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Nielsbohrite, a new potassium uranyl arsenate from the uranium deposit of Menzenschwand, southern Black Forest, Germany

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Abstract: Nielsbohrite, ideally $K(UO_2)_3(AsO_4)(OH)_4 \cdot H_2O$, is a new mineral species belonging to the secondary mineral assemblage of the uranium deposit of Menzenschwand in the southern Black Forest, Baden-Württemberg, Germany. It is associated with hematite, pyrite, schoepite, metazeunerite and the gangue minerals quartz and barite. Nielsbohrite occurs mainly in euhedral rhombohedron-like crystals reaching 0.15 mm in size, often altered, and showing the forms {001}, {100} or {010}, and {210} or {120}. The mineral is yellow with a vitreous to dull lustre and with a yellowish streak. It is non-fluorescent in ultraviolet light, brittle, and shows an irregular fracture without any visible cleavage. The estimated Mohs hardness is about two, and the calculated density is 5.45–5.65 g/cm^3. Nielsbohrite is biaxial negative, with $n\alpha = 1.756(2)$, $n\beta = 1.764(2)$, and $n\gamma = 1.765(2)$. No pleochroism was observed. The measured 2V angle is 35(5)°, and the calculated 2V angle is 39°, orientation $Y = c$. A strong $r > v$ dispersion has been observed, with anomalous blue-green and reddish brown interference colours. Electron-microprobe analysis gives K_2O 1.90, UO_3 83.34, As_2O_5 10.64, H_2O* 5.07, total 100.95 wt% (*: calculated value). The resulting empirical formula, calculated on the basis of 10 O + 4 OH structural anions, is $(K_{0.430}\square_{0.570})(AsO_4)_{0.987}(UO_2)_{3.106}(OH)_4 \cdot 1.00H_2O$. The single-crystal unit-cell parameters are $a = 8.193(3)$, $b = 11.430(4)$, $c = 13.500(5)$ Å, and $V = 1264.1(8)$ Å^3, with $Z = 4$, space group *Cccm*. The strongest lines of the powder X-ray diffraction pattern [d(in Å)(I)(hkl)] are: 6.71(80)(110), 6.03(100)(111), 3.78(70)(113), 3.33(80)(220), 2.96(60)(024), 2.63(50)(204), 1.942(50)(244). The original crystal structure of nielsbohrite is related to those of minerals of the phosphuranylite group, and was refined to a R_1 factor of 11.04 %. The mineral species and its name were approved by the Commission on New Minerals, Nomenclature and Classifications of the International Mineralogical Association (# IMA 2002-045b).

Key-words: nielsbohrite, new mineral, optical properties, infrared spectrum, crystal structure, potassium uranyl arsenate, Black Forest, Germany.

1. Introduction

Nielsbohrite was found in the uranium deposit situated in the Krunkelbach valley, near the village of Menzenschwand, in the southern Black Forest, Baden-Württemberg, Germany. This locality is a famous occurrence of secondary minerals, in which more than 40 uranium-bearing mineral species were described. Five minerals have been first described from Menzenschwand as new species: arsenuranospathite, joliotite, uranosilite, uranotungstite and arsenovanmeersscheite (Walenta, 1992; Walenta & Theye, 2007). Nielsbohrite now increases this number to six.

The sample, from the collection of W. Oppelt, Triberg, was received by the first author in 1983, and it was soon established, from the Debye-Scherrer X-ray powder diffraction pattern and preliminary electron-microprobe analyses, that we were dealing with a new mineral species. Further single-crystal X-ray diffraction and infrared spectroscopic studies were difficult as only a small amount of material was available. Finally, the new mineral and its name were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (# IMA 2002-045b). The mineral is named for the Danish physicist Niels Hendrik David Bohr (1885–1962). Material is deposited at the Staatliches Museum für Naturkunde in Stuttgart, Germany, and the single crystal used for the structural study at the Laboratory of Mineralogy, University of Liège, Belgium (no 20355).

