Cuatrocapaite-(NH₄) and cuatrocapaite-(K), two new minerals from the Torrecillas mine, Iquique Province, Chile, related to lucabindiite and gajardoite.

Anthony R. Kampf¹*, Nikita V. Chukanov², Gerhard Möhn³, Maurizio Dini⁴, Arturo A. Molina Donoso⁵ and Henrik Friis⁶

¹Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA
²Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Moscow region, 142432 Russia
³Dr.-J.-Wittemannstrasse 5, 65527 Niedernhausen, Germany
⁴Pasaje San Agustin 4045, La Serena, Chile
⁵Los Algarrobos 2986, Iquique, Chile
⁶Natural History Museum, University of Oslo, Postboks 1172, Blindern, 0318, Oslo, Norway
*E-mail: akampf@nhm.org

Abstract

The new minerals cuatrocapaite-(NH₄) (IMA2018-083) and cuatrocapaite-(K) (IMA2018-084) are the NH₄- and K-dominant members of a series with the general formula (NH₄,K)₃(NaMg□)(As₂O₅)₆Cl₆·16H₂O. Both minerals were found at the Torrecillas mine, Iquique
Province, Chile, where they occur as secondary alteration phases. Both minerals occur as hexagonal tablets up to about 0.3 mm in diameter. They are transparent, with vitreous lustre and white streak. For both, the Mohs hardness is ca. 2½, the crystals are somewhat flexible, but not elastic, the fracture is irregular and the cleavage is perfect on {001}. The measured densities are 2.65(2) and 2.76(2) g/cm³ for the NH₄- and K-dominant species, respectively.

Optically, cuatrocapaite-(NH₄) is uniaxial (−) with ω = 1.779(3) and ε = 1.541(3) and cuatrocapaite-(K) is uniaxial (−) with ω = 1.777(3) and ε = 1.539(3) (white light). The minerals are insoluble in acids, but decompose in NaOH(aq). The empirical formulas, determined from electron-microprobe analyses, are

\[(NH_4)_{2.48}Na_{1.66}Mg_{0.87}K_{0.09}(As_{12}O_{18.05})Cl_{5.88}·16.02H_2O\] and

\[K_{2.68}Na_{1.33}Mg_{0.93}(NH_4)_{0.31}(As_{12}O_{18.01})Cl_{6.16}·16.04H_2O\]. The minerals are trigonal, space group \(R-3m\); the cuatrocapaite-(NH₄) cell parameters are \(a = 5.25321(19)\) Å, \(c = 46.6882(19)\) Å, \(V = 1115.80(9)\) Å³ and \(Z = 1\); the cuatrocapaite-(K) cell parameters are \(a = 5.2637(15)\) Å, \(c = 46.228(8)\) Å, \(V = 1109.2(7)\) Å³ and \(Z = 1\). The structures, refined for cuatrocapaite-(NH₄) to \(R_1 = 1.78%\) for 544 \(I_o > 2σI\) reflections, contain four types of layers: (1) a planar neutral As₂O₃ (arsenite) sheet, (2) an \((NH_4^+,K^+)\) layer that links adjacent arsenite sheets, (3) a Cl⁻ layer placed on the As side of each arsenite and (4) a layer containing partially occupied Na, Mg and H₂O sites that is flanked on either side by Cl layers. The layer sequence for the type 1, 2 and 3 layers is identical to the Cl–As₂O₃–K–As₂O₃–Cl layer sequence in the structures of lucabindiite and gajardoite.

**Keywords:** cuatrocapaite-(NH₄); cuatrocapaite-(K); new mineral; arsenite; crystal structure; lucabindiite; gajardoite; Torrecillas mine, Chile
Introduction

The small, long-inactive Torrecillas mine in the northern Atacama Desert of Chile was probably discovered and first worked during the guano mining boom of the early 19th century (Mortimer, et al., 1971). The once-important Pabellón de Pica guano deposit is only about 7 km north of Torrecillas Hill. Although the veins that were exploited at Torrecillas are particularly rich in arsenic, the early miners were most likely working the veins for copper and, perhaps, were hoping to find gold. The deposit apparently was worked later for arsenic, as reported by Pimentel (1978), who also noted that the mine was probably finally abandoned several years prior to 1950. Based upon the very limited extent of the workings, the mine clearly was never a significant producer.

