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Schlegelite, $Bi_7O_4(MoO_4)_2(AsO_4)_3$, a new mineral from Schneeberg, Saxony, Germany

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Abstract: Schlegelite is a new bismuth molybdate arsenate from the dumps of the Pucher Richtschacht, near Schneeberg, Saxony, Germany. Associated minerals are quartz, petitjeanite, pucherite, bismuth and sillenite. Schlegelite forms dense spherical aggregates that are composed of small lath-like crystals up to 0.3 mm in length. Crystallographic forms are {010} (dominant), {001} and {100}; the elongation is parallel to [100]. The colour is yellow, the streak is pale yellow; Vickers hardness is VHN_{25} = 285 kg/mm^2, corresponding to a Mohs' hardness of 31/2; good cleavage parallel to {010} and {001}. Schlegelite is biaxial negative, 2V = 40(5)°, n_x = 2.22, n_y = 2.255 (calc.), and n_z = 2.26 (calculated from reflectance data); non-pleochroic; orientation X = *a*, Y = *b*, Z = *c*. Electron-microprobe analyses gave Bi_2O_3 70.20, PbO 0.48, CaO 0.05, P_2O_5 0.51, As_2O_5 15.38, V_2O_5 0.21, MoO_3 12.13, total 98.96 wt.-%. The empirical formula based on 24 oxygen atoms is $Bi_{6.78}Pb_{0.05}Ca_{0.02}O_{3.51}(MoO_4)_{1.90}(PO_4)_{0.16}(VO_4)_{0.05}(AsO_4)_{3.01}$, the idealized formula is $Bi_7O_4(MoO_4)_2(AsO_4)_3$. Schlegelite is orthorhombic, space group *Pnca*, with *a* = 5.299(1), *b* = 16.133(4), *c* = 23.948(5) Å, V = 2047.2(7) Å^3, *Z* = 4, D_{calc} = 7.23 g/cm^3. The crystal structure refinement converged for 2378 reflections and 166 variable parameters at R1 = 0.045. The atomic arrangement is characterized by ribbons of Bi atoms shortly linked by oxo-oxygen atoms parallel to [100]. The ribbons are connected to AsO_4 and MoO_4 tetrahedra forming layers parallel to (001). The chemical composition of schlegelite is remarkable as minerals containing both the anion groups, arsenate and molybdate, are rare; furthermore, Bi arsenates with a second anion group were found only occasionally. The mineral name is for Fritz Schlegel, a dedicated mineral collector and finder of the new species, in recognition of his contributions to the mineral assemblage of the Schneeberg area in Saxony, Germany.

Key-words: schlegelite, Schneeberg, Germany, new mineral, microprobe analysis, crystal chemistry, crystal structure.

Introduction

In the course of investigations of minerals from the Schneeberg area in Saxony, Germany, a single specimen with a few spherical aggregates was found that could not be identified by means of X-ray powder diffraction data. According to preliminary micro-chemical tests it was considered a new bismuth arsenate. Subsequent electron-microprobe analyses showed also molybdenum to be an additional major constituent. Trials to investigate single-crystals with various X-ray techniques (Weissenberg and Buerger film methods, conventional 4-circle diffractometer) failed. The small size as well as the poor crystal quality did not allow to determine unit-cell metrics or any structural features. In 1994 it was decided to postpone the description as a new mineral species until new finds of more suitable material would be available. Unfortunately, further samples of this probably very rare material have not been discovered until now. Nonetheless, a new attempt was started in 2002 by using very small crystal fragments of the original material, which could now be measured successfully by means of a four-circle X-ray diffractometer equipped with a CCD area detector, revealing not only the crystal symmetry and cell metrics but also the complete crystal structure information.

The new mineral was named schlegelite in honour of the dedicated mineral collector Fritz Schlegel (born in 1938) in recognition of his contributions to the knowledge about the mineral assemblage of the Schneeberg area in Saxony, Germany (Schlegel *et al*., 1992; Schlegel, 2000, 2002). He is not only the finder of this new mineral; he discovered also a number of other recently described new mineral species in this area, such as brendelite (Krause *et al*., 1998), cobaltlotharmeyerite (Krause *et al*., 1999), nickellotharmeyerite (Krause *et al*., 2001), schneebergite, nickelschneebergite (Krause *et al*., 2002a), neustädtelite, and cobaltneustädtelite (Krause *et al*., 2002b). Both, mineral and mineral name have been approved by the IMA Commission on New Minerals and Mineral Names (#2003-051). Type material is preserved in the collection of the

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Table 1. Physical data of schlegelite.

Morphology	2/*m* 2/*m* 2/*m*, {010}, {100}, {001}
Habit	tabular on {010}, elongated // [100]
Twinning	none observed
Lustre	adamantine
Diaphaneity	transparent to translucent
Colour	yellow
Streak	pale yellow
Fluorescence	none
Hardness	Mohs 3½, VHN_{25} = 285(20) kg/mm²
Tenacity	brittle
Cleavage	{010} good, {001} good
Fracture	uneven
Density (calc.)	7.23 g/cm³
Optical character	negative
n_x[1]	2.22
n_y (calc.)[2]	2.255
n_z[1]	2.26
2V [3]	40(5)°
Dispersion	not determined
Pleochroism	none
Orientation	X = *a*, Y = *b*, Z = *c*

[1] Calculated from reflectance data.
[2] Calculated from n_x, n_z and 2V.
[3] Calculated from extinction curves using spindle-stage measurements.

Table 2. Reflectance data[1] of schlegelite.

λ (nm)	Air R_{max}	Air R_{min}	Oil R_{max}	Oil R_{min}
400	17.82	16.93	5.10	4.70
420	17.14	16.30	4.81	4.45
440	16.76	15.69	4.59	4.36
460	16.35	15.40	4.52	4.28
470 (COM)	16.20	15.31	4.43	4.21
480	16.05	15.23	4.34	4.15
500	15.85	14.89	4.27	4.04
520	15.59	14.78	4.11	3.99
540	15.47	14.56	3.98	3.90
546 (COM)	15.41	14.53	3.96	3.86
560	15.26	14.50	3.99	3.80
580	15.12	14.35	3.84	3.64
589 (COM)	15.06	14.21	3.83	3.64
600	14.99	14.03	3.82	3.64
620	14.82	13.96	3.72	3.63
640	14.80	13.76	3.71	3.52
650 (COM)	14.76	13.74	3.68	3.51
660	14.73	13.73	3.66	3.53
680	14.54	13.51	3.52	3.43
700	14.59	13.60	3.58	3.39

[1] Standard SiC; immersion oil DIN 58.884; LEITZ ORTHOPLAN microscope, combined with a photometer similar to that described by Bernhardt (1987).

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Occurrence

Schlegelite has been discovered on a small specimen from the dumps of the Pucher Richtschacht, approximately 3.6 km south-west of the centre of Schneeberg, Saxony, Germany. The type specimen was found in 1988 and consists mainly of coarse quartz. It was approximately 20 × 40 × 50 mm in size and was broken into several pieces; one of them showed a few spherical schlegelite aggregates grown within a small vug. The dense aggregates have a maximum diameter of 1 mm and are composed of small lath-like crystals up to 0.3 mm in length. These can only be observed on fracture surfaces since the schlegelite aggregates are overgrown by a thin coating of quartz (approximately 50 µm in thickness). A few yellow petitjeanite aggregates are on top of the coating. This proves the successive crystallisation of (1) schlegelite, (2) quartz and (3) petitjeanite. A formation under supergene or hydrothermal conditions might be possible but could not be verified from the present investigations. At least the presence of the three elements arsenic, molybdenum and vanadium in their highest naturally occurring valence states besides oxo-oxygen atoms indicates a highly oxidising environment during the formation of the schlegelite paragenesis. Other associated minerals on the original specimen are pucherite and bismuth; the latter is seen as a hint that schlegelite is an alteration product from native ores. In addition, sillenite occurs around the bismuth grains as small colourless to pale yellow xenomorphic masses. It was identified by means of

Table 3. Electron-microprobe analyses[1] of schlegelite and petitjeanite.