2. Occurrence and descriptive mineralogy

As already mentioned the new mineral originated from the uranium deposit in the Krunkelbach valley near

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Menzenschwand, but details about its discovery are not known. Probably it was found on the mine dumps. The two specimens on which the following description is based have been provided by W. Oppelt from his collection which in the meantime has changed of hands. The first author (K.W.) received the first specimen in 1983, when the mine was still in operation.

The new mineral occurs mostly in euhedral crystals which are orthorhombic according to the single-crystal study. However, this is not evident from their rhombohedron-like appearance, which could also be interpreted otherwise and indeed was originally considered to be monoclinic. The forms are, in accordance with the orthorhombic setting, {001} bordered by {100} or {010}, and by {210} or {120}. The single-crystal study did not allow to determine the direction of *a* and *b*, and this means that the forms cannot be indexed unequivocally. Under the microscope the interfacial angle between the {001} and the prisms could be measured roughly as 108(1)° in rather good agreement with the angle of 108.9° derived from the X-ray data, if the faces are considered as {210} or {120}. The size of the crystals reaches 0.15 mm. They occur as single crystals or in clusters on quartz and barite in cavities, and are associated with hematite, pyrite, schoepite and metazeunerite.

We obtained two different samples containing nielsbohrite, and while the morphology of the crystals on the two samples is similar, their appearance and transparency are distinct. On the sample first provided, the crystals are not solid but mostly somewhat altered and they disintegrate into powdery aggregates when one attempts to isolate them. They are not transparent and have a dull lustre. In the second sample provided the crystals are well preserved, in part transparent, but unfortunately smaller. Whereas some material of the altered crystals could be obtained later, it was not possible to obtain another sample of the unaltered crystals.

The hydrous solutions in the oxidized zone of the Menzenschwand deposit contain sufficient uranium as $(UO_2)^{2+}$ for the formation of nielsbohrite, which was released by alteration of uraninite. Arsenic can be derived from primary arseniferous minerals such as arsenopyrite, löllingite or safflorite, and K is derived from orthoclase of the granitic country rock.

3. Physical and optical properties

Nielsbohrite is yellow in somewhat different shades; generally it is lemon yellow. The streak is yellowish, the lustre of the transparent crystals is vitreous, that of the altered crystals is dull. Crystals are brittle, without cleavage, and the fracture is irregular. The hardness is about two, that of the altered crystals less. The density has not been measured due to the small size of the crystals, but the calculated density is 5.45 (calculated from structural data) or 5.65 g/cm^3 (calculated from chemical data). No fluorescence could be observed in ultraviolet light.

Optically, nielsbohrite is biaxial negative, with $n\alpha$ 1.756(2), $n\beta$ 1.764(2), $n\gamma$ 1.765(2). The measured 2V angle is 35(5)°, and the calculated 2V angle is 39°, orientation $Y = c$. No pleochroism was observed. The mineral exhibits anomalous blue-green and reddish brown interference colours, due to a strong $r > v$ dispersion.

The compatibility index is 0.101 (poor), according to Mandarino (1981), and by using the *k* (UO_3) value of 0.134 (Piret & Deliens, 1989). This poor compatibility probably results from the low K-content measured by electron-microprobe analysis (see below). By using the ideal composition of nielsbohrite and the density obtained from the structural data, a compatibility index of 0.037 (excellent) is obtained, thus confirming the consistency of the structural model of nielsbohrite.

4. Chemical composition

Chemical analyses (Table 1) were carried out with a Cameca SX 100 electron microprobe (WDS mode), using 15 kV acceleration voltage, 10 nA beam current, and 10 μm beam diameter. A preliminary WDS scan of the new mineral gave U, As, K and O as major constituents. No additional elements are present in amounts detectable by the electron microprobe. The following standards were used: orthoclase (K), synthetic U glass (U) and synthetic GaAs (As). For the determination of U the $M\alpha$ line was used, for that of K the $K\alpha$ line. Due to the unavoidable overlap between the K $K\alpha$ and U $M\beta$ lines, an interference correction for K was applied by measuring pseudo-K on the U standard. The water content could not be measured directly due to lack of material. The mineral is rapidly soluble in cold HNO_3 1:1, H_2SO_4 1:1 and HCl 1:5 without effervescence, thus confirming the absence of CO_2.