In recent years, our investigations on the minerals of this unusual deposit have yielded many new mineral species. Including the two new minerals reported herein, cuatrocapaite-(NH₄) and cuatrocapaite-(K), seventeen new minerals have now been described from this deposit. All of these, except leverettite, CoCu₃Cl₂(OH)₆ (Kampf et al., 2013), contain essential arsenic. Twelve are arsenates and four are arsenites [see Kampf et al. (2019) for a complete listing]; cuatrocapaite-(NH₄) and cuatrocapaite-(K) are arsenites.

The name “cuatrocapaite” is in allusion to the structure, which consists of four (cuatro in Spanish) different types of layers (capa in Spanish): (1) [As₂O₃], (2) [(NH₄),K], (3) [Cl₆] and (4) [(Na,Mg,□)₃(H₂O)₁₆]. The -(NH₄) and -(K) suffixes indicate the dominant cations in the large-cation layer (2). The IPA pronunciation of cuatrocapaite is (/kwaˈtroʊ ˈkaː paː art/).

The new minerals and their names, cuatrocapaite-(NH₄) (IMA2018-083) and cuatrocapaite-(K) (IMA2018-084), have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association. The description of cuatrocapaite-(NH₄) is based upon four cotype specimens. Three are deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition...
Boulevard, Los Angeles, CA 90007, USA, catalogue numbers 66984, 66985 and 66986. One is deposited in the collection of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 5255/1. The description of cuatrocapaite-(K) is based upon one holotype specimen deposited in the collections of the Natural History Museum of Los Angeles County, catalogue number 66987.

**Occurrence**

The Torrecillas mine is located on Torrecillas Hill, Iquique Province, Tarapacá Region, Chile (approximately 20°58′13″S, 70°8′17″W). Four different rock units are exposed on the hill. The Coastal Range Batholith (mainly gabbros) extends from the seashore to the Pan-American Road along the base of Torrecillas Hill. At the foot of Torrecillas Hill is a small area of contact metamorphic rocks in which garnet crystals occur in metamorphosed shales. Higher on the hill, the rocks are predominantly porphyritic andesitic lavas of the Jurassic La Negra Formation (cf. Oliveros et al., 2007). The Torrecillas deposit, in which the new mineral is found, consists of two main veins rich in secondary arsenic and copper minerals that intersect metamorphosed marine shales and lavas. These mineralized veins are genetically related to the aforementioned porphyritic andesitic lavas. More information on the geology and mineralogy of the area is provided by Gutiérrez (1975).

The rare secondary chlorides, arsenates and arsenites have been found at three main sites on the hill: an upper pit measuring about 8 m long and 3 m deep, a lower pit about 100 m from the upper pit and measuring about 5 m long and 3 m deep, and a mine shaft adjacent to the lower pit and lower on the hill. Cuatrocapaite-(NH₄) was found in November of 2015 in a recent excavation a few meters above the shaft by one of the authors (AAMD). Cuatrocapaite-(K) was found in January of 2016 near the upper pit by another of the authors (GM), who also collected additional cuatrocapaite-(NH₄) specimens.
Both new minerals are low-temperature secondary alteration phases occurring on matrix consisting of native arsenic, arsenolite and pyrite. Cuatrocapaite-(NH₄) is also associated with lavendulan, lucabindiite (I-rich), magnesiokoritnigite and torrecillasite. Cuatrocapaite-(K) is also associated with anhydrite, gypsum, lavendulan and torrecillasite. The secondary arsenic-rich assemblages at the Torrecillas deposit are interpreted as having formed under hyperarid conditions from the oxidation of native arsenic, and possibly other As-bearing primary phases, coupled with reaction with underground brines rich in mobile cations such as K⁺, Na⁺, NH₄⁺, Ca²⁺ and Mg²⁺ (cf. Cameron et al., 2007). Following the exhumation of Torrecillas Hill, it is possible that long-term exposure to the frequent dense coastal fogs (cf. Rech et al., 2003; Wang et al., 2014) caused continued near-surface alteration coupled with very late-stage secondary mineral formation.

Physical and optical properties

Both cuatrocapaite-(NH₄) and cuatrocapaite-(K) occur as hexagonal plates, flattened on {001} and bounded by {100}, up to about 300 μm in diameter. The pyramidal forms {10ℓ} and {01ℓ} are present on some crystals, with measurements on cuatrocapaite-(NH₄) plates indicating ℓ values in the 12 to 18 range. Cuatrocapaite-(NH₄) plates sometimes grow in vermiciform stacks (Fig. 1) and in satin-spar-like vein fillings (Fig. 2) and the mineral is also found as white powdery coatings. Most cuatrocapaite-(K) crystals have been observed in massive intergrowths, but freestanding crystals in vugs do occur (Fig. 3). No twinning was observed for either mineral. Lucabindiite crystals, occurring in association with cuatrocapaite-(NH₄), are very similar in appearance, but exhibit apparent twinning by rotation on [001] (Fig. 4).