	schlegelite[2]			petitjeanite[3]		
constituent	wt.%	range	std. dev.	wt.%	range	std. dev.
CaO	0.05	0.00 - 0.09	0.02	0.41	0.19 - 0.90	0.33
PbO	0.48	0.14 - 0.83	0.22	0.40	0.25 - 0.59	0.13
Bi_2O_3	70.20	69.28 - 71.78	0.62	78.91	78.55 - 79.38	0.36
P_2O_5	0.51	0.27 - 0.72	0.12	8.21	6.08 - 11.25	2.39
V_2O_5	0.21	0.06 - 0.56	0.11	6.26	2.32 - 9.26	2.93
As_2O_5	15.38	14.47 - 16.51	0.52	5.63	4.98 - 6.31	0.46
MoO_3	12.13	11.29 - 13.34	0.58			
H_2O (calc.)				1.04		
Total	98.96			100.87		

[1] 20 kV, 10 nA, beam diameter 2 µm; standards: andradite (Ca), mimetite (Pb, As), Bi_2S_3 (Bi), $AlPO_4$ (P), V (V), Mo (Mo).
[2] Mean of 27 analyses; empirical formula based on 24 O atoms: $(Bi_{6.78}Ca_{0.02}Pb_{0.05})_{\Sigma 6.85}O_{3.51}(MoO_4)_{1.90}[(AsO_4)_{3.01}(PO_4)_{0.16}(VO_4)_{0.05}]_{\Sigma 3.22}$.
[3] Mean of 6 analyses; empirical formula based on 10 O atoms: $(Bi_{2.92}Ca_{0.06}Pb_{0.02})_{\Sigma 3.00}(OH)_{1.00}O_{0.94}[(PO_4)_{1.00}(AsO_4)_{0.42}(VO_4)_{0.59}]_{\Sigma 2.01}$.

its high bismuth content and its X-ray powder diffraction pattern; the refined lattice parameter *a* is 10.175(1) Å.

Physical properties

Physical and optical properties are summarized in Table 1; reflectance values are compiled in Table 2. The optical axial angle 2V and the orientation were derived from extinction measurements using a spindle stage; the orientation with respect to the crystallographic axes was checked by single-crystal X-ray investigations. The refractive indices n_x and n_z were calculated from the mean values of the reflectance data in air and in oil at 590 nm using the Fresnel formula and neglecting absorption; n_y was calculated from n_x, n_z, and 2V (meas.). The value for the birefringence ($\Delta n = 0.04$) derived from the reflectance data was confirmed during the spindle-stage measurements.

Chemical composition

An electron-microprobe analysis of schlegelite (Table 3) was obtained from a polished and carbon-coated section of the same aggregate that yielded the crystal fragment used for the structure analysis. The main components of the new mineral are Bi_2O_3, As_2O_5 and MoO_3. The occurrence of Mo as a main constituent seems to be rather uncommon for the Schneeberg mineral assemblage. However, it should be mentioned that the Schneeberg area is the type locality for koechlinite, Bi_2MoO_6, (Schaller, 1916; Hyršl, 1992). In addition, a few minor finds of molybdenite, MoS_2, have also been reported (Massanek & Michalski, 2005).

The idealized formula of schlegelite is $Bi_7O_4(MoO_4)_2(AsO_4)_3$. Small amounts of Ca and Pb substitute for Bi; also small amounts of phosphate and vanadate substitute for arsenate. No other elements with atomic numbers greater than 8 could be detected. The empirical formula based on 24 oxygen atoms is $Bi_{6.78}Pb_{0.05}Ca_{0.02}O_{3.51}(MoO_4)_{1.90}(PO_4)_{0.16}(VO_4)_{0.05}(AsO_4)_{3.01}$. The compatibility index according to the Gladstone-Dale relationship (Mandarino, 1981) is –0.043, which is rated as good. Substitutions involving (Bi,Pb,Ca) and (P,As,V) are common for lead and bismuth minerals of the Schneeberg area; compare for example petitjeanite (Table 3; Krause *et al*., 1993) and brendelite (Krause *et al*., 1998). To achieve charge balance a coupled substitution involving $(Pb,Ca)^{2+}$ on the Bi^{3+} sites and $(MoO_4)^{2-}$ on the $(AsO_4)^{3-}$ sites is assumed. End member compositions of a solid solution series in case of Mo:(As,P,V) ratios greater than 2:3 may be formulated as: $Bi_7O_4(MoO_4)_2(AsO_4)_3 \leftrightarrow$ "$Bi_6(Pb,Ca)O_4(MoO_4)_2[(AsO_4)_2(MoO_4)]$". In case of Mo:(As,P,V) ratios below 2:3 an oxo/hydroxo substitution might be a possible mechanism to achieve charge balance.

X-ray investigation

X-ray powder diffraction data for schlegelite are compiled in Table 4. The differences between observed and

Table 4. X-ray powder diffraction data[1] of schlegelite.

h	*k*	*l*	d_{calc}	I_{calc}	d_{obs}	I_{obs}
0	0	2	11.974	8	12.018	3
0	2	0	8.067	8	8.072	12
0	2	2	6.690	6	6.691	3
0	0	2	5.987	1	5.983	2
0	3	1	5.247	2	5.244	4
1	1	1	4.926	2	4.923	1
1	0	2	4.845	2	4.837	2
0	2	4	4.808	2	4.803	2
1	1	2	4.641	5	4.645	2
0	3	3	4.460	7	4.459	6
1	2	1	4.355	4	4.349	3
1	1	3	4.258	3	not obs.[2]	
1	0	4	3.968	5	3.969	3
0	4	2	3.822	2	3.825	3
1	3	1	3.728	1	93.729	8
0	3	5	3.577	2	3.577	3
1	3	3	3.412	95	3.413	37
1	0	6	3.188	4	3.190	7
1	4	1	3.181	2		
1	1	6	3.128	2	3.125	4
0	0	8	2.993	35	2.996	69
1	2	6	2.965	2	2.963	48
1	3	5	2.965	100		
0	3	7	2.887	1	2.884	3
1	1	7	2.830	3	2.831	4
0	2	8	2.806	2	2.804	3
0	6	0	2.689	26	2.688	100
1	5	2	2.686	2		
2	0	0	2.649	22	2.648	12
1	5	3	2.605	2	2.607	2
2	1	2	2.554	3	2.554	2
1	3	7	2.535	5	2.535	3
1	5	5	2.389	3	2.393	3
1	3	8	2.345	2	2.346	2
2	3	3	2.278	3	not obs.[2]	
2	2	5	2.228	2	2.227	2
1	6	4	2.226	4		
2	1	6	2.187	2	2.175	2
1	3	9	2.175	3		
1	5	7	2.146	2	2.148	1
2	4	3	2.134	2	not obs.[2]	
2	3	5	2.129	2		
0	4	10	2.059	2	2.058	3
1	6	6	2.055	2		
2	5	2	2.018	2	2.020	9
0	3	11	2.018	3		
0	6	8	2.000	30	2.001	28
2	0	8	1.984	26	1.983	12
2	6	0	1.887	24	1.887	13
1	3	11	1.886	9		
1	0	12	1.868	2	1.867	3
1	7	7	1.798	2	not obs.	
2	1	10	1.766	2	not obs.	
3	1	2	1.737	2	not obs.	
3	2	1	1.721	2	not obs.	
2	7	2	1.721	2		
1	8	6	1.704	2	not obs.	
1	9	1	1.694	2	not obs.	
1	9	3	1.661	12	1.657	14
1	3	1	31.655	22		
3	3	3	1.642	9	1.643	3
3	4	1	1.614	2	not obs.	
3	1	6	1.607	2	1.600	9
2	3	11	1.605	2		
1	9	5	1.600	17		
2	6	8	1.586	23		
3	3	5	1.584	13	1.584	4

[1] Philips PW 1710 powder diffractometer, Cu*K*α radiation; internal standard: Si; I_{calc} was calculated with the programme LAZY PULVERIX (Yvon *et al.*, 1977); reflections with $I_{calc} \geq 2$ are listed. Observed intensities are not corrected for texture effects.

[2] Overlap due to quartz impuritiy.