The empirical formula, calculated on the basis of 10 O + 4 OH structural anions per formula unit (*pfu*), is $(K_{0.430}\square_{0.570})(AsO_4)_{0.987}(UO_2)_{3.106}(OH)_4\cdot1.00H_2O$. However, the structural investigation of nielsbohrite (see below) showed a K-content higher than that expected from the electron-microprobe measurements. This discrepancy probably results from the poor stability of hydrated uranyl minerals under the electron beam, which can produce dehydration and migration of the

Table 1. Electron-microprobe analysis of nielsbohrite.

	Wt%	Range
K_2O^*	1.90	1.79–2.01
UO_3	83.34	83.04–83.63
As_2O_5	10.64	10.26–11.02
H_2O^{**}	5.07	
Total	100.95	
Cation numbers		
K	0.430	
U	3.106	
As	0.987	
H	6.000	

Analyst T. Theye. Average of two point analyses.
*Corrected for overlap with U.
**Calculated value.

alkalis. As a consequence, the simplified formula of nielsbohrite, $K(UO_2)_3(AsO_4)(OH)_4 \cdot H_2O$, was established taking the structural results into account. This formula requires K_2O 4.38, As_2O_5 10.70, UO_3 79.89, H_2O 5.03, Total 100.00 wt%.

5. Infrared spectroscopy

The infrared spectrum of nielsbohrite was recorded on a IFS-48 Bruker Fourier transform infrared spectrometer, equipped with a IR microscope (Bruker). A beam spot of ~100 μm size, with a wavenumber resolution of 2 cm^{-1}, was applied on the sample. Sample preparation was done by crushing and grinding carefully selected nielsbohrite crystals of 100–200 μm in diameter, between cleaved halite plates. The infrared spectra of thin sample layers were recorded in transmission mode, from 5000 to 600 cm^{-1}.

As shown in Fig. 1, the spectrum is characterized by a very large absorption band centred around 3500 cm^{-1} and corresponding to the OH stretching vibrations, as well as a large domain located around 1000 cm^{-1} and corresponding to UO_2 and AsO_4 vibrations. The detailed assignment of the UO_2 bands (Table 2) was performed in comparison with the IR spectra of haynesite, $(UO_2)_3(OH)_2(SeO_3)_2.5H_2O$ (Čejka *et al.*, 1999) and of vandenbrandeite, $CuUO_2(OH)_4$ (Čejka, 1994). The assignments of AsO_4, OH and H_2O bands were performed according to Farmer (1974). Starting from the antisymmetric stretching vibrations of UO_2 groups at 919 and 854 cm^{-1}, the correlations established by Glebov (1989) and Veal *et al.* (1975) served us to calculate U—O bond distances of 1.75 and 1.80 Å, which are very close the measured bond distances U1—O2 (1.751 Å) and U3—O4 (1.82 Å), respectively (see below).

6. X-ray structural investigation

The X-ray powder-diffraction data were obtained with a 57.3 mm diameter Debye-Scherrer camera using Fe-*K*α radiation (Table 3). The powder pattern was indexed by comparison with the X-ray powder pattern calculated from the structural model, with the program Powdercell (Kraus & Nolze, 1999). This program was also used for obtaining

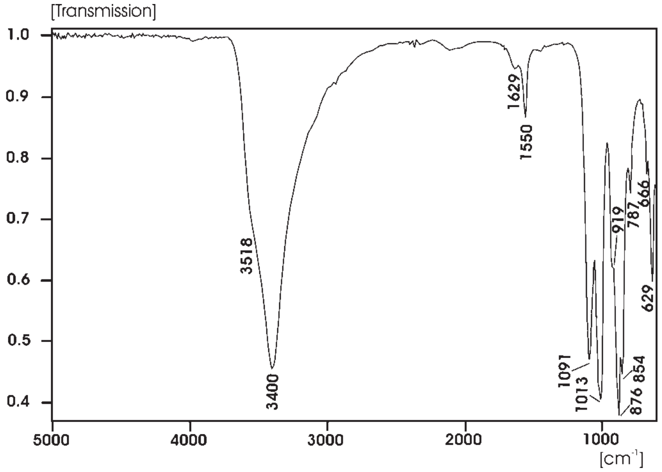

Fig. 1. The infrared spectrum of nielsbohrite.