Crystals are colourless and transparent, with a white streak. Crystals have vitreous to pearly lustre, while vein fillings of cuatrocapaite-(NH₄) have silky lustre. The minerals do not
fluoresce in long- or short-wave ultraviolet light. The Mohs hardness for both is 2½, based on scratch tests, and thin plates are flexible, but not elastic. Cleavage is perfect on {001}. The densities for cuatrocapaite-(NH₄) and cuatrocapaite-(K), measured by floatation in methylene iodide - toluene are 2.65(2) and 2.76(2) g/cm³, respectively, and their calculated densities, based on the empirical formulas, are 2.667 and 2.771 g/cm³, respectively.

At room temperature, the minerals are not readily soluble in water or acids (including concentrated HCl, H₂SO₄ and HNO₃). They rapidly decompose in aqueous solution of NaOH forming a nearly transparent residue of Mg(OH)₂. As added confirmation for the presence of NH₄⁺ in cuatrocapaite-(NH₄), a microchemical test was performed. The mineral was heated in a melting-point tube, yielding sublimates (from hot to cold) presumed to be (1) As₂O₅ (as arsenolite octahedra), (2) NH₄Cl and (3) H₂O. When placed in Na₃[Co(NO₂)₆] solution, the presumed NH₄Cl sublimate yielded an orange precipitate of (NH₄)₂Na[Co(NO₂)₆], thereby confirming the presence of NH₄⁺.

Optically, both minerals are uniaxial (−) and nonpleochroic. The indices of refraction for cuatrocapaite-(NH₄) are ω = 1.779(3) and ε = 1.541(3) and those for cuatrocapaite-(K) are ω = 1.777(3) and ε = 1.539(3) (measured in white light). The Gladstone-Dale compatibilities 1 – (Kᵣ/Kᵅ) for the empirical formulas are both 0.019, in the range of superior compatibility (Mandarino, 2007).

**Infrared spectroscopy**

In order to obtain IR absorption spectra, powdered samples were mixed with anhydrous KBr, pelletized, and analyzed using an ALPHA FTIR spectrometer (Bruker Optics) at a resolution of 4 cm⁻¹. Sixteen scans were collected for each mineral. The IR spectrum of an analogous pellet of pure KBr was used as a reference.
Absorption bands in the IR spectrum of cuatrocapaite-(NH₄) (curve 1 in Figure 5) and their assignments are (cm⁻¹; s – strong band, w – weak band, sh – shoulder): 3440sh, 3413s, 3370sh (O–H stretching vibrations of H₂O molecules), 3259 (N–H stretching vibrations of ammonium cations), 2035w (combination mode), 1652, 1630sh (bending vibrations of H₂O molecules), 1425sh, 1410 (bending vibrations of ammonium cations), 1125w (broad; possibly, overlapping bands of combination modes), 673s, 593s (As³⁺–O stretching vibrations), 455 (Mg–O stretching vibrations combined with librational vibrations of H₂O molecules). The assignment was made based in accordance with ranges for characteristic bands of NH₄⁺ cations, H₂O molecules, Mg–O and As³⁺–O bonds indicated by Chukanov and Chervonnyi (2016) based on a representative collection of IR spectra of minerals (Chukanov, 2014). In particular, the strongest band of Mg–O stretching vibrations is observed in the range 430 – 460 cm⁻¹; the strongest band of As³⁺–O stretching vibrations of isolated AsO₃³⁻ groups are observed in the range 500 – 610 cm⁻¹ and shift towards somewhat higher values as a result of polymerization of AsO₃ triangles. In particular, the strongest IR bands of As³⁺–O stretching vibrations are observed at 545 and 610 cm⁻¹ for Pb₅(AsO₃)Cl₇, 556, 605 and 641 cm⁻¹ for leiteite, 628 and 654 cm⁻¹ for manganarsite, 532, 568 and 656 cm⁻¹ for stenhuggarite (Chukanov, 2014). It is to be noted that characteristic bands of As⁴⁺–O stretching vibrations are observed in the range from 750 to 900 cm⁻¹.

