

The crystal structure of namibite, $\text{Cu}(\text{BiO})_2\text{VO}_4(\text{OH})$, and revision of its symmetry

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ABSTRACT

The crystal structure of namibite, $\text{Cu}(\text{BiO})_2\text{VO}_4(\text{OH})$ [triclinic, space group $P\bar{1}$, $a = 6.210(1)$, $b = 7.398(1)$, $c = 7.471(1)$ Å, $\alpha = 90.10(1)$, $\beta = 108.73(1)$, $\gamma = 107.47(1)^\circ$, $V = 308.22(8)$ Å³, $Z = 2$] was determined using single-crystal X-ray diffraction data. The refinement, based on 2140 unique reflections with $F_o > 4\sigma(F_o)$, gave $R1 = 3.61\%$. The structure determination showed namibite to be triclinic-pseudomonoclinic; the previously reported C -centered monoclinic cell is a pseudocell. The structure contains two unique Bi atoms, with nine Bi-O bonds between 2.17 and 3.39 Å. The Bi coordinations show some stereochemical influence of the lone pair of electrons on Bi^{3+} . A three-dimensional network is formed by linkages of Bi-O polyhedra to one slightly distorted V^{5+}O_4 tetrahedron that decorates chains of corner-sharing CuO_6 polyhedra extending parallel to the b axis. The CuO_6 polyhedra show the Jahn-Teller-distorted [4+2]-coordination of Cu^{2+} . Layers of Bi atoms parallel to (100) alternate with layers of parallel heteropolyhedral $[\text{Cu}(\text{VO}_4)\text{O}_2(\text{OH})]$ chains. According to bond-valence calculations and geometrical considerations, the H atom of the OH group is probably involved in disordered or trifurcated H bonding. The structure of namibite represents a slightly distorted ordered variant of the monoclinic structure of brendelite, $(\text{Bi,Pb})_2(\text{Fe}^{3+},\text{Fe}^{2+})\text{O}_2(\text{OH})(\text{PO}_4)$. Further relations to synthetic $\text{Cu}_3\text{Bi}_4\text{V}_2\text{O}_{14}$, to the 7 Å chain-structure phosphates and sulfates, and to linarite are outlined.

INTRODUCTION

Namibite is a rare dark-green Cu-Bi-V-mineral originally described from Namibia (von Knorring and Sahama 1981). Recently, it has been found at an increasing number of localities (see overview by Dunning and Cooper 1998). Originally assumed to be an oxide with the formula CuBi_2VO_6 , namibite was redefined by Mrázek et al. (1994) as a vanadate with the formula $\text{Cu}^{2+}(\text{BiO})_2\text{V}^{5+}\text{O}_4(\text{OH})$, based on a new wet chemical analysis, IR spectroscopical and thermoanalytical data, and a hydrothermal preparation of synthetic namibite. The suggested presence of vanadate is also corroborated by the fact that namibite forms as a secondary mineral under oxidizing conditions, with commonly associated minerals including secondary Bi carbonates, Bi vanadates and Cu minerals. Both von Knorring and Sahama (1981) and Mrázek et al. (1994) report that crystals of namibite are monoclinic (C -/, probably $C2/m$), on the basis of precession photographs obtained by the first authors. A platy {100} habit and cleavage parallel to (100) were reported by von Knorring and Sahama (1981), but Mrázek et al. (1994) inferred that the cleavage is parallel to (001), based on an X-ray powder pattern strongly affected by preferred orientation of the cleavage fragments. According to von Knorring and Sahama (1981), type namibite shows common interpenetration twinning on (011), often in a polysynthetic manner. An IR absorption spectrum of namibite did not indicate "any notable H_2O or OH" (von Knorring and Sahama 1981), whereas Mrázek et al. (1994) report clear evidence for a hydroxyl group, based on their IR investigations and chemical analyses of both natural and synthetic material. To clarify these inconsistencies,

we determined the atomic arrangement of namibite and report the results here.