Table 2. Assignment of the infrared absorption bands of nielsbohrite.

Wavenumber (cm^{-1})	Assignment
3518 (sh)	ν OH (stretching)
3400 (vs)	ν OH (stretching)
1629 (w)	ν_2 H_2O (bending)
1550 (s)	δ UOH (?) (in-plane bending)
1091 (vs)	δ UOH (in-plane bending)
1013 (vs)	δ UOH (in-plane bending)
919 (sh)	ν_3 UO_2 (antisymmetric stretching – U1—O2)
876 (vs)	ν_3 AsO_4 (antisymmetric stretching)
854 (vs)	ν_3 UO_2 (antisymmetric stretching – U3—O4)
787 (w)	ν_1 UO_2 (symmetric stretching)
666 (w)	γ UOH (out-of-plane bending)
629 (s)	γ UOH (out-of-plane bending)

vs = very strong, s = strong, w = weak, sh = shoulder.

Table 3. X-ray powder diffraction data for nielsbohrite.

$I_{meas.}$	$d_{meas.}$	$I_{calc.}$	$d_{calc.}$	*hkl*
80	6.71	51	6.66	110
100	6.03	100	5.99	111
5	4.83	7	4.78	112
20	4.61	–	–	–
70	3.78	45	3.78	113
20	3.48	10	3.48	130
80	3.33	80	3.33	220
20	3.06	12	3.06	114
60	2.96	56	2.95	024
40	2.88	21	2.89	040
20	2.77	11	2.77	133
50	2.63	30	2.63	204
5	2.55	3	2.54	115
20	2.28	6	2.29	313
20	2.22	11	2.23, 2.19	242, 331
5	2.09	2	2.10	314
10	2.03	7	2.04	400
30	1.993	7	1.998	333
50	1.942	29	1.944	244
10	1.886	5	1.888	226
5	1.854	1	1.854	062
20	1.741	10	1.741	260
40	1.677	16	1.678	424
10	1.664	9	1.665	440
5	1.606	2	1.604	511
5	1.572	1	1.572	512
30	1.524	2	1.523	513

Data obtained with a 53.7 mm Debye-Scherrer camera (Fe*K*α). Intensities estimated visually.

The powder pattern, calculated from the structural data with the program Powdercell (Kraus & Nolze, 1999), served to index the observed pattern and to obtain the calculated intensities.

The calculated *d* values were obtained with the program LCLSQ version 8.4 (Burnham, 1991), and correspond to the unit-cell parameters: *a* = 8.154(9), *b* = 11.55(2), and *c* = 13.75(3) Å.

the calculated intensities. The parameters of the orthorhombic unit cell were refined with the program LCLSQ version 8.4 (Burnham, 1991): $a = 8.154(9)$, $b = 11.55(2)$, $c = 13.75(3)$ Å, $V = 1264.1(8)$ Å^3, a:b:c = 0.7168 : 1:1.1811, $Z = 4$, space group *Cccm*. As may be seen from the powder data (Table 3) there is one line that can neither be indexed on the basis of the assumed cell with space group *Cccm*, nor on the basis of the alternative unit cell with space group *P*2/*m* (see discussion below). This line is regarded as due to an impurity or an alteration product of nielsbohrite. The X-ray investigation of the altered crystals did not show any sign of a phase transformation, since powder patterns of the altered and the unaltered crystals are identical.