Table 5. Single-crystal X-ray data collection and structure refinements of schlegelite.

a [Å]	5.302(1)
b [Å]	16.154(3)
c [Å]	23.981(5)
V [Å^3]	2056.1(7)
Z	4{$Bi_7O_4(MoO_4)_2(AsO_4)_3$}
space group	*Pnca* (no. 60)
crystal dimensions [µm]	8 x 42 x 130
range of data collection [°]	3° < 2ϑ < 60°
number of frames	840
scan time [s / °]	260
µ(MoK_α) [mm^{-1}]	66
$R_{int} = \Sigma \mid F_o^2 - F_o^2(mean)\mid / \Sigma F_o^2$	0.092
$R1 = \Sigma(\mid\mid F_o\mid - \mid F_c\mid\mid)/\Sigma\mid F_o\mid$	0.045
$wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	0.114
extinction parameter	0.00004(1)
absorption correction	multi-scan method
measured reflections	21914
observed unique reflections (n)	3022
reflections with $F_o > 4\sigma(F_o)$	2378
variable parameters (p)	166
$GooF = \{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{0.5}$	1.069
max Δ/σ	≤ 0.001
final difference Fourier map [eÅ^{-3}]	–3.49 to + 4.45

NONIUS KappaCCD four-circle diffractometer equipped with a CCD detector and a 300µm diameter capillary-optics collimator, Mo tube, graphite monochromator, φ-scans for distinct ω-angles, Δφ = 2°/frame, frame size: binned mode, 621×576 pixels, detector-to-sample distance: 30 mm; range of data collection: $-7 \geq h \leq 7$, $-22 \leq k \leq 22$, $-33 \leq l \leq 33$. Corrections for background, Lorentz-polarization and absorption effects. Programmes COLLECT (Nonius, 1999), DENZO-SMN (Otwinowski & Minor, 1997), SHELXS-97, SHELXL-97 (Sheldrick, 1997a,b). Neutral-atomic complex scattering functions (Wilson, 1992).
$w = 1 / \{\sigma^2(F_o^2) + [0.050*P]^2 + 75*P\}$; $P = ([\max(0,F_o^2)] + 2*F_c^2) / 3$.

calculated intensities are most probably due to preferred orientation. Unit-cell parameters refined from powder data are *a* = 5.299(1), *b* = 16.133(4), *c* = 23.948(5) Å, V = 2047.2(7) Å^3. This is slightly smaller than the cell parameters derived from the single-crystal investigations (Table 5) and might be due to minor differences in the chemical composition (*e.g.* Ca, P, V).

Single-crystal data collections were performed on two thin, lath-like samples of schlegelite. The results are very similar; during this paper only the results from the refinement yielding the smaller standard deviations for the structural parameters are considered. Details on the data collection are compiled in Table 5. The intensity distribution indicated orthorhombic symmetry, the space group was found from the extinction rules to be *Pnca* (no. 60). The Bi atoms as well as the centres of the XO_4 tetrahedra (*X* = Mo, As) were located by direct methods; successive Fourier and difference Fourier maps revealed the positions of the oxygen atoms. For all atoms anisotropic displacement parameters were allowed to vary. The electron density in the final difference Fourier map amounts –4.50 to +5.57 eÅ^{-3}; the highest peaks are in the surrounding of the Bi atoms. From the refinement of the site occupation factors it is evident that the sites *X*1 and *X*2 are occupied predominantly by Mo atoms. This is in agreement with the size and shape of the coordination polyhedra around these positions (see below). The sites *X*3 and *X*4 contain the arsenic atoms and small amounts of phosphorus and vanadium as well as molybdenum in case of a Mo surplus. Different refinement models using distinct scattering functions for the atom sites *X*3 and *X*4 were applied. However, the results did not significantly deviate from a full occupation with As atoms. Consequently, for the final refinement neutral-atomic complex scattering functions of As were

Table 6. Atomic coordinates and anisotropic displacement parameters for schlegelite (e.s.d.'s in parentheses).

Atom	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Bi1	0.25	0.0	0.82100(3)	0.0263(4)	0.0333(4)	0.0181(3)	0.0	0.0	0.0049(3)	0.0259(2)
Bi2	0.20136(11)	0.17526(3)	0.31301(2)	0.0231(3)	0.0257(3)	0.0227(3)	–0.0023(2)	0.0031(2)	–0.0020(2)	0.0238(2)
Bi3	0.30289(10)	0.16056(3)	0.56105(2)	0.0181(3)	0.0240(3)	0.0216(2)	0-0.0021(2)	0.0011(2)	–0.0017(2)	0.0213(1)
Bi4	0.25882(10)	0.32375(3)	0.44420(2)	0.0228(3)	0.0215(3)	0.0199(2)	0.0002(2)	–0.0015(2)	–0.0017(2)	0.0214(2)
Mo1	0.25	0.0	0.07488(7)	0.0153(7)	0.0178(7)	0.0186(7)	0.0	0.0	0.0001(6)	0.0172(3)
Mo2	0.25	0.0	0.67760(7)	0.0216(8)	0.0173(8)	0.0181(7)	0.0	0.0	–0.0031(6)	0.0190(3)
As3	0.25	0.0	0.42911(8)	0.0173(9)	0.0167(8)	0.0156(8)	0.0	0.0	–0.0040(7)	0.0165(4)
As4	0.2509(3)	0.16929(8)	0.17204(5)	0.0194(6)	0.0195(7)	0.0149(6)	0.0009(4)	0.0016(5)	0.0045(5)	0.0179(3)
O11	0.146(2)	–0.0785(7)	0.0312(4)	0.031(6)	0.030(6)	0.030(6)	–0.003(4)	0.004(5)	–0.003(5)	0.030(2)
O12	–0.025(2)	0.0481(6)	0.1072(4)	0.028(5)	0.018(5)	0.028(5)	0.005(4)	0.010(4)	–0.004(4)	0.025(2)
O21	0.029(2)	0.0383(6)	0.7251(4)	0.024(5)	0.021(5)	0.030(5)	0.004(4)	–0.004(4)	0.005(4)	0.025(2)
O22	0.400(2)	0.1008(6)	0.6553(4)	0.023(5)	0.025(5)	0.019(4)	0.002(4)	–0.007(4)	–0.012(4)	0.023(2)
O31	0.025(2)	–0.0473(7)	0.3899(4)	0.040(7)	0.027(6)	0.026(5)	0.006(4)	–0.014(5)	–0.013(5)	0.031(3)
O32	0.383(2)	–0.0743(6)	0.4695(4)	0.026(5)	0.030(5)	0.016(4)	–0.002(4)	–0.003(4)	0.0112(4)	0.024(2)
O41	0.420(2)	0.2337(7)	0.2139(4)	0.028(5)	0.038(6)	0.013(4)	0.001(4)	0.004(4)	–0.012(5)	0.026(2)
O42	0.452(2)	0.1013(7)	0.1438(4)	0.040(7)	0.038(6)	0.017(5)	–0.002(4)	0.002(4)	0.020(5)	0.032(3)
O43	0.047(2)	0.1261(7)	0.2166(4)	0.046(7)	0.026(6)	0.021(5)	0.000(4)	0.010(5)	–0.011(5)	0.031(2)
O44	0.102(2)	0.2249(6)	0.1231(4)	0.025(5)	0.014(5)	0.026(5)	0.005(4)	–0.012(4)	0.000(4)	0.022(2)
O1	0.495(2)	0.2481(6)	0.4980(4)	0.019(4)	0.030(5)	0.014(4)	0.003(4)	0.002(3)	0.001(4)	0.021(2)
O2	0.116(2)	0.2231(6)	0.3972(4)	0.024(5)	0.024(5)	0.017(4)	–0.003(4)	0.009(4)	–0.007(4)	0.022(2)

[1] The anisotropic displacement parameters are defined as: $\exp[-2\pi^2 \Sigma^3_{i=1} \Sigma^3_{j=1} U_{ij} \mathbf{a}^*_i \mathbf{a}^*_j h_i h_j]$; equivalent isotropic displacement parameter according to Fischer & Tillmanns (1988).

applied for the *X*3 and *X*4 sites and of Mo for the *X*1 and *X*2 sites. Final structure parameters are given in Table 6, some interatomic bond distances and bond angles in Table 7.