CRYSTAL STRUCTURE DETERMINATION AND REFINEMENT

Namibite crystals were taken from a small specimen from the Iron Monarch deposit, South Australia (Pring et al. 1992, 2000). The platy crystals are black-green, translucent, and occur in intimate association with finely crystalline beyerite. Energy-dispersive spectroscopic chemical analyses of the namibite showed that the crystals are of ideal composition within detection limits. Preliminary investigations of selected crystal fragments were done with a Nonius KappaCCD diffractometer equipped with a 300 mm diameter capillary-optics collimator to provide increased resolution. They showed that subparallel intergrowth is common. Optically, no twinning features were recognizable. Tiny grains of high crystal quality clearly showed a triclinic cell, $a = 6.210(1)$ $b = 7.398(1)$, $c = 7.471(1)$ Å, $\alpha = 90.10(1)$, $\beta = 108.73(1)$, $\gamma = 107.47(1)^\circ$, $V = 308.22(8)$ Å³, that has pseudo-monoclinic symmetry, with a C -centered pseudocell $a \sim 10.51$, $b \sim 10.52$, $c \sim 6.21$ Å, $\alpha \sim 91.0$, $\beta \sim 116.1$, $\gamma \sim 89.4^\circ$, $V \sim 616.5$ Å³, the transformation matrix being (011,0 $\bar{1}$ 1,100). Frames obtained from poor-quality fragments resulted in large errors and did not allow distinction between the triclinic and the pseudomonoclinic cells. The previously reported, smaller monoclinic C -centered cell, $a \approx 11.87$, $b \approx 3.70$, $c \approx 7.49$ Å, $\beta \approx 109.7^\circ$, $V \approx 310$ Å³ (von Knorring and Sahama 1981; Mrázek et al. 1994) is a monoclinic pseudocell that shows interesting relations to the true triclinic cell (see discussion below).

A tiny, irregular, somewhat platy fragment with approximate dimensions $0.05 \times 0.03 \times 0.02$ mm³ was selected for the

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intensity-data collection (experimental details are listed in Table 1). A full sphere was measured. The recorded intensity data were processed with the Nonius program suite DENZO-SMN and corrected for Lorentz, polarization, and background effects. No superstructure reflections were seen on the recorded frames. Because of the very small size of the fragment and its irregular shape, no absorption correction was applied. Merging of the reflections showed the internal agreement factor R_{int} to be 2.3%, whereas for the (presently determined) pseudomonoclinic cell, R_{int} was 35%, again providing evidence for the distinct deviation from monoclinic symmetry. Normalized structure factor statistics indicated the centrosymmetric space group $P\bar{1}$. However, the structure could only be solved by Patterson methods (SHELXS-97, Sheldrick 1997a) in $P1$, and the center of symmetry was then located using the program ADDSYM within the PLATON98 suite of programs (Spek 1998). The revised formula of Mrázek et al. (1994) was confirmed. The refinement, using SHELXL-97 (Sheldrick 1997b), proceeded smoothly and converged to the final parameters in Table 1. As expected, it was impossible to locate the H atom. The maximum peaks in the final difference-Fourier maps were -3.9 and $5.8 \text{ e}/\text{\AA}^3$, and the most positive peaks were all close to the Bi atoms. The final positional and displacement parameters are given in Table 2, selected bond lengths in Table 3, and a bond-valence analysis is presented in Table 4. A list of observed and calculated structure factors has been deposited (Table 5).¹

¹For a copy of Table 5, document item AM-00-051, contact the Business Office of the Mineralogical Society of America for price information. Deposit items may also be available on the MSA web site (<http://www.minsocam.org>).

TABLE 1. Crystal data, data-collection information and structure-refinement details for namibite

Formula	Cu(BiO) ₂ VO ₄ (OH)
Space group	$P\bar{1}$
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.210(1), 7.398(1), 7.471(1)
α , β , γ (°)	90.10(1), 108.73(1), 107.47(1)
<i>V</i> (Å ³)	308.22(8)
<i>Z</i>	2
<i>F</i> (000)	550
ρ_{calc} (g/cm ³)	6.955
μ (mm ⁻¹)	61.8
Diffractometer	Nonius KappaCCD system
Temperature (K)	293
λ (MoK α) (Å)	0.71073
Detector distance (mm)	30
Rotation axes	ϕ , ω
Rotation width	2.0
Total no. of frames	504
Collect. time per frame (s)	220
$2\theta_{\text{max}}$ (°)	66.22
<i>h</i> , <i>k</i> , <i>l</i> ranges	$-9 \rightarrow 9$, $-11 \rightarrow 11$, $-11 \rightarrow 11$
Total reflections measured	4520
Unique reflections	2326
<i>R</i> 1(<i>F</i>), <i>wR</i> 2(<i>F</i> ²)*	3.61%, 8.87%
Unique reflections	2140 [$F_o > 4\sigma(F_o)$]
Extinction factor	0.0021(3)
No. of refined parameters	104
Goof	1.092
(Δ/σ) _{max}	0.0001
$\Delta\rho_{\text{min}}$, $\Delta\rho_{\text{max}}$ (e/Å ³)	-3.93 , 5.78