For the single-crystal study, two tiny crystals of nielsbohrite were measured on an Oxford Diffraction Xcalibur 4-circle diffractometer (Mo$K\alpha$ radiation, $\lambda = 0.71073$ Å), equipped with a Sapphire2 CCD-area detector (Ruhr-Universität Bochum, Germany). Both crystals were poorly crystalline, and exhibited a strong powder-like behaviour. However, one of the crystals (size 40 × 50 × 65 μm) showed some distinct diffraction spots overprinted on the powder pattern. 859 frames with a spatial resolution of 0.75° were collected by the ϕ/ω scan technique, with a counting time of 35 s per frame, in the range $6.82° < 2\theta < 82.90°$ ($-13 \leq h \leq 15, -19 \leq k \leq 18, -23 \leq l \leq 23$). 9563 reflections were extracted from these frames, corresponding to 1919 unique reflections. The unit-cell parameters refined from these reflections are $a = 8.193(3)$, $b = 11.430(4)$, $c = 13.500(5)$ Å, and $V = 1264.1(8)$ Å^3. Data were corrected for Lorenz polarisation and absorption effects, the latter with a numerical method included in the CrysAlisRED package (Oxford Diffraction, 2002).

The crystal structure of nielsbohrite was solved in space group *Cccm,* which was confirmed from systematic absences. Scattering curves for neutral atoms, together with anomalous dispersion corrections, were taken from the *International Tables for X-ray Crystallography, Vol. C* (Wilson, 1992). All atoms were refined anisotropically, except O5 and O6 which showed an extremely anisotropic thermal ellipsoid. For this reason, O6 was split into two close positions, O6 and O6*, which show occupancy factors of 0.67(3) and 0.33(3), respectively. The final conventional R_1 factor, 0.1104, is rather high due to the poor crystallinity of the nielsbohrite crystal. Further details on the intensity data collection and structure refinement are given in Table 4. Final positional and isotropic thermal parameters are given in Table 5, and selected bond distances are given in Table 6. Anisotropic displacement parameters are available from the authors or through the EJM editorial office in Paris.

Table 4. Experimental details for the single-crystal X-ray diffraction study of nielsbohrite.

Dimensions of the crystal (mm)	*ca.*, 0.040 × 0.050 × 0.065
a (Å)	8.193(3)
b (Å)	11.430(4)
c (Å)	13.500(5)
Space group	*Cccm*
Z	4
Calculated density	5.449
Diffractometer	Oxford diffraction Xcalibur with Sapphire2 CCD-area detector
Operating conditions	45 kV, 25 mA
Radiation	Mo$K\alpha$ ($\lambda = 0.71073$ Å)
Scan mode	ϕ/ω scans
$2\theta_{min}$, $2\theta_{max}$	6.82°, 82.90°
Range of indices	$-13 \leq h \leq 15, -19 \leq k \leq 18, -23 \leq l \leq 23$
Measured intensities	9563
Unique reflections	1919
Independent non-zero [$I > 2\sigma(I)$] reflections	741
Absorption correction	Numerical
μ (mm^{-1})	41.17
Extinction coefficient	0.0012(3)
Structure solution program	SHELXS-97 (Sheldrick, 1990)
l.s. refinement program	SHELXL-97 (Sheldrick, 1997)
Refined parameters	55
R_1 (on $I > 2\sigma(I)$)	0.1104
R_1 (all)	0.2197
wR_2 (all)	0.3339
S (goodness of fit)	1.004
Max Δ/σ in the last l.s. cycle	0.000
Max peak and hole in the final ΔF map (e/Å^3)	+5.65 and –5.42

Table 5. Atomic coordinates and isotropic displacement parameters (Å^2) for nielsbohrite.

Site	*x*	*y*	*z*	*Uiso*
U1	0.25	0.25	0.36478(8)	0.0308(4)
K2	0	0	0.5	0.041(3)
U3	0	0.5	0.5	0.0334(5)
As4	0	0.5	0.25	0.0492(12)
O1	0.113(2)	0.4233(15)	0.3272(13)	0.049(4)
O2	0.066(2)	−0.1716(17)	0.1339(10)	0.041(4)
O3	0.677(4)	−0.146(3)	−3.5	0.062(7)
O4	−0.172(3)	0.399(3)	0.5	0.048(6)
O5	0	0	0.25	0.023(5)
O6[a]	0.25	−0.25	0.3816(14)	0.005(3)
O6*[b]	0.25	−0.25	0.315(3)	0.005(3)