Results and discussion

There are each four crystallographically independent Bi and *X* atoms in the crystal structure of schlegelite. The cations Bi1, Mo1, Mo2, and As3 are located on the two-fold axis running parallel to [001] (Fig. 1). The atoms Bi2, Bi3, Bi4, and As4 as well as all the oxygen atoms are on general positions. Ten crystallographically different O atoms belong to the XO_4 groups; two oxo-oxygen atoms are coordinated only to the Bi atoms.

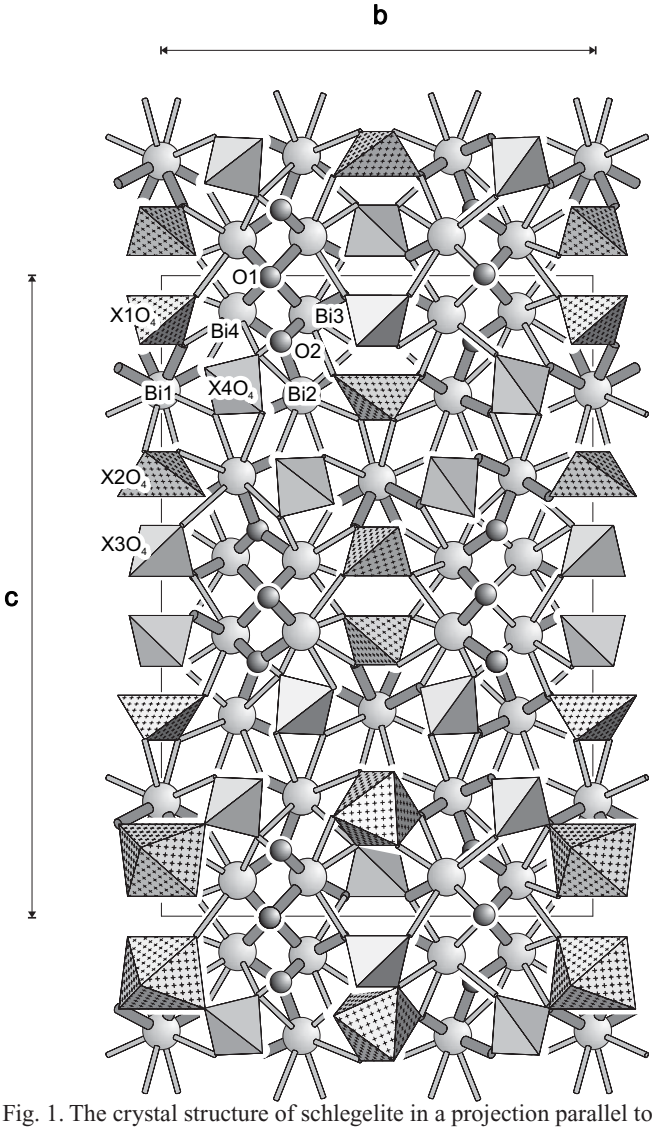

Fig. 1. The crystal structure of schlegelite in a projection parallel to [100]. At the top MoO_4 tetrahedra are shown whereas at the bottom the distorted MoO_6 octahedra are indicated (programme ATOMS, Dowty 1999).

Table 7. Interatomic bond lengths, common O—O edge lengths shared between the coordination figures around the Bi atoms (in Å) bond angles (in °) and distorsion parameters (Fleet, 1976) for schlegelite.

Bi1—O12$^{vii, i}$	2.237(10)		Bi2—O22^{vi}	2.139(9)
Bi1—O42$^{ii, vi}$	2.428(11)		Bi2–O41^{iii}	2.193(10)
Bi1—O21$^{0, v}$	2.659(10)		Bi2–O2	2.210(9)
Bi1—O43$^{i, vii}$	2.731(11)		Bi2–O43	2.581(11)
O12^{vii}–Bi1–O12^{i}	79.2(6)		Bi2–O41	2.812(10)
O12^{vii}–Bi1–O42^{ii}	67.6(4)		Bi2–O21^{vii}	2.959(10)
O12^{vii}–Bi1–O42^{vi}	81.1(4)		Bi2–O44^{iv}	3.072(10)
O12^{i}–Bi1–O42^{ii}	81.1(4)		Bi2–O31^{v}	3.132(12)
O12^{i}–Bi1–O42^{vi}	67.6(4)		O22^{vi}–Bi2–O41^{iii}	88.6(4)
O42^{ii}–Bi1–O42^{vi}	139.3(5)		O22^{vi}–Bi2–O2	73.7(4)
			O41^{iii}–Bi2–O2	84.0(4)
Bi3–O2^{vii}	2.189(9)		Bi4–O2	2.121(10)
Bi3–O32^{ii}	2.293(10)		Bi4–O1	2.177(10)
Bi3–O1	2.311(10)		Bi4–O1^{vi}	2.318(10)
Bi3–O22	2.515(9)		Bi4–O44^{iv}	2.552(9)
Bi3–O1^{vi}	2.584(10)		Bi4–O11^{ix}	2.667(11)
Bi3–O44^{viii}	2.610(10)		Bi4–O12^{iv}	2.672(10)
Bi3–O32^{v}	2.785(10)		Bi4–O11^{x}	2.731(11)
Bi3–O31^{i}	2.785(11)		Bi4–O42^{iii}	2.929(11)
O2^{vii}–Bi3–O32^{ii}	82.9(4)		O2–Bi4–O1	95.2(4)
O2^{vii}–Bi3–O1	71.4(4)		O2–Bi4–O1^{vi}	72.5(4)
O32^{ii}–Bi3–O1	80.0(4)		O1–Bi4–O1^{vi}	72.3(2)
$Bi3O_3$...$Bi4O_3$	O1–O2	2.629(14)		
$Bi2O_8$...$Bi3O_8$	O2–O22	2.609(13)	O31—O44	3.754(14)
$Bi2O_8$...$Bi4O_8$	O2–O44	2.745(13)		
$Bi3O_8$...$Bi3O_8$	O1–O32	2.989(14)		
$Bi3O_8$...$Bi4O_8$	O1–O1	2.654(10)	O1—O44	2.993(14)
$Bi4O_8$...$Bi4O_8$	O1–O11	3.009(15)		
$Bi1O_8$...$Bi2O_8$	O21–O43	3.398(15)		
$Bi1O_8$...$Bi4O_8$	O12–O42	3.035(15)		
Mo1–O11$^{0, v}$	1.738(11)		Mo2–O21$^{0, v}$	1.751(10)
Mo1–O12$^{0, v}$	1.825(10)		Mo2–O22$^{0, v}$	1.892(10)
Mo1–O42$^{0, v}$	2.564(11)		Mo2–O31^{i,vii}	2.310(11)
O11^{0}–Mo1–O11^{v}	105.7(7)		O21^{0}–Mo2–O21^{v}	98.8(6)
O11^{0,v}–Mo1–O12^{0,v}	108.3(5)		O21^{0,v}–Mo2–O22^{0,v}	99.4(5)
O11^{0,v}–Mo1–O12^{v,0}	101.5(5)		O21^{0,v}–Mo2–O22^{v,0}	101.8(5)
O12^{0}–Mo1–O12^{v}	129.6(7)		O22^{0}–Mo2–O22^{v}	147.2(6)
As3–O32$^{0, v}$	1.698(10)		As4–O43	1.675(10)
As3–O31$^{0, v}$	1.703(10)		As4–O42	1.676(10)
O32^{0}–As3–O32^{v}	110.3(6)		As4–O44	1.682(9)
O32^{0,v}–As3–O31^{0,v}	109.9(6)		As4–O41	1.703(10)
O32^{0,v}–As3–O31^{v,0}	106.9(5)		O43–As4–O42	113.4(6)
O31^{0}–As3–O31^{v}	113.80(8)		O43–As4–O44	111.2(6)
			O43–As4–O41	102.7(5)
			O42–As4–O44	111.8(5)
			O42–As4–O41	107.7(6)
			O44–As4–O41	109.6(5)
	σ^2_{tet}	σ^2_{oct}	Δ^2_{tet}	Δ^2_{oct}
$Mo1O_4$ / $Mo1O_6$	110.0	240.4	1.000596	1.72
$Mo2O_4$ / $Mo2O_6$	371.3	100.7	1.001498	1.81
$As3O_4$	5.4		1.000002	
$As4O_4$	14.7		1.000045	