Note: Unit-cell parameters were refined from all recorded reflections. Scattering factors for neutral atoms were employed in the refinement.

* $w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 7.00P]$; $P = (\max \text{ of } (0 \text{ or } F_o^2)) + 2F_o^2/3$.

DESCRIPTION OF THE STRUCTURE

Cation coordination and structure connectivity

The structure contains two unique Bi atoms, one slightly distorted VO₄ tetrahedron ($\langle V-O \rangle = 1.714 \text{ \AA}$, range 1.677–1.757 Å; angles O-V-O = 105.5–114.0°), and two elongate CuO₆ octahedra. The Cu atoms exhibit the characteristic Jahn-Teller distorted [4+2]-coordination (Table 3). All Bi, V, and O atoms are on general positions, whereas Cu1 and Cu2 are on special positions with site symmetry $\bar{1}$. The Bi atoms each have nine oxygen neighbors within the range of 2.171 to 3.387 Å (Table 3). Both Bi coordinations show the influence of the lone pair of electrons on the Bi³⁺ cation, especially Bi1, which has six closer and three rather remote neighbors. The lone pairs of electrons of two adjacent Bi1 atoms seem to be located between the Bi atoms (Bi1-Bi1 distance = 3.61 Å).

The dominant structure elements are chains of corner-sharing, alternately tilted CuO₆ octahedra parallel to the *b* axis, and decorated with VO₄ tetrahedra in a staggered arrangement (Fig. 1). Bi atoms connect the chains to form a three-dimensional framework. The Bi atoms can also be considered as forming chains parallel to both the *b* axis and, in a less pronounced manner, the *a* axis. Layers of Bi atoms parallel to (100) alternate with layers of parallel heteropolyhedral [Cu(VO₄)O₂(OH)] chains (Fig. 2). The fairly good cleavage of the mineral is parallel to (001), in agreement with the observed preferred orientation in the X-ray powder-diffraction pattern (Mrázek et al. 1994).

The oxygen atom OH6, which represents the shared corner of two CuO₆ octahedra, has a bond-valence sum of 1.32 valence units (v.u.), indicating that it represents the donor of an OH group (Table 4). Based on O-O distances, the following O

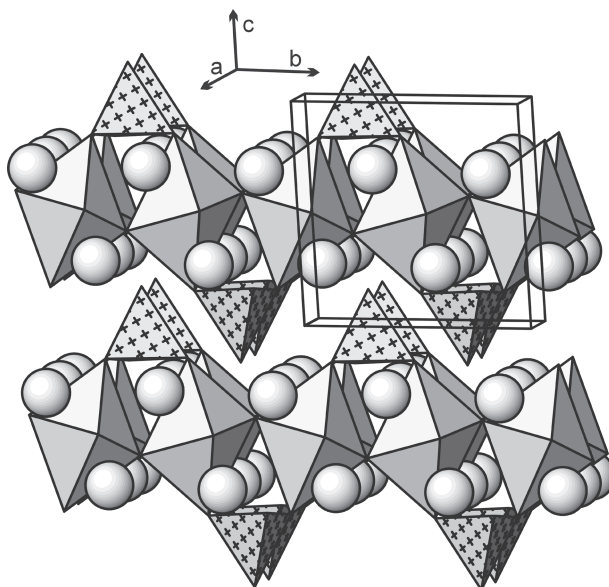
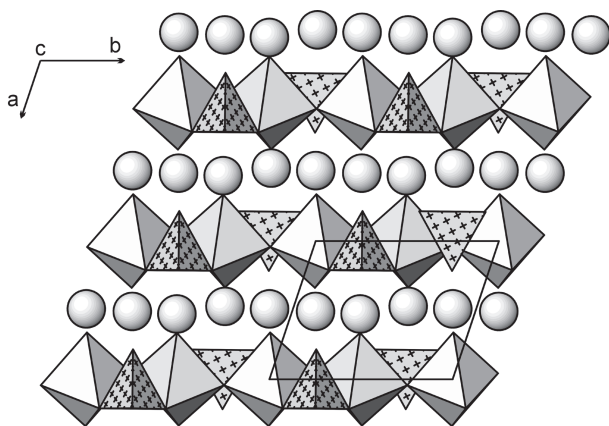