[a] 0.67(3) O
[b] 0.33(3) O

The structural formula of nielsbohrite is $K(AsO_4)(UO_2)_3(OH)_4{\cdot}H_2O$, with $Z = 4$. The structure consists of a uranyl arsenate framework composed of $As4O_4$ tetrahedra ($As4{-}O = 1.646$ Å), $U3O_8$ elongated hexagonal bipyramids ($U3{-}O = 1.82$–2.657 Å), and $U1O_7$ pentagonal bipyramids ($U1{-}O = 1.751$–2.43 Å) (Fig. 2). Pairs of uranyl pentagonal bipyramids are connected *via* edge-sharing to two adjacent hexagonal bipyramids (Fig. 2), producing a heteropolyhedral chain topologically identical to those observed in minerals of the phosphuranylite group (Demartin *et al.*, 1991; Locock & Burns, 2003; Locock, 2007). These uranyl chains, which extend parallel to (110)

Table 6. Selected bond distances (Å) for nielsbohrite.

U1—O2	1.751(18) (× 2)	U3—O4	1.82(2) (× 2)
U1—O3	2.258(19) (× 2)	U3—O3	2.21(3) (× 2)
U1—O1	2.334(17) (× 2)	U3—O1	2.657(18) (× 4)
U1—O6*	2.43(4)	Mean	2.336
Mean	2.162		
K2—O2	2.723(17) (× 4)	As4-O1	1.646(17) (× 4)
K2—O4	2.92(2) (× 2)		
Mean	2.789		

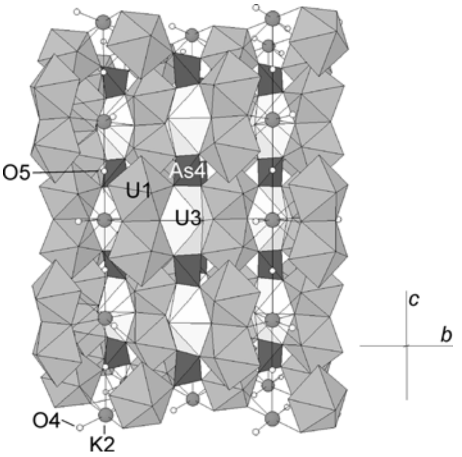

Fig. 2. The crystal structure of nielsbohrite. $As4O_4$ tetrahedra are dark grey, $U1O_7$ pentagonal bipyramids are light grey, and $U3O_8$ hexagonal bipyramids are white. K atoms are grey and (O, OH, H_2O) anions are white.

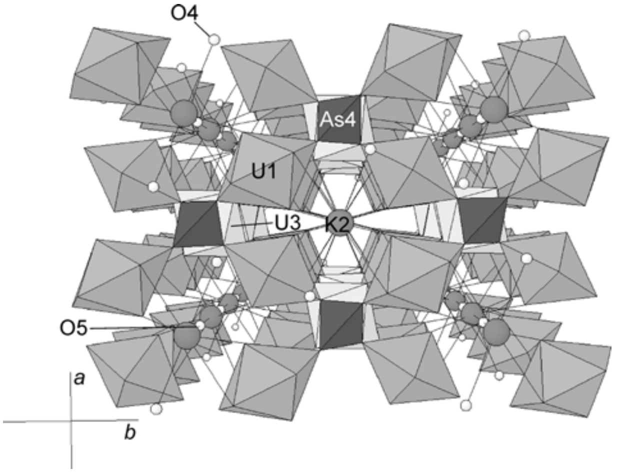

Fig. 3. The crystal structure of nielsbohrite, projected perpendicular to the *c* axis. For key see Fig. 2.

and $(\bar{1}10)$, are connected by edge-sharing with arsenate tetrahedra to form a framework. Each arsenate tetrahedron is linked to two chains by sharing two tetrahedral edges with uranyl hexagonal bipyramids of adjacent chains (Fig. 2). A projection perpendicular to the *c* axis (Fig. 3) shows that the large $K2—O_6$ site (K2—O = 2.723–2.92 Å) and the O5 anion (H_2O molecule, see below) occur in large channels running along the *c* axis, channels that are located between the heteropolyhedral phosphuranylite-type chains.