Symmetry code: not specified and ^{0} *x*, *y*, *z*; ^{i} -*x*, -*y*, -*z*+1; ^{ii} -*x*+1, -*y*, -*z* + 1; ^{iii} *x*-1/2, -*y* +1/2, -*z* + 1/2; ^{iv} *x* + 1/2, -*y* + 1/2, -*z* + 1/2; ^{v} -*x* + 1/2, -*y*, *z*; ^{vi} *x*-1/2, *y*, -*z* + 1; ^{vii} *x* +1/2, *y*, -*z* +1; ^{viii} *x*, -*y* +1/2, *z* +1/2; ^{ix} -*x* +1/2, *y* +1/2, *z* +1/2; ^{x} -*x*, *y* +1/2, -*z* + 1/2

The distortion parameters (bond-angle variance σ^2 and mean-square relative deviation from average bond length Δ^2) are defined as

$\sigma^2_{tet} = \frac{1}{5}\Sigma^6_{i=1}(\theta_i - 109.47°)^2$ and $\Delta_{tet} = \frac{1}{4}\Sigma^4_{i=1}(l_i/\bar{l})^2$ for a tetrahedron ($\sigma^2_{tet} = 0$ and $\Delta_{tet} = 1.0$ in case of an ideal tetrahedron)

$\sigma^2_{oct} = \frac{1}{11}\Sigma^{12}_{i=1}(\theta_i - 90°)^2$ and $\Delta_{oct} = \frac{1}{6}\Sigma^6_{i=1}(li/\bar{l})^2$ for an octahedron $\sigma^2_{oct} = 0$ and $\Delta_{oct} = 1.0$ in case of an ideal octahedron)

θ_i, l_i and $\bar{l}$ are the individual bond angles, the individual and mean bond lengths (Fleet, 1976).

Table 8. Bond valence analysis for schlegelite calculated with the parameters given by Brese & O'Keeffe (1991).

	O11	O12	O21	O22	O31	O32	O41	O42	O43	O44	O1	O2	Σ ν
Bi1		0.67 2x →	0.21 2x →					0.40 2x →	0.18 2x →				2.93
Bi2			0.10	0.88	0.06		0.76+0.14		0.27	0.07		0.72	2.99
Bi3				0.32	0.15	0.58+0.15				0.25	0.55+0.26	0.77	3.02
Bi4	0.21+0.18	0.21						0.10		0.29	0.79+0.54	0.92	3.24
Mo1	1.58 2x →	1.25 2x →						0.17 2x →					5.99
Mo2			1.52 2x →	1.04 2x →	0.34 2x →								5.80
As3					1.21 2x →	1.19 2x →							4.79
As4							1.19	1.28	1.28	1.26			5.01
Σ ν	1.96	2.13	1.83	2.23	1.74	1.94	2.09	1.95	1.72	1.86	2.14	2.41	

Table 9. Principal mean square atomic displacements *U* for schlegelite.

Bi1	0.0358	0.0239	0.0181	O11	0.038	0.027	0.026
Bi2	0.0289	0.0228	0.0197	O12	0.038	0.025	0.012
Bi3	0.0257	0.0204	0.0176	O21	0.032	0.027	0.015
Bi4	0.0244	0.0206	0.0192	O22	0.039	0.019	0.010
Mo1	0.0186	0.0178	0.0153	O31	0.056	0.021	0.016
Mo2	0.0232	0.0181	0.0157	O32	0.040	0.017	0.015
As3	0.0210	0.0156	0.0130	O41	0.046	0.022	0.011
As4	0.0243	0.0153	0.0142	O42	0.059	0.021	0.016
O1	0.031	0.020	0.013	O43	0.053	0.024	0.015
O2	0.035	0.019	0.011	O44	0.038	0.017	0.010

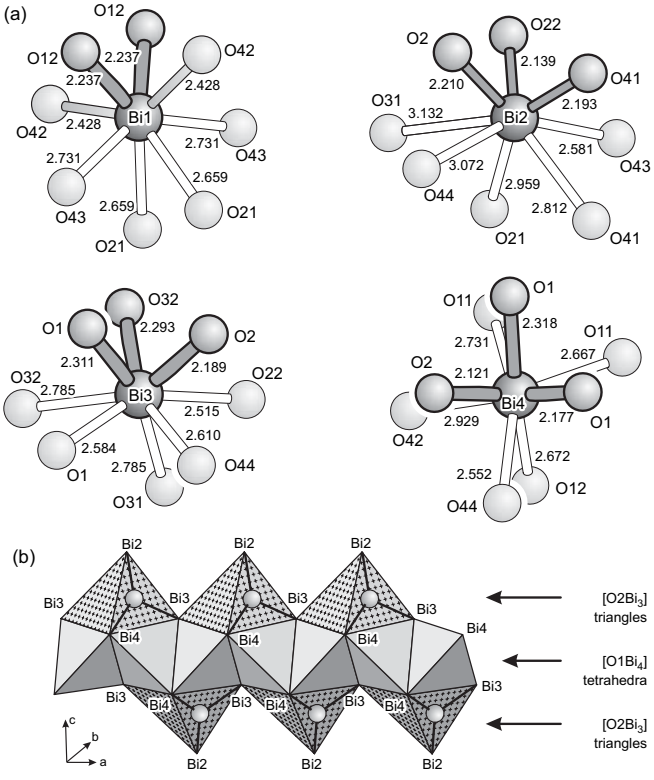

Fig. 2. The stereochemistry of the Bi atoms in schlegelite. (a) Interatomic bond distances are given in Å. The tetragonal antiprisms $Bi1O_8$, $Bi2O_8$ and $Bi3O_8$ as well as the $Bi4O_8$ cube are in projections parallel to their approximate four-fold axes. (b) The $[Bi_4]$ tetrahedra are edge-connected to rows parallel [100]. The central tetrahedron surrounds the O1 atom; the O2 atom is located at a face of the branched $[Bi_4]$ tetrahedron (programme ATOMS, Dowty 1999).

The Bi atoms have a one-sided coordination to account for the space requirements of their lone-pair electrons (Fig. 2a). The Bi1 atom exhibits a [2+2+4] coordination with Bi1—O = 2.237 Å, 2x, and 2.428 Å, 2x; four further ligands have Bi1—O = 2.659 Å, 2x and 2.731 Å, 2x. The atoms Bi2, Bi3 and Bi4 have three ligands with short Bi—O bond distances ranging from 2.121 to 2.318 Å, the coordination is completed by each five additional ligands between 2.515 and 3.132 Å. Further O atoms have Bi—O distances ≥ 3.582 Å indicating only weak interactions. The coordination figure around the Bi1 atom is solely formed by oxygen atoms belonging to XO_4 tetrahedra. For the other Bi sites the oxo-oxygen atoms O1 and O2 are involved in the coordination; as usually found, the oxo-oxygen atoms are predominantly shortly bounded ligands. The coordination figures $[Bi1O_8]$, $[Bi2O_8]$, $[Bi3O_8]$ are distorted tetragonal antiprisms whereas $[Bi4O_8]$ forms an approximate cube.

The bond valence sums for the atoms Bi1, Bi2 and Bi3 in schlegelite are balanced considering eight neighbours each; only the Bi4 atom is somewhat overestimated (Brese & O'Keeffe, 1991; Table 8). The calculations are based on the formula $\nu_{ij} = \exp[(R_{ij}-d_{ij})/b]$; Brese & O'Keeffe (1991) suggested b = 0.37 to be valid for a very large variety of cations bound to different anions and they fitted the parameters R_{ij} to obtain $\nu_i = \Sigma_j \nu_{ij}$ and $\nu_j = \Sigma_i \nu_{ij}$; ν_i and ν_j are the valences of cations and anions, respectively. However, this generalization causes an overestimation of the short and an underestimation of the long Bi—O bond lengths (Table 8). Such systematic deviations are responsible for some erroneous bond-valence sums frequently found for the O atoms coordinating Bi atoms with a pronounced steric activity of the lone-pair electrons. Using always the same value of b gives no proper credit to the changes in the interatomic bond character in case of a variable environment of a single kind of atoms. Bi is a very critical atom because it may exhibit steric active lone-pair electrons like in schlegelite, but also regular coordinations are known (*cf.* schneebergite and nickelschneebergite, $BiM_2(AsO_4)_2[(H_2O)(OH)]$, M = Co, Ni , Krause *et al.* (2002a), where the $Bi^{[6+2]}$ atoms have site symmetry 2/*m* and Bi—O bond lengths range only from 2.386(8) to 2.439(6) Å for the six atoms in the first coordination sphere).