FIGURE 1. The crystal structure of namibite viewed in a direction close to the *a* axis (the unit cell is outlined). Chains of (OH6) corner-sharing CuO₆ octahedra extend parallel to the *b* axis and are decorated with VO₄ tetrahedra in a staggered arrangement. Large balls represent Bi atoms. All drawings were done with ATOMS (Shape Software 1999).

TABLE 2. Fractional atom coordinates and displacement parameters ($\times 10^4$) for namibite

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1	0.50921(5)	0.12785(4)	0.29598(4)	102.5(1.0)	122.3(1.5)	96.6(1.5)	96.9(1.4)	12.2(1.0)	48.3(1.0)	34.4(1.0)
Bi2	0.47248(5)	-0.37572(4)	0.28136(4)	108.3(1.0)	112.5(1.5)	102.6(1.5)	116.5(1.5)	2.8(1.0)	59.1(1.0)	21.6(1.0)
Cu1	0.0	0.5	0.5	83(2)	45(5)	47(5)	159(6)	-4(4)	53(5)	-4(4)
Cu2	0.0	0.0	0.5	86(2)	45(5)	61(5)	154(6)	26(5)	41(5)	12(4)
V	0.0960(2)	0.2764(2)	0.9244(2)	114(3)	103(6)	120(6)	104(6)	-5(4)	20(5)	29(5)
O1	0.2153(13)	0.4896(10)	0.8588(10)	214(13)	210(30)	180(30)	240(30)	50(30)	70(30)	40(30)
O2	0.2105(13)	0.1250(10)	0.8489(10)	204(13)	240(30)	200(30)	180(30)	-10(20)	60(30)	110(30)
O3	-0.2166(12)	0.2010(9)	0.8288(9)	150(12)	140(30)	160(30)	140(30)	20(20)	20(20)	50(20)
O4	0.2093(11)	0.3043(8)	0.1742(9)	122(11)	110(30)	100(20)	130(30)	00(20)	20(20)	20(20)
O5	0.6647(9)	0.4108(8)	0.4834(8)	85(10)	10(20)	130(20)	90(20)	-17(19)	08(18)	-01(18)
OH6	0.9568(11)	0.2369(8)	0.4109(9)	134(11)	110(30)	60(20)	230(30)	40(20)	60(20)	16(19)
O7	0.6612(10)	-0.0815(8)	0.4842(8)	87(10)	60(20)	110(20)	70(20)	28(18)	15(18)	-01(19)

atoms are candidates for being the acceptor atom of an H bond: O1, O2, O4, O5, and O7. However, both O5 and O7 are already saturated (2.23 and 2.21 v.u., respectively) and the bonds O1-OH6 and O4-OH6 represent edges of the CuO_6 octahedra. Nonetheless, all three O1, O2, and O4 atoms have low incident bond-valence sums (1.75, 1.78, and 1.88 v.u., respectively) and thus might all participate in weak H bonding, suggesting the possibility of a trifurcated bond or a somewhat disordered H position. Geometrical considerations would support this scheme, as estimated OH6-H-O angles for the three possible O acceptor atoms would be similar. The reported infrared spectrum of both natural and synthetic namibite (Mrázek et al. 1994) shows a flat absorption band at around 2900 cm^{-1} that seems to support the presence of H bonds with variable distances. The band position would correspond to an approximate OH...O distance of ca. 2.62 \AA , suggesting that the dominant H bond acceptor is O4. A disordered H position would also explain the somewhat elongate displacement ellipsoids of the two Cu atoms and their close equatorial O ligands (Table 2). (Note that isotropic refinement of the O atoms did not result in significant changes of the anisotropic-displacement parameters of the Cu atoms.)