The bond-valence sums for nielsbohrite were calculated as $s = \exp[(R_0 - R)/B]$, by using R_0 and B values of Brown & Altermatt (1985) or of Burns *et al.* (1997) (U). The bond-valence sums for cations (U1 = 6.46, K2 = 1.05, U3 = 5.72, and As4 = 5.55) are in fairly good agreement with the expected values. O1, O2, and O4 show bond-valence sums of 2.24, 1.98, and 1.67, respectively, indicating that they correspond to O^{2-}, while O3 and O6/O6* show bond-valence sums of 1.38 and 0.47, respectively, confirming their identification as OH^- groups. It is noteworthy that the low bond-valence sum for O4 and the high bond-valence sum for O3, compared to the expected values, probably result from the mixed donor-acceptor roles of these anions. The bond-valence sum for O5 is 0.00, thus indicating that it corresponds to the H_2O molecule occurring in the channels of the nielsbohrite structure (Fig. 3).

The main problem occurring during the structural investigation was the space group determination. A first attempt to determine the unit-cell dimensions of nielsbohrite by using a crystal of another sample suggested a monoclinic unit-cell with $a = 7.11$, $b = 13.76$, $c = 6.98$, $\beta = 108.9°$, $Z = 1$, space group *P*2/*m*. This unit-cell is related to the orthorhombic unit-cell by the matrix [½ ½ 0 \ 0 0 1 \ ½ -½ 0]. Attempts to refine the structure in space group *P*2/*m* did not significantly improve the R_1 factor (11.30 %), induce ''Non Positive Definite'' atoms, and necessitate the introduction of one supplementary K position, thus increasing the K-content of nielsbohrite to *ca.*, 1.5 atoms *pfu*. Starting from the atomic coordinates obtained with the monoclinic model, the program ADDSYM (Le Page, 1987) immediately identified supplementary symmetry elements, thus confirming the orthorhombic *Cccm* space group. Further refinements with a twinned monoclinic model failed, and a careful examination of the X-ray reconstructed photographs did not show supplementary reflections indicative of a larger unit-cell. As a consequence, this orthorhombic model was chosen, even if the monoclinic model can not be definitely ruled out. Unfortunately, the extreme scarcity of the material does not allow us to clarify this point.

7. Comparison with other mineral species and synthetic compounds

The original crystal structure of nielsbohrite has not been previously reported among minerals or synthetic compounds. The only mineral that also contains As, K and U as major constituents is abernathyite, $K_2(UO_2)(AsO_4)_2{\cdot}8H_2O$, which shows a crystal structure related to that of natroautunite (Ross & Evans, 1964). The synthetic tetragonal compounds $K(H_2O)(UO_2AsO_4)_2{\cdot}6H_2O$ (Ross & Evans, 1964) and $KAsUO_6{\cdot}3H_2O$ (Alekseev *et al.*, 2005) have also been reported, but their crystal structure is significantly different from that of nielsbohrite.

As previously mentioned in the crystal structure description, the heteropolyhedral uranyl chains observed in the nielsbohrite structure are topologically identical to those observed in minerals of the phosphuranylite group (Demartin *et al.*, 1991; Locock & Burns, 2003; Locock, 2007). However, the chains of nielsbohrite are assembled to form a framework, while the chains of phosphuranylite-group minerals are linked into sheets by the sharing of polyhedra vertices and edges. In the literature, only two crystal structures based on a framework constituted by phosphuranylite-type chains are reported: the synthetic uranyl phosphate $[(UO_2)_3(PO_4)O(OH)(H_2O)_2](H_2O)$ (Burns *et al.*, 2004), and the mineral althupite, $AlTh(UO_2)[(UO_2)_3O(OH)(PO_4)_2]_2(OH)_3 \cdot 15H_2O$ (Piret & Deliens, 1987). These structures are distinct from that of nielsbohrite.

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