The four crystallographically different XO_4 tetrahedra split into two groups with respect to their shape, size and scattering power of the central atom. To sum up, the $X1O_4$

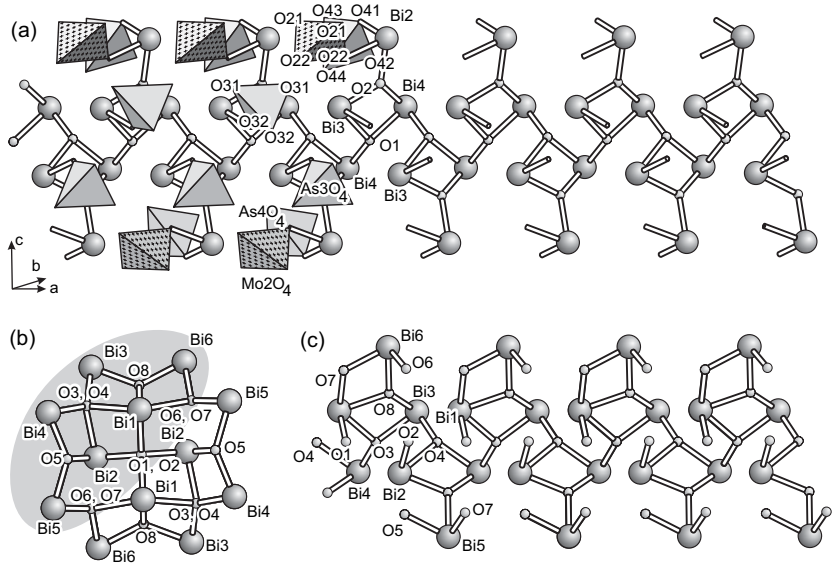

Fig. 3. (a) The connection of the Bi atoms in schlegelite in a projection approximaely parallel to [010]; parts of the neighbouring XO_4 tetrahedra are shown. (b) A $(Bi_{12}O_{14})_n$ column in $PbBi_{12}Mo_5O_{34}$ (Enjalbert *et al*., 1997) in a projection on (010). Part of this column is marked and shown in (c) in a projection approximately parallel to [100]. Bi and oxo-oxygen atoms are shown as large and small circles, respectively; O atoms of XO_4 tetrahedra are not separately marked (programme ATOMS, Dowty 1999).

and $X2O_4$ tetrahedra are larger and stronger distorted as compared to the $X3O_4$ and the $X4O_4$ tetrahedra going along with an occupation by predominantly Mo and As atoms, respectively. The coordination figures around the two $Mo^{[4]}$ atoms exhibit two short and two long Mo—O bond lengths, the difference is 5.0 % within the $Mo1O_4$ and 8.1% within the $Mo2O_4$ polyhedron. As usual, the stronger distorted polyhedron exhibits larger average bond lengths: The average $<Mo1^{[4]}—O>$ bond length of 1.782 Å is slightly shorter as compared to $<Mo2^{[4]}—O>$ which amounts 1.822 Å. In addition, for the Mo1 and Mo2 atoms some interactions with each two additional ligands are evident; these Mo—O distances of 2.564 and 2.310 Å correlate negatively with the average $<Mo^{[4]}—O>$ bond lengths. Formal bond-valence calculations indicate significant contributions even of these further ligands (Table 8). Their steric influence cause the large deviation of the O—Mo1/Mo2—O bond angles from that expected for a regular tetrahedron: 129.6 and 147.2° were observed at the Mo atoms between the two longer bonds within each tetrahedron; the other O—Mo1/Mo2—O bond angles are only in the range from 98.8 to 108.3°. The additional ligands complete the coordination figures in the area of the more separated ligands. Considering all six neighbours, both coordination figures can be regarded alternatively as strongly distorted octahedra as supported by comparison of the bond-angle variances σ^2_{tet} and σ^2_{oct} (Table 7). In general, the values are very large for both, the tetrahedral and the octahedral coordination figure indicating that both descriptions fit only poorly with the environment. However, for the coordination figures around the Mo1 atom $\sigma^2_{tet} < \sigma^2_{oct}$ whereas $\sigma^2_{tet} > \sigma^2_{oct}$ for that around the Mo2 atom. Consequently, the bond angles of the Mo2 atoms match with the description as a $Mo2O_6$ octahedron rather than the description as a $Mo2O_4$ tetrahedron. However, the bond lengths (cf. the bond-length distortions given in Table 7) as well as the bond valences (Table 8) indicate a predominantly tetrahedral coordination with markedly interactions to two further ligands in both cases.

The sizes of the $X3O_4$ and the $X4O_4$ tetrahedra agree with the expectation for an occupation predominantly by As atoms. The average bond length $<X3—O>$ of 1.701 Å is slightly longer whereas the $X4O_4$ tetrahedron with $<X4—O>$ of 1.684 Å accords with the expectations for a pure AsO_4 tetrahedron. The chemical analyses revealed small amounts of P and V; it is assumed that these elements substitute at the *X*3 and *X*4 sites. Solid solution for the central atoms of the $X3O_4$ and the $X4O_4$ tetrahedra is supported by the analysis of the principal mean-square displacements of the anisotropic displacement parameters (Table 9). The oxygen atoms O31, O32, O41, O42, O43, and O44 exhibit stronger anisotropies as compared to all the other atoms. It has to be mentioned that the anisotropies of the central atoms *X*3 and *X*4 are in the same range as those of the Mo1 and Mo2 atoms. It indicates that the size of the tetrahedron varies according to the space requirement of the respective central atom. The accuracy of the structure determination does not allow a detailed refinement of the scattering power at the *X* sites considering minor substitutions.

The atoms Bi2, Bi3 and Bi4 are closely connected to each other *via* the oxo-oxygen atoms. Considering solely these Bi atoms, they are at the corners of edge sharing tetradehra forming ribbons in [100], *i.e.*, the direction of the elongation of the lath-like crystals. As shown in Fig. 2b, the central tetrahedra formed by each two Bi3 and Bi4 atoms are more or less regular. They surround the O1 atoms forming $[O1Bi_4]$ tetrahedra with Bi—O1—Bi angles between 101.4(4)° and 118.6(5)°. The branched $[Bi3_2Bi4Bi2]$ tetrahedra are rather flattened. The O2 atom is in the Bi2-Bi3-Bi4 face within limits of error; the three Bi—O2—Bi angles are 112.4(4)°, 114.4(4)° and 133.1(4)° (sum 359.9°).

The $Bi3^{[3]}O_3$ and $Bi4^{[3]}O_3$ groups are connected *via* an O1—O2 edge to a dimer. These dimers are corner-linked among each other and with the $Bi2^{[3]}O_3$ groups forming Bi_6O_{10} rods (two O atoms belong to molybdate tetrahedra, four to arsenate tetraheda and four represent oxo-oxygen

atoms); a Bi_6O_{10} rod (partly with the linked XO_4 tetrahedra) is shown in Fig. 3a. Including the additional neighbours around the Bi atoms an extensive connection is observed (see Table 7). These rods are corner-connected among each other by the O41 atoms only. As a result, layers parallel to (010) are formed, which are connected by XO_4 tetrahedra to a three-dimensional net-work.