Absorption bands in the IR spectrum of cuatrocapaite-(K) (curve 2 in Figure 5) and their assignments are (cm⁻¹): 3530sh, 3478sh, 3406s, 3355sh (O–H stretching vibrations of H₂O molecules), 3254 (N–H stretching vibrations of ammonium cations), 2035w (combination mode), 1652, 1622 (bending vibrations of H₂O molecules), 1419w (bending vibrations of ammonium cations), 1125w (broad; possibly, overlapping bands of combination modes), 670s, 598s (As³⁺–O stretching vibrations), 455 (Mg–O stretching vibrations combined with librational vibrations of H₂O molecules).
For both minerals, splitting of the band of bending vibrations of H$_2$O molecules (a non-degenerate mode) indicates the presence of locally non-equivalent water molecules in the structure. The IR spectrum of cuatrocapaite-(NH$_4$) differs from that of cuatrocapaite-(K) in much higher intensities of the NH$_4^+$ bands.

**Composition**

Chemical analyses (3 points for each mineral) were carried out using an electron microprobe (EDS mode, 20 kV, 600 pA. Attempts to use WDS mode, with higher beam current, were unsuccessful because of the instability of the minerals. For cuatrocapaite-(NH$_4$), the beam was rasterized on an area 16 x 16 μm to minimise sample damage. Also for cuatrocapaite-(NH$_4$), N was analysed by gas chromatography of products of ignition at 1200°C in oxygen flow in oxygen flow, by means of a Vario Micro cubeanalyser (Elementar GmbH, Germany). For cuatrocapaite-(K), it was possible to estimate the content of NH$_4$ from the IR spectrum using cuatrocapaite-(NH$_4$) as a standard because in both minerals NH$_4^+$ has identical local environments.

For both minerals, H$_2$O was calculated from the idealized formula. Contents of other elements with atomic numbers >8 are below detection limits. Analytical data are given in Table 1.

The charge-balanced empirical formulas for cuatrocapaite-(NH$_4$) and cuatrocapaite-(K) (based on 12 As apfu) are (NH$_4$)$_{2.48}$Na$_{1.66}$Mg$_{0.87}$K$_{0.09}$(As$_{12}$O$_{18.05}$)Cl$_{5.88}$·16.02H$_2$O and K$_{2.68}$Na$_{1.33}$Mg$_{0.93}$(NH$_4$)$_{0.31}$(As$_{12}$O$_{18.01}$)Cl$_{6.16}$·16.04H$_2$O, respectively. The simplified formula for both minerals is (NH$_4$,K)$_3$(Na,Mg,□)$_3$(As$_2$O$_3$)$_6$Cl$_6$·16H$_2$O (with K preceding NH$_4$ in the formula of the K-dominant phase). The ideal formula for cuatrocapaite-(NH$_4$) is (NH$_4$)$_3$NaMg·(As$_{12}$O$_{18}$)Cl$_6$·16H$_2$O, which requires (NH$_4$)$_2$O 4.37, Na$_2$O 1.73, MgO 2.25,
As₂O₃ 66.34, Cl 11.89, H₂O 16.11, –O=Cl –2.68, total 100.00 wt%. The idealized formula for cuatrocapaite-(K) is K₃NaMg₋₋₋₋(As₁₂O₁₈)Cl₆·16H₂O, which requires K₂O 7.63, Na₂O 1.67, MgO 2.18, As₂O₃ 64.07, Cl 11.48, H₂O 15.56, –O=Cl –2.59, total 100.00 wt%.

X-ray crystallography and structure refinement

Powder X-ray studies were carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with monochromatic MoKα radiation. A Gandolfi-like motion on the φ and ω axes was used to randomize the samples and observed d-values and intensities were derived by profile fitting using JADE 2010 software (Materials Data, Inc.). The powder data for cuatrocapaite-(NH₄) and cuatrocapaite-(K), presented in Tables 2 and 3, respectively, are quite similar and show good agreement with the patterns calculated from the structure refinements. Unit-cell parameters refined from the powder data using JADE 2010 with whole pattern fitting are \(a = 5.2501(7)\) Å, \(c = 46.639(8)\) Å and \(V = 1113.3(4)\) Å³ for cuatrocapaite-(NH₄) and \(a = 5.2637(16)\) Å, \(c = 46.228(19)\) Å and \(V = 1109.2(8)\) Å³ for cuatrocapaite-(K).

