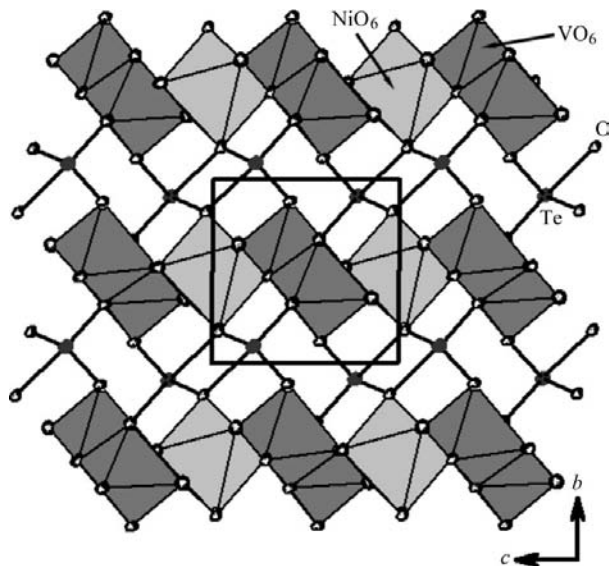


Figure 3
A view of the structure of $\text{NiV}_2\text{Te}_2\text{O}_{10}$ along [100].

pair, E , and two such units share edges to form Te_2O_6E_2 units, where the $\text{Te}^{\text{IV}}\cdots\text{Te}^{\text{IV}}$ distance [symmetry code: (ii) $-x + 1, -y + 2, -z$] is 3.312 (6) Å. The crystal structure can be described as being layered, and the Te_2O_6E_2 groups connect the metal–oxide layers by corner sharing (Fig. 3). The stereochemically active Te^{IV} lone pairs are located in voids in the structure.

Experimental

Single crystals of $\text{NiV}_2\text{Te}_2\text{O}_{10}$ are nonhygroscopic and were synthesized *via* chemical vapour transport reactions in sealed evacuated silica tubes. The starting materials were NiO (Alfa Aesar, 99%), NiCl_2 (Sigma–Aldrich, 98%), V_2O_5 (ABCR, 99.9%) and TeO_2 (Sigma–Aldrich, >99%) mixed in a 1:1:1:2 molar ratio. The starting mixture was loaded at one end of a silica tube, which was subsequently evacuated, sealed and heat treated in a muffle furnace at 793 K for 72 h. The synthesized products were a mixture of red–brown $\text{NiV}_2\text{Te}_2\text{O}_{10}$ single crystals and a yellow–brown powder of undetermined composition. The crystals used for analysis were selected manually on the basis of colour and morphology. Attempts to synthesize the compound from a stoichiometric mixture were unsuccessful.

Crystal data

$\text{NiV}_2\text{Te}_2\text{O}_{10}$	$\gamma = 72.011 (4)^\circ$
$M_r = 575.79$	$V = 178.76 (2) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 1$
$a = 4.7961 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 6.3747 (3) \text{ \AA}$	$\mu = 13.21 \text{ mm}^{-1}$
$c = 6.5643 (5) \text{ \AA}$	$T = 293 \text{ K}$
$\alpha = 84.651 (2)^\circ$	$0.07 \times 0.06 \times 0.05 \text{ mm}$
$\beta = 69.490 (3)^\circ$	

Data collection

Oxford Xcalibur3 diffractometer
Absorption correction: analytical
(*CrysAlis RED*; Oxford Diffraction, 2007), based on expressions derived by Clark & Reid (1995)
 $T_{\text{min}} = 0.413, T_{\text{max}} = 0.599$

6322 measured reflections
723 independent reflections
713 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.071$
 $S = 1.00$
723 reflections

71 parameters
 $\Delta\rho_{\text{max}} = 1.40 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.43 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

Te1–O3 ⁱ	1.887 (4)	V1–O4	1.643 (4)
Te1–O2	1.895 (4)	V1–O5	1.719 (4)
Te1–O1	1.974 (3)	V1–O3	1.867 (3)
Te1–O2 ⁱⁱ	2.291 (3)	V1–O1	1.990 (3)
Ni1–O5	2.030 (3)	V1–O1 ^{iv}	2.013 (4)
Ni1–O4 ^{iv}	2.068 (4)	V1–O5 ^v	2.332 (4)
Ni1–O2 ⁱⁱⁱ	2.111 (3)		

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 2, -z$; (iii) $x - 1, y, z$; (iv) $-x + 1, -y + 1, -z + 1$; (v) $-x, -y + 1, -z + 1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: LG3009). Services for accessing these data are described at the back of the journal.

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