Topologically, the connection of the atom Bi1 within the crystal structure is distinct; it is not shortly linked to any other Bi atom. The Bi1 atoms are only connected to the other three Bi atoms *via* the second coordination sphere of the Bi2 and Bi4 atoms. Considering [8] coordination around all four Bi atoms, they form a three-dimensional network. However, in $z \sim 1/4$ and $3/4$ only Bi—O distances longer than 2.50 Å are observed which cause the good cleavage parallel to (001) (Fig. 1). The *X* atoms are in tetrahedral cavities within this framework; they maintain the loose connection in $\sim xy1/4$ and $\sim xy3/4$. Considering [6] coordination around the Mo1 and Mo2 atoms, each of the $Mo1O_6$ octahedra is corner connected to two $As4O_4$ tetrahedra forming $Mo1As4_2O_{12}$ groups. In contrast, the $Mo2O_6$ octahedra are corner connected to $As3O_4$ tetrahedra forming $Mo2As3O_8$ chains.

Minerals containing both, arsenate and molybdate anion groups, are rare. Up to now only a few examples have been mentioned: betpakdalite, $Ca_2MgFe^{3+}{}_3Mo_8O_{28}(OH)(AsO_4)_2{\cdot}23H_2O$, which was recently reinvestigated by Cooper & Hawthorne (1999), sodium betpakdalite, formula given as $(Na,Ca)_3Fe^{3+}{}_2Mo_6As_2O_{28}{\cdot}15H_2O$ (Skvortsova *et al*., 1971), molybdofornacite, $Pb_2Cu(OH)(AsO_4)(MoO_4)$ (Medenbach *et al*., 1983) and its unnamed phosphate analogue (Nickel & Hitchen, 1994), and obradovicite, formula given as $H_4(K,Na)CuFe^{3+}{}_2(AsO_4)(MoO_4)_5{\cdot}12H_2O$ (Finney *et al*., 1986). Arsenite groups besides molybdate were found in vajdakite, $(MoO_2)_2(H_2O)_2As^{3+}{}_2O_5{\cdot}H_2O$ (Ondruš *et al*., 2002) and biehlite, $Sb^{3+}{}_{1.79}As^{3+}{}_{0.21}MoO_6$ (Adiwidjaja *et al*., 2000). The only well described bismuth-molybdate found in nature so far is koechlinite, Bi_2MoO_6 (Pertlik & Zemann, 1982, Theobald *et al*., 1984, Teller *et al*., 1984). It forms sheets of corner-sharing MoO_6 octahedra alternating with sheets of corner sharing $Bi^{[2+4]}O_6$ polyhedra; both are linked by O atoms. Here the Mo atom is coordinated in a [4+2] coordination, but the bond-length distribution and shape of the coordination figure is rather an octahedron as compared to the $Mo^{[4+2]}O_6$ polyhedra in schlegelite. Chiluite mentioned as $Bi_6Te_2Mo_2O_{21}$ by Xiuzhen Yong *et al.* (1989) needs further investigations. Bismuth arsenates were found more frequently, for a number of these minerals the crystal structure was described during the last years: rooseveltite and tetrarooseveldite, $BiAsO_4$ (Bedlivy & Mereiter, 1982a; Mooney 1958), preisingerite, $Bi_3O(OH)(AsO_4)_2$ (Bedlivy & Mereiter, 1982b), atelestite, $Bi_2O(OH)AsO_4$ and mixite, $BiCu_6(OH)_6(AsO_4)_3{\cdot}3H_2O$ (Mereiter & Preisinger, 1986; see also Krause *et al*., 1997), paganoite, $NiBi^{3+}As^{5+}O_5$ (Roberts *et al*., 2001), walpurgite and orthowalpurgite, $(UO_2)Bi_4O_4(AsO_4)_2{\cdot}2H_2O$ (Mereiter, 1982; Krause *et al*., 1995), schneebergite and nickelschneebergite, $BiM_2(AsO_4)_2[(H_2O)(OH)]$, M = Co, Ni, (Krause *et al*., 2002a), neustädtelite, $Bi_2Fe_2O_2(OH)_2(AsO_4)_2$, cobaltneustädtelite and medenbachite, $Bi_2FeMO(OH)_3(AsO_4)_2$, M = Cu, Co (Krause *et al*., 2002b). It should be mentioned that these are oxo-, oxo-hydroxo-, or hydroxoarsenates; none of them was described to include a second anion group.

Only synthetically known is the compound $PbBi_{12}O_{14}(MoO_4)_5$ (Enjalbert *et al*., 1997a). The crystal structure consists of $(Bi_{12}O_{14})_n$ columns linked by Pb atoms and MoO_4 tetrahedra. These $(Bi_{12}O_{14})_n$ columns (Fig. 3b) show some topological similarities with that in $Bi_{13}O_{14}(MoO_4)_4(VO_4)$ (Enjalbert *et al*., 1997b), $Bi(Bi_{12-x}Te_xO_{14})Mo_{4-x}V_{1+x}O_{20}$ ($0 \le x < 2.5$) (Castro *et al*., 1998), and $\gamma(H)Bi_2MoO_6$ (Bégué *et al*., 2000). The $(Bi_{12}O_{14})_n$ columns in $PbBi_{12}O_{14}(MoO_4)_5$ can be described as formed by two Bi_6O_{10} rods of schlegelite rotated around a twofold axis parallel to the direction of the rods and linked by six oxygen atoms (Fig. 3b,c). The oxygen atoms of schlegelite shortly bonded to Bi atoms and belonging to XO_4 tetrahedra are shared between three Bi atoms in $PbBi_{12}O_{14}(MoO_4)_5$; they become oxo-oxygen atoms. Some torsion of the BiO_3 and BiO_4 figures cause that Bi_6 octahedra are formed in $PbBi_{12}O_{14}(MoO_4)_5$ whereas Bi_4 tetrahedra in schlegelite.

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References

Adiwidjaja, G., Friese, K., Klaska, K.H., Schlüter, J., Czank, M. (2000): Crystal structure and crystal chemistry of biehlite, $Sb_{1.79}As_{0.21}MoO_6$. *Z. Krist.*, **215**, 529-535.

Bedlivy, D. & Mereiter, K. (1982a): Structure of α-$BiAsO_4$ (Rooseveltite). *Acta Cryst*., **B38**, 1559-1561.

—,— (1982b): Preisingerite, $Bi_3O(OH)(AsO_4)_2$, a new species from San Juan Province, Argentina: its description and crystal structure. *Am. Mineral.*, **67**, 833-840.

Bégué, P., Enjalbert, R., Galy, J., Castro, A. (2000): Single-crystal X-ray investigations of the structures of $\gamma(H)Bi_2MoO_6$ and its partially substituted As^{3+} and Sb^{3+} homologues. *Solid State Sci.*, **2**, 637-653.

Bernhardt, H.-J. (1987): A simple fully-automated system for ore mineral identification. *Mineral. Petrol.*, **36**, 241-245.

Brese, N.E. & O'Keeffe, M. (1991): Bond-valence parameters for solids. *Acta Cryst*., **B47**, 192-197.

Castro, A., Enjalbert, R., Baules, P., Galy, J. (1998): Synthesis and structural evolution of the solid solution $Bi(Bi_{12-x}Te_xO_{14})Mo_{4-x}V_{1+x}O_{20}$ ($0 \le x < 2.5$). *J. Solid State Chem.*, **139**, 185-193.

Cooper, M.A. & Hawthorne, F.C. (1999): The crystal structure of betpakdalite, and a new chemical formula: $(Mg(H_2O)_6)Ca_2(H_2O)_{13}(Mo^{6+}{}_2As^{5+}{}_2Fe^{3+}{}_3O_{36}(OH))(H_2O)_4$. *Can. Mineral.*, **37**, 61-66.

Dowty, E. (1999): ATOMS 5.0, a computer program. Kingsport, TN.

Enjalbert, R., Hasselmann, G., Galy, J. (1997a): A new mixed oxide with $(Bi_{12}O_{14})_n$ columns: $PbBi_{12}Mo_5O_{34}$. *Acta Cryst.*, **C53**, 269-272

—,— (1997b): $[Bi_{12}O_{14}E_{12}]_n$ columns and lone pairs E in $Bi_{13}Mo_4VO_{34}E_{13}$: synthesis, crystal structure, and chemistry of

the Bi_2O_3—MoO_3—V_2O_5 - system. *J. Solid State Chem.*, **131**, 236-245.