Initial single-crystal X-ray studies were carried out for both cuatrocapaite-(NH₄) and cuatrocapaite-(K) using the same diffractometer and radiation used for the powder studies. Crystals of cuatrocapaite-(K) are generally of poorer quality than those of cuatrocapaite-(NH₄) and our structure data for cuatrocapaite-(K), while confirming it to be isostructural with cuatrocapaite-(NH₄), yielded a much poorer refinement \(R_1 = 6.97\%\) for 263 reflections with \(I_o > 2\sigma I\). Rather than report this refinement, herein we provide the details only for the structure refinement for cuatrocapaite-(NH₄). Nevertheless, we confirm that the refinement for cuatrocapaite-(K) is consistent with nearly full occupancy of K at the (K,NH₄) site.

The final cuatrocapaite-(NH₄) structure data were collected on a Rigaku Synergy-S diffractometer equipped with a HyPix-6000HE detector at the Natural History Museum,
University of Oslo using monochromatized MoKα radiation. The Rigaku CrysAlisPro software package was used for processing the structure data, including the application of a shape-based absorption correction. An initial structure model was obtained by the charge-flipping method using SHELXT (Sheldrick, 2015a) in the space group \( R-3m \). Refinement proceeded by full-matrix least-squares on \( F^2 \) using SHELXL-2016 (Sheldrick, 2015b). A difference Fourier map failed to reveal the locations of the H atoms associated with the NH\(_4^+\) cation or with the two partially occupied OW sites. The H sites associated with the NH\(_4^+\) are presumed to be disordered, as is commonly the case. The only difference-Fourier peak \( > 0.42 \) \( e/\text{Å}^3 \) has a magnitude of 1.21 \( e/\text{Å}^3 \) (which refines to \( <5\% \) occupancy by O). This peak at \([\frac{1}{3}, \frac{1}{3}, 0.391]\), in the centre of the “cavities” in the As\(_2\)O\(_3\) (arsenite) sheet and only 1.42 Å from the Cl site, is assumed to be a refinement artefact. The data collection and refinement details are given in Table 4, atom coordinates and displacement parameters in Table 5 and selected bond distances in Table 6.

**Description of the structure**

The structure of cuatrocapaite-(NH\(_4\)) (Fig. 6) contains four types of layers: (1) a planar neutral As\(_2\)O\(_3\) (arsenite) sheet with hexagonal symmetry (Figure 7a), (2) an NH\(_4^+\) layer that links adjacent arsenite sheets via bonds to their O atoms, (3) a Cl\(^-\) layer placed on the As side of each arsenite sheet with the Cl atoms forming long bonds to the As atoms and (4) a layer containing partially occupied Na, Mg and H\(_2\)O sites (Figs. 7b, 7c and 7d) that is flanked on either side by Cl layers. The Cl–As\(_2\)O\(_3–\)NH\(_4^+–\)As\(_2\)O\(_3–\)Cl layer sequence is identical to the Cl–As\(_2\)O\(_3–\)K–As\(_2\)O\(_3–\)Cl layer sequence in the structures of lucabindiite (Garavelli *et al.*, 2013) and gajardoite (Kampf *et al.*, 2016). In lucabindiite, this sequence repeats itself with no intervening layers, while gajardoite incorporates a disordered Ca-H\(_2\)O layer and cuatrocapaite-(NH\(_4\)) incorporates a disordered Na-Mg-H\(_2\)O layer. Based on the low
occupancies of the sites in the Na-Mg-H\(_2\)O layer and the placements of the H\(_2\)O groups around the cations (Figs. 7b, 7c and 7d), the Na and Mg coordination polyhedra in this layer appear to be isolated, that is, not to be linked to one another. Note that the short Mg–OW\(_a\) distance of 1.985 Å and the short Na–OW\(_b\) distance of 1.721 Å do not correspond to bonds; these OW sites are vacant when the nearby cation sites are occupied.

The bond valences sums based on the As\(^{3+}\)–O parameters from Gagné and Hawthorne (2015), As\(^{3+}\)–Cl from Brese and O'Keeffe (1991) and NH\(_4\)\(^+\)–O from García-Rodríguez et al. (2000) are As1 = 2.98, As2 = 3.00, O = 2.08, N(NH\(_4\)) = 1.00 and Cl = 0.24 \(vu\). The Cl BVS does not include hydrogen bond contributions from the partially occupied H\(_2\)O groups; however, very low BVS values are also observed for Cl in the lucabindiite (0.31 \(vu\)) and gajardoite (0.24 \(vu\)) structures, a phenomenon likely caused by the repulsive effect of the lone electron pair of the As\(^{3+}\). The calculation of the BVS values for the components of the Na-Mg-H\(_2\)O layer is problematic because of the disorder and partial occupancies. Note that, while the Na and Mg site assignments are based upon bond lengths, the Mg–OW\(_b\) distance (2.230 Å) suggests that some Na may occupy this site, as well.