**FIGURE 2.** View of the structure of namibite approximately along the *c* axis (symbols as in Fig. 1). The alternation of Bi layers with layers of parallel $[\text{Cu}(\text{VO}_4)\text{O}_2(\text{OH})]$ chains is clearly seen.**TABLE 3.** Selected interatomic distances (\AA) in namibite

Bi1-O7	2.199(6)	V-O1	1.677(7)
Bi1-O5	2.277(6)	V-O2	1.677(7)
Bi1-O7	2.302(6)	V-O3	1.746(7)
Bi1-OH6	2.496(6)	V-O4	1.757(6)
Bi1-O3	2.518(6)	<V-O>	1.714
Bi1-O4	2.525(6)		
Bi1-O2	3.255(7)		
Bi1-O1	3.263(7)	Cu1-O5	1.948(5) $\times 2$
Bi1-O2	3.295(7)	Cu1-OH6	1.967(6) $\times 2$
<Bi-O>	2.681	Cu1-O1	2.596(7) $\times 2$
		<Cu1-O>	2.170
Bi2-O5	2.171(6)		
Bi2-O3	2.296(6)	Cu2-OH6	1.938(6) $\times 2$
Bi2-O7	2.392(6)	Cu2-O7	1.970(6) $\times 2$
Bi2-O4	2.397(6)	Cu2-O2	2.537(7) $\times 2$
Bi2-O5	2.486(6)	<Cu2-O>	2.148
Bi2-O2	2.703(7)		
Bi2-O1	2.801(8)		
Bi2-O1	3.051(7)		
Bi2-OH6	3.387(6)		
<Bi-O>	2.632		

TABLE 4. Bond-valence analysis for namibite

	Bi1	Bi2	Cu1	Cu2	V	Sum*
O1	0.04	0.15	0.08 $\downarrow \times 2$	-	1.41	1.75
		0.07				
O2	0.04	0.19	-	0.10 $\downarrow \times 2$	1.41	1.78
	0.04					
O3	0.31	0.57	-	-	1.17	2.06
O4	0.31	0.44	-	-	1.13	1.88
O5	0.60	0.80	0.48 $\downarrow \times 2$	-	-	2.23
		0.34				
OH6	0.33	0.03	0.46 $\downarrow \times 2$	0.50 $\downarrow \times 2$	-	1.32
O7	0.75	0.44	-	0.46 $\downarrow \times 2$	-	2.21
	0.56					
Sum*	2.99	3.04	2.05	2.10	5.11	

Note: Bond-valence parameters used are from Brese and O'Keeffe (1991). * Sum values are derived from unrounded bond-valence contributions.

Discussion and relation to other compounds

A published SEM micrograph of sharp namibite crystals from the type locality (von Knorring and Sahama 1981) is in accordance with the triclinic symmetry found here, because no mirror plane seems to be present. A calculated X-ray powder-diffraction pattern shows good agreement with the measured powder data of Knorring and Sahama (1981). The intensities of the powder pattern given by Mrázek et al. (1994) are strongly affected by preferred orientation, as noted by them. The chemical formula is unchanged and the redefinition of the mineral as a hydroxyl-bearing vanadate by Mrázek et al. (1994) is confirmed.

The basic topology of the structure of namibite, $\text{Cu}(\text{BiO})_2\text{VO}_4(\text{OH})$, is almost the same as that in the recently described