Finney, J.J., Williams, S.A., Hamilton, R.D. (1986): Obradovicite, a new complex arsenate-molybdate from Chuquicamata, Chile. *Min. Mag.*, **50**, 283-284.

Fischer, R.X. & Tillmanns, E. (1988): The equivalent isotropic displacement factor. *Acta Cryst.*, **C44**, 775-776.

Fleet, M.E. (1976): Distortion parameters for coordination polyhedra. *Min. Mag.*, **40**, 531-533.

Hyršl, J. (1992): Über das Vorkommen von Russelit und Koechlinit im sächsisch-böhmischen Erzgebirge. *Mineralien-Welt*, **3**(3), 31-33.

Krause, W., Belendorff, K., Bernhardt, H.J. (1993): Petitjeanite, $Bi_3O(OH)(PO_4)_2$, a new mineral and additional data for the corresponding arsenate and vanadate, preisingerite and schumacherite. *N. Jb. Mineral. Mh.*, **1993**, 487-503.

Krause, W., Effenberger, H., Brandstaetter, F. (1995): Orthowalpurgite, $(UO_2)Bi_4O_4(AsO_4)_2{\cdot}2H_2O$, a new mineral from the Black Forest, Germany. *Eur. J. Mineral.*, **7**, 1313-1324.

Krause, W., Bernhardt, H.-J., Blass, G., Effenberger, H., Graf, H.-W. (1997): Hechtsbergite, $Bi_2O(OH)(VO_4)$, a new mineral from the Black Forest, Germany. *N. Jb. Miner. Mh.*, **1997**, 271-287.

Krause, W., Bernhardt, H.-J., McCammon, C., Effenberger, H. (1998): Brendelite, $(Bi,Pb)_2Fe^{3+,2+}O_2(OH)(PO_4)$, a new mineral from Schneeberg, Germany: description and crystal structure. *Mineral. Petrol.*, **63**, 263-277.

Krause, W., Effenberger, H., Bernhardt, H.-J., Martin, M. (1999): Cobaltlotharmeyerite, $Ca(Co,Fe,Ni)_2(AsO_4)_2(OH,H_2O)_2$, a new mineral from Schneeberg, Germany. *N. Jb. Mineral. Mh.*, **1999**, 505-517.

Krause, W., Bernhardt, H.-J., Effenberger, H., Martin, M. (2001): Cobalttsumcorite and nickellotharmeyerite, two new minerals from Schneeberg, Germany: description and crystal structure. *N. Jb. Mineral. Mh.*, **2001**, 558-576.

Krause, W., Bernhardt, H.-J., Effenberger, H., Witzke, T. (2002a): Schneebergite and nickelschneebergite from Schneeberg, Saxony, Germany: the first Bi-bearing members of the tsumcorite group. *Eur. J. Mineral.*, **14**, 115-126.

Krause, W., Bernhardt, H.-J., McCammon, C., Effenberger, H. (2002b): Neustädtelite and cobaltneustädtelite, the Fe^{3+}- and Co^{2+}-analogues of medenbachite. *Am. Mineral.*, **87**, 726-738.

Mandarino, J. A. (1981): The Gladstone-Dale relationship: part IV. The compatibility concept and its application. *Can. Mineral.*, **19**, 441-450.

Massanek, A. & Michalski, S. (2005): Die Mineralien des Schneeberger Reviers. *Lapis*, **30**(7/8), 41-66.

Medenbach, O., Abraham, K., Gebert, W. (1983): Molybdofornacit, ein neues Blei-Kupfer-Arsenat-Molybdat-Hydroxid von Tsumeb, Namibia. *N. Jb. Mineral. Mh.*, **1983**, 289-295.

Mereiter, K. (1982): The crystal structure of walpurgite, $(UO_2)Bi_4O_4(AsO_4)_2{\cdot}2H_2O$. *Tschermaks Miner. Petrogr. Mitt.*, **30**, 129-139.

Mereiter, K. & Preisinger, A. (1986): Kristallstrukturdaten der Wismutminerale Atelestit, Mixit und Pucherit. *Österr. Akad. Wiss., Mathem.-Naturwiss. Kl., Sitzungsberichte*, **123**, 79-81.

Mooney, R.C.L. (1958): Crystal structure of tetragonal bismuth arsenate, $BiAsO_4$. *Acta Cryst.*, **1**, 163-165.

Nickel, E.H. & Hitchen, G.J. (1994): The phosphate analog of molybdofornacite. *Mineral. Rec.*, **25**, 203-204.

Nonius (1999): "Collect" data collection software. Nonius, B. V.

Ondruš, P., Skála, R., Císařová, I., Veselovský, F., Frýda, J., Čejka, J. (2002): Description and crystal structure of vajdakite, $[(Mo^{6+}O_2)_2(H_2O)_2As^{3+}{}_2O_5]{\cdot}H_2O$ - a new mineral from Jáchymov, Czech Republic. *Am. Mineral.*, **87**, 983-990.

Otwinowski, Z. & Minor, W. (1997): Processing of X-ray diffraction data collected in oscillation mode. Methods in Enzymology, 276, Macromolecular crystallography A (eds. Carter, C.W. Jr.; Sweet, R.M.) Academic Press 307-326.

Pertlik, F. & Zemann, J. (1982): Neubestimmung der Kristallstruktur des Köchlinits. *Fortschr. Miner. Beih.*, **60**, 162-163

Roberts, A.C., Burns, P.C., Gault, R.A., Criddle, A.J., Feinglos, M.N., Stirling, J.A.R. (2001): Paganoite, $NiBi^{3+}As^{5+}O_5$, a new mineral from Johanngeorgenstadt, Saxony, Germany: description and crystal structure. *Eur. J. Mineral.*, **13**, 167-175.

Schaller, W.T. (1916): Koechlinite (bismuth molybdate), a new mineral. *U.S. Geol. Surv. Bull.*, **610**, 10-34.

Schlegel, F. (2000): Neufunde aus dem Bergrevier Schneeberg/Sachsen, 1995-99 (I). *Lapis*, **25**(2), 31-38.

— (2002): Neufunde und Neubestimmungen aus dem Bergrevier Schneeberg/Sachsen, 1990-2002 (II). *Lapis*, **27**(7/8), 67-72.

Schlegel, F., Schumann, K., Siemroth, J. (1992): Haldenfunde sekundärer Wismutminerale von Schneeberg im Erzgebirge. *Lapis*, **17**(11), 29-36.

Sheldrick, G.M. (1997a): SHELXS-97 Program for the solution of crystal structures. Univ. Göttingen, Germany.

— (1997b): SHELXL-97 Program for crystal structure refinement. Univ. Göttingen, Germany.

Skvortsova, K.V., Sidorenko,G.A., Nesterova, Yu.S., Arapova, G.A., Dara, A.D., Rybakova, L.I. (1971) Sodium betpakdalite and conditions of its formation. *Zap. Vses. Miner. Obshch.*, **100**, 603-611 (cited in Fleischer, M. (1972): New mineral names *Am. Mineral.*, **57**, 1312).

Teller, R.G., Brazdil, J.F., Grasselli, R.K., Jorgensen, J.D. (1984): The structure of gamma-Bismuth Molybdate, Bi_2MoO_6, by powder neutron diffraction. *Acta Cryst.*, **C40**, 2001-2005

Theobald, F.R., Laarif, A., Hewat, A.W. (1984): The structure of koechlinite bismuth molybdate. A controversy resolved by neutron diffraction. *Ferroelectrics*, **56**, 219-237

Wilson, A.J.C. (editor) (1992): International Tables for Crystallography, Vol. C. Kluver, Dordrecht, The Netherlands.

Xiuzhen Yong, Deren Li, Guanxin Wang, Mengxiang Deng, Nansheng Chen, Shuzhen Wang (1989): A study of chiluite - a new mineral in Chilu, Fujian, China. *Acta Miner. Sin.*, **9**, 9-14 (cited in Jambor, J.L. & Puziewicz, J. (1972): New mineral names, *Am. Mineral.*, **76**, 666).

Yvon, K., Jeitschko, W., Parthé, E. (1977): LAZY PULVERIX, a computer program, for calculating X-ray and neutron powder patterns. *J. Appl. Cryst.*, **10**, 73-74.

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