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Barium divanadium(V) tellurite(IV)

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A new three-dimensional bimetallic tellurite, BaV_2TeO_8, was synthesized by the hydrothermal reaction of $Ba(OH)_2$, TeO_2 and V_2O_5, and characterized by single-crystal X-ray diffraction. The three-dimensional framework is built up from anionic $[V_2TeO_8]_n^{2n-}$ layers parallel to (101) and connected *via* Ba—O bonds. The anionic layers are formed by three types of polyhedra, namely VO_5 tetragonal pyramids, VO_4 tetrahedra and TeO_{4+2} 'folded square' polyhedra.

Comment

Both vanadium and tellurium exhibit a variety of coordination geometries, such as the VO_4 tetrahedron, the VO_6 octahedron, the VO_5 square pyramid, the TeO_3 trigonal pyramid, the TeO_4 folded square and the TeO_5 square pyramid, which lead to the rich structural chemistry of vanadium tellurites. A series of compounds have been obtained, such as $Te_2V_2O_9$ (Darriet & Galy, 1973), $TeVO_4$ (Meunier *et al.*, 1972), $TeVO_4$ (Meunier *et al.*, 1973), $NaVTeO_5$ (Darriet *et al.*, 1972), $KVTeO_5$ (Darriet *et al.*, 1972), $Cs(VO_2)_3(TeO_3)_2$ (Harrison & Buttery, 2000), $M(phen)V_2TeO_8$ (M = Cu and Ni, and phen = phenanthroline; Xiao, Li *et al.*, 2003) and $V_4Te_4O_{18}$ (Xiao, Wang *et al.*, 2003). Thus, the preparation of novel vanadium tellurites continues to be an intriguing endeavor.

Recently, the hydrothermal method has found increased application in the syntheses of a variety of inorganic oxide materials, such as metal phosphates (Soghomonian *et al.*, 1995), phosphonates (Bonavia *et al.*, 1996) and selenites (Vaughey *et al.*, 1994). The metastable materials thus prepared possess novel low-dimensional or three-dimensional framework structures. We have attempted to introduce the hydrothermal method into the synthesis of vanadium tellurites, in order to obtain compounds with novel structures. In this paper, we report the crystal structure of the new vanadium tellurite BaV_2TeO_8.

There are two crystallographically independent V atoms, one Te atom and one Ba atom in this structure (Fig. 1). Atom V1 exhibits a distorted tetrahedral coordination geometry, with two terminal O atoms (O1 and O2), and two μ_2-O atoms (O3 and O4) linked to Te atoms. The V1—O bond lengths are in the range 1.651 (3)–1.833 (3) Å, and the O—V1—O angles range from 107.46 (14) to 111.51 (14)°. Atom V2 has square-pyramidal coordination, with two terminal O atoms (O5 and O6), one μ_2-O atom (O8) shared with Te, and two μ_3-O atoms [O7 and O7^{vi}; symmetry codes: (vi) $-x - 1$, $-y + 1$, $-z + 1$] linked with Te and V2^{vi}. The V2—O bond lengths are in the range 1.645 (3)–1.990 (3) Å, and the O—V2—O angles range from 77.55 (11) to 143.55 (15)°. The Te atom has a folded square coordination geometry, with three μ_2-O atoms (O3, O4 and O8), two of which are shared with V1 atoms and the third bridging atoms Te and V2, and one μ_3-O atom (O7) shared with V2 and V2^{vi}. This geometry can be rationalized simply in valence-shell electron-pair repulsion (VSEPR) theory as an AX_4E trigonal bipyramid, with the lone pair of electrons occupying an equatorial position. The Te—O bond lengths range from 1.891 (3) to 2.125 (3) Å, and the two axial bonds are longer than the two equatorial bonds. The O—Te—O angles are in the range 73.77 (11)–152.78 (11)°. Moreover,