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Mortimer C., Saric N. and Cáceres R. (1971) *Apuntes sobre algunas minas de la región costera de la provincia de Tarapacá*. Instituto de Investigaciones Geológicas, Santiago de Chile, Chile.


Figure 1. Cuatrocapaite-(NH$_4$) tablets, some in vermiform stacks, with acicular torrecillasite; field of view 0.6 mm across.

Figure 2. Cuatrocapaite-(NH$_4$) satin-spar-like vein filling; field of view 1.7 mm across.
Figure 3. Cuatrocapaite-(K) tablets; field of view 0.4 mm across.

Figure 4. Lucabindiite tablets exhibiting apparent twinning by rotation on [001]; field of view 0.63 mm across.
Figure 5. Powder IR absorption spectra of (1) cuatrocapaite-(NH₄) and (2) cuatrocapaite-(K).
Figure 6. The structure of cuatrocapaite-(NH$_4$).
Figure 7. Selected layer components in the structure of cuatrocapaita-(NH₄) viewed down c: (a) the As₂O₃ (arsenite) layer, (b) the Na-Mg-H₂O layer, (c) the Na-H₂O portion of the Na-Mg-H₂O layer, (d) the Mg-H₂O portion of the Na-Mg-H₂O layer. The unit cell outline is shown.
Table 1. Analytical data (wt%) for cuatrocapaite-(NH₄) and cuatrocapaite-(K).

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* Measured by gas chromatography for cuatrocapaite-(NH₄); estimated by IR spectroscopy for cuatrocapaite-(K).

§ Calculated based on the ideal formula.
Table 2. Powder X-ray data (d in Å) for cuatrocapaite-(NH₄).

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Table 3. Powder X-ray data (d in Å) for cuatrocapaite-(K).

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Table 4. Data collection and structure refinement details for cuatriopaite-(NH₄).

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<td>X-ray radiation</td>
<td>MoKα (λ = 0.71073 Å)</td>
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<tr>
<td>Temperature</td>
<td>293(2) K</td>
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<td>Structural Formula*</td>
<td>[(NH₄)₂.65K₀.35]Σ₂(Na₀.72Mg₀.79)Σ₂.51(As₂O₃)₆Cl₆·15.44H₂O</td>
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<tr>
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<td>Unit cell dimensions</td>
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<tr>
<td>V</td>
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<td>Density (for above formula)</td>
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<tr>
<td>Absorption coefficient</td>
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<td>F(000)</td>
<td>850</td>
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<tr>
<td>Crystal size</td>
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<td>0 range</td>
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<td>Index ranges</td>
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<td>Reflections with I₀ &gt; 2σI</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
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<td>Parameters / restraints</td>
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<td>R indices (all data)</td>
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<tr>
<td>Largest diff. peak / hole</td>
<td>+1.21 / −0.67 e/A³</td>
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\[
R_{\text{int}} = \frac{\Sigma|F_o^2 - F_c^2|/\Sigma|F_o^2|}{\Sigma|F_o^2|}. \text{GoF} = S = \left\{ \Sigma[w(F_o^2 - F_c^2)^2/(n-p)] \right\}^{1/2}. R_1 = \Sigma|F_o^2|/|F_c^2|/\Sigma|F_o^2|. wR_2 = \left\{ \Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\right\}^{1/2}. w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP] where a is 0.0305, b is 0 and P is [2F_o^2 + Max(F_o^2,0)]/3.
\]

* The structural formula reflects the refined site occupancies; no effort has been made to balance the net charge of this formula, which has a net charge of +0.3.
Table 5. Atom coordinates and displacement parameters (Å²) for cuatrocapaite-(NH₄).

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* Site occupancies: N = 0.884(9)N/0.116(9)K, Na = 0.287(9), Mg = 0.264(10), OWa = 0.303(13), OWb = 0.277(8).

Table 6. Selected bond distances (Å) for cuatrocapaite-(NH₄).

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* Too short for cation–O bonds.