brendelite, $(\text{Bi,Pb})_2(\text{Fe}^{3+}, \text{Fe}^{2+})\text{O}_2(\text{OH})(\text{PO}_4)$, which is monoclinic, $C2/m$, with $a = 12.278$, $b = 3.815$, $c = 6.899$ Å, $\beta = 111.14^\circ$, $V = 301.4$ Å³ (Krause et al. 1998). The crystal data of brendelite are quite close to those originally given for namibite (monoclinic, $C-1$, $a \approx 11.87$, $b \approx 3.70$, $c \approx 7.49$ Å, $\beta \approx 109.7^\circ$, $V \approx 310$ Å³; von Knorring and Sahama 1981; Mrázek et al. 1994). We found that this monoclinic cell is a pseudocell of namibite, which is based on the positions of the strongly scattering Bi and Cu atoms. The relation between the triclinic and monoclinic cells is depicted in Figure 3. In brendelite, the P atoms and two of the O atoms are disordered, thereby giving rise to the higher symmetry and the halved b axis (Krause et al. 1998). The true monoclinic pseudosymmetry of the atomic arrangement in namibite (i.e., including the positions of the O atoms) can be described by a pseudomonoclinic supercell with $a = 23.694$ (2×11.857), $b = 7.398$ (2×3.699), $c = 7.471$ Å, $\alpha = 90.10(1)$, $\beta = 109.71$, $\gamma = 90.14^\circ$. This supercell is derived from the true triclinic cell via transformation with the matrix (410,010,001). The reported plane of the common interpenetration twinning in type namibite, $(011)_{\text{mon}}$ (von Knorring and Sahama 1981), must be considered doubtful; twinning is more likely to occur parallel to one of the pseudo-mirror planes in the structure (compare Fig. 3).

The deviation of the namibite structure from monoclinic symmetry is relatively small, and the influence of possible incorporation of foreign cations (such as Pb, Ca, Zn, Fe, As, P) or disorder on the symmetry of the structure might be an interesting question. A recently identified Ca-bearing variety of namibite (Kolitsch, in preparation) unfortunately did not provide crystals suitable for structure investigation.

The atomic arrangement in namibite may be compared to that of $\text{Cu}_3\text{Bi}_4\text{V}_2\text{O}_{14}$ (Deacon et al. 1994), which is also triclinic and has a similar unit-cell volume. The red-black pleochroic

$\text{Cu}_3\text{Bi}_4\text{V}_2\text{O}_{14}$ is characterized by an infinite three-dimensional structure that contains eightfold-coordinated Bi^{3+} , fivefold- and sixfold-coordinated Cu^{2+} , and fourfold-coordinated V^{5+} cations. A layered arrangement of cations is present, but is not as pronounced as that in namibite. The $[\text{Cu}(\text{VO}_4)\text{O}_2(\text{OH})]$ chain-motif in namibite is also found as $[\text{M}(\text{TO}_4)(\text{O}, \text{OH}, \text{H}_2\text{O})_3]$ ($\text{M} = \text{metal}$, $\text{T} = \text{P}$, S) chains in a larger number of 7 Å chain-structure phosphate and sulfate minerals (Moore 1984; Hawthorne 1997, 1998). Linarite, $\text{PbCu}(\text{OH})_2(\text{SO}_4)$ (Effenberger 1987), has $[\text{Cu}(\text{SO}_4)\text{O}(\text{OH})_2]$ chains similar to the $[\text{Cu}(\text{VO}_4)\text{O}_2(\text{OH})]$ chains in namibite. However, the CuO_6 octahedra in linarite share edges whereas in namibite they share corners.

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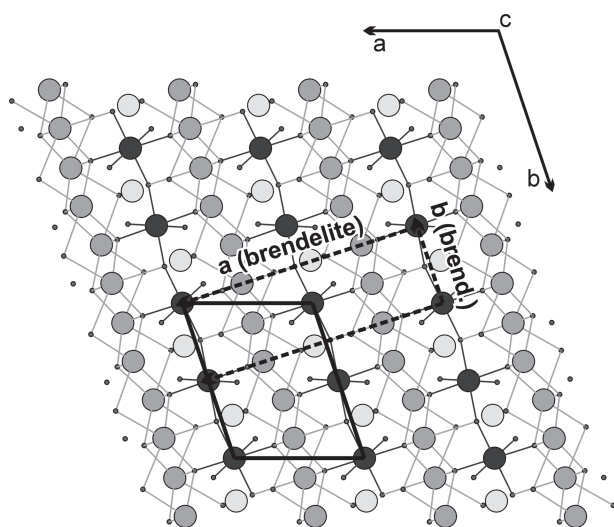


FIGURE 3. Schematic view of a 7 Å thick slice of the structure of namibite along the c axis (black balls = Cu, dark gray balls = Bi, light gray balls = V, very small balls = O). Only the strongest bonds are drawn. The relation between the true triclinic cell (bold lines) and the pseudomonoclinic cell (= monoclinic cell in brendelite; dashed lines) is indicated; see text for details.