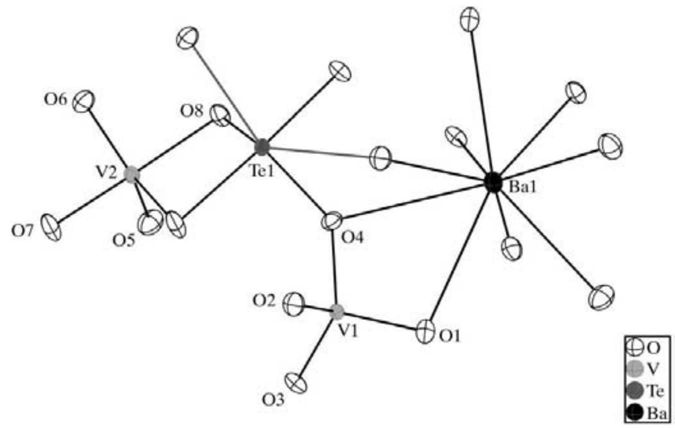

Figure 1
The coordination environments of the V, Te and Ba atoms, showing the atom-labeling scheme and 50% probability displacement ellipsoids.

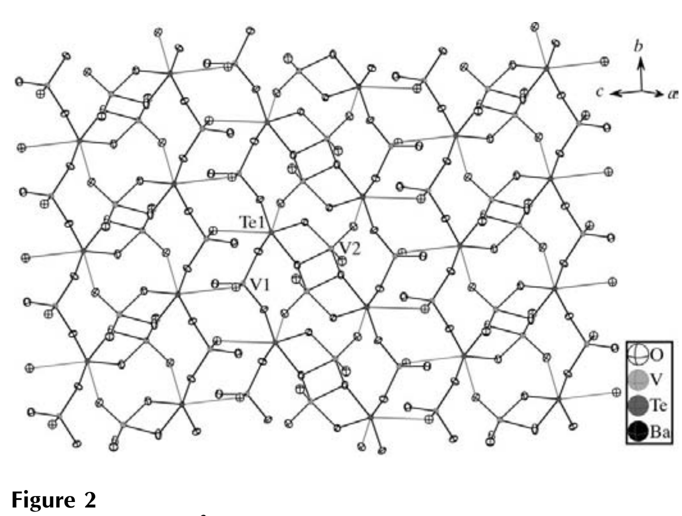

Figure 2
Infinite $[V1V2TeO_8]_n^{2n-}$ layers parallel to (101). The light lines represent weak Te—O interactions.

there are two long Te—O contacts, namely Te—O2[ii] [2.942 (3) Å] and Te—O6[vii] [2.644 (3) Å] (Table 1). The overall shape of this TeO_{4+2} group approximates to a distorted octahedron. The Ba atom adopts a nine-coordination mode.

The title compound exhibits a three-dimensional framework. The framework contains two-dimensional $[V1V2TeO_8]_n^{2n-}$ folded anionic layers (Fig. 2) formed by VO_5 square pyramids, VO_4 tetrahedra and TeO_4 polyhedra, which share corners and edges, with Ba atoms located between the layers. The TeO_4 polyhedra and VO_4 tetrahedra share corners to form an infinite $[V1TeO_6]_n$ chain parallel to the *b* axis. Two $V2O_5$ square pyramids share an edge to form a $V2_2O_8$ moiety. The $V2_2O_8$ moieties connect two $[V1TeO_6]_n$ chains into a complex $[V1V2TeO_8]_n^{2n-}$ band by sharing an edge with neighboring TeO_4 groups. Taking the weak Te—O interaction into account, neighboring $[V1V2TeO_8]_n^{2n-}$ infinite bands combine with each other to form $[V1V2TeO_8]_n^{2n-}$ infinite layers parallel to (101). Successive layers are linked by Ba—O interactions into a three-dimensional framework.

Experimental

A mixture of V_2O_5 (0.0455 g), TeO_2 (0.795 g), $Ba(OH)_2{\cdot}8H_2O$ (0.0947 g) and H_2O (5 ml) was sealed in a 23 ml Teflon-lined stainless steel autoclave. The Ba/V/Te/H_2O molar ratio was 3:5:5:278. The mixture was heated at 473 K for five days and then cooled to room temperature. Bright-yellow block-shaped crystals of the title compound were obtained, washed with distilled water and dried at room temperature.

Crystal data

BaV_2TeO_8	D_x = 4.548 Mg m^{-3}
M_r = 494.82	Mo *Kα* radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
a = 9.6380 (8) Å	*θ* = 12–18°
b = 5.6665 (3) Å	*μ* = 11.88 mm^{-1}
c = 13.8866 (11) Å	*T* = 293 (2) K
β = 107.642 (4)°	Block, yellow
V = 722.73 (9) Å^3	0.30 × 0.15 × 0.05 mm
Z = 4	

Data collection

Rigaku Weissenberg IP diffractometer	1663 independent reflections
φ scans	1538 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)	R_{int} = 0.033
T_{min} = 0.13, T_{max} = 0.55	θ_{max} = 27.5°
1663 measured reflections	$h = 0 \rightarrow 12$
	$k = 0 \rightarrow 7$
	$l = -18 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 1.1787P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.017	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.056	$\Delta\rho_{max}$ = 0.79 e Å^{-3}
S = 1.23	$\Delta\rho_{min}$ = −1.00 e Å^{-3}
1663 reflections	Extinction correction: *SHELXL97*
110 parameters	Extinction coefficient: 0.0112 (3)

Table 1
Selected interatomic distances (Å).

Ba1—O8[i]	2.701 (3)	Te1—O7[vi]	2.125 (3)
Ba1—O2[ii]	2.791 (3)	Te1—O6[vii]	2.644 (3)
Ba1—O6[iii]	2.802 (3)	Te1—O2[ii]	2.942 (3)
Ba1—O5[iv]	2.838 (3)	V1—O1	1.651 (3)
Ba1—O5[iii]	2.900 (3)	V1—O2	1.651 (3)
Ba1—O3[iv]	2.914 (3)	V1—O3	1.785 (3)
Ba1—O1	2.954 (3)	V1—O4	1.833 (3)
Ba1—O1[v]	3.014 (3)	V2—O5	1.645 (3)
Ba1—O4	3.090 (3)	V2—O6	1.652 (3)
Te1—O8	1.891 (3)	V2—O7	1.894 (3)
Te1—O4	1.943 (3)	V2—O8	1.956 (3)
Te1—O3[v]	2.017 (3)	V2—O7[vi]	1.990 (3)

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x, -y+1, -z+1$; (v) $x, y-1, z$; (vi) $-x-1, -y+1, -z+1$; (vii) $-x-1, -y, -z+1$.

Space group $P2_1/n$ was established from the systematic absences.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97-2* (Sheldrick, 1997).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FA1130). Services for accessing these data are described at the back of the journal.

References

Bonavia, G., Haushalter, R. C., O'Connor, C. J. & Zubieta, J. (1996). *Inorg. Chem.* **35**, 5603–5612.
Darriet, J. & Galy, J. (1973). *Cryst. Struct. Commun.* **2**, 237–238.
Darriet, J., Guillaume, G., Wilhelmi, K. A. & Galy, J. (1972). *Acta Chem. Scand.* **26**, 59–70.
Harrison, W. T. A. & Buttery, J. H. N. (2000). *Z. Anorg. Allg. Chem.* **626**, 867–870.
McArdle, P. (1995). *J. Appl. Cryst.* **28**, 65.
Meunier, G., Darriet, J. & Galy, J. (1972). *J. Solid State Chem.* **5**, 314–320.
Meunier, G., Darriet, J. & Galy, J. (1973). *J. Solid State Chem.* **6**, 67–74.
Molecular Structure Corporation (1999). *TEXSAN* (Version 1.10) and *TEXRAY*. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXL97*, *SHELXS97* and *SHELXL97-2*. University of Göttingen, Germany.
Soghomonian, V., Chen, Q., Zhang, Y., Haushalter, R. C., O'Connor, C. J., Tao, C. & Zubieta, J. (1995). *Inorg. Chem.* **34**, 3509–3519.
Vaughey, J. T., Harrison, W. T. A., Dussack, L. L. & Jacobson, A. J. (1994). *Inorg. Chem.* **33**, 4370–4375.
Xiao, D. R., Li, Y. G., Wang, E. B., Wang, S. T., Hou, Y., De, G. J. H. & Hu, C. W. (2003). *Inorg. Chem.* **42**, 7652–7657.
Xiao, D. R., Wang, S. T., Wang, E. B., Hou, Y., Li, Y. G., Hu, C. W. & Xu, L. (2003). *J. Solid State Chem.* **176**, 159–164.