

Zeitschrift: Archives des sciences et compte rendu des séances de la Société
Herausgeber: Société de Physique et d'Histoire Naturelle de Genève
Band: 54 (2001)
Heft: 1

Artikel: Theoparacelsite, Cu₃(OH)₂As₂O₇, a new mineral : its description and crystal structure
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DOI: <https://doi.org/10.5169/seals-740511>

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THEOPARACELSITE, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, A NEW MINERAL: ITS DESCRIPTION AND CRYSTAL STRUCTURE

BY

Halil SARP¹ & Radovan ČERNÝ²

ABSTRACT

Theoparacelsite, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, a new mineral: its description and crystal structure. - Theoparacelsite, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, was found in the old copper mines of Roua (Alpes-Maritimes, France), associated with olivenite, cornubite, clinotyrolite, connellite, brochantite, malachite, trippkeite, pharmacosiderite, strashimirite, gilmarite, native copper, cuprite, algodonite and domeykite. It forms aggregates in geodes of cuprite (1mm diameter) formed by xenomorph crystals (0.2 x 0.1 x 0.05 mm maximum dimension), rectangular elongated crystals (90 x 10 x 5 μm), perfect little rectangular crystals (10 x 7 x 2 μm), equidimentional crystals blunted at their extremities (20 μm), pseudomorphs after thin acicular crystals of olivenite, or finally in very fine grained aggregates. The dark pistachio green rectangular crystals are elongated along b , flattened on {001}, and have a perfect cleavage on {001}. They are not twinned. The mineral is orthorhombic, $Pmma$, $a = 8.3212(8)$, $b = 2.9377(3)$, $c = 4.6644(5)$ \AA , $V = 114.02(2)$ \AA^3 , $Z = 2/3$, and $D_{\text{calc}} = 4.72$ (1) g/cm^3 . The strongest lines in the X-ray powder diffraction pattern (d_{obs} in \AA , (hkl), I_{vis}) are: 3.104, (201), 100; 2.486, (011), 70; 2.400, (210), 25; 1.672, (212), 30; 1.596, (411), 25; 1.330, (601)(221), 25. The Mohs' hardness could not be measured. Luster is vitreous to adamantine, streak is yellowish green; crystals are biaxial (+) with $\alpha = 1.81(1)$, $\beta = 1.82(1)$, $\gamma = 1.86(1)$ at 590 nm; $2V_{\text{obs}} = 57(3)^\circ$, $2V_{\text{calc}} = 54(1)^\circ$. Pleochronism is moderate with $\gamma =$ dark green pistachio, $\beta =$ olive green, $\alpha =$ light olive green. The crystal structure was solved by direct methods (MoK α radiation) and refined using 207 observed unique reflections to $R = 0.063$, $R_w = 0.064$. The structure of theoparacelsite is disordered and formed by (001) sheets of CuO_6 octahedra with the composition CuO_3 . The sheets are linked in the c direction by chains of AsO_4 tetrahedra parallel to b and occupied from 2/3 giving so the composition $\text{As}_{2/3}\text{O}_3$.

Key-words: theoparacelsite, new mineral, powder pattern, crystal structure, arsenate, copper.

INTRODUCTION

Theoparacelsite, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, is a new mineral discovered in samples collected by Danielle Mari, Gilbert Mari and Pierre Rolland in the old copper mines of Roua (North and South group, municipality of Guillaumes and Daluis respectively), which are situated NW of the Alpes-Maritimes department (France), about 50 km from Nice.

The mineral name honors Philippus Theophrastus Aureolus Bombastus von Hohenheim, called Paracelse (1493-1541). The name Paracelse is a Greek-roman translation of Hohenheim which means «close to the sky». He was an important Swiss

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physician, chemist, alchemist and doctor who also worked in mineralogy (*De Mineralibus*, *De Elemento Aquae & Fructibus eius*). He is often misunderstood by people ignoring vocabulary, customs and difficulties encountered by scientists of the XVIth century. The history learns us that his purposes were warped! Even now, some contemporary journals criticized him wrongly. Nowadays, he is known in toxicology for having said: «All is poison, nothing is poison, it is the dosage which makes the poison».

The mineral and mineral name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association.

The type material is preserved in the Department of Mineralogy of the Natural History Museum of Geneva, Switzerland, under reference no. 447.010.

OCCURRENCE

The Barrot Dome, in the north-eastern part of the Alpes-Maritimes area (France), is characterized by the presence of numerous showings of cupriferous ore. The metallogeny and geology of this Dome has been studied by VINCHON (1984) and MARI (1992). The new mineral described occurs in the Roua copper occurrences (North and South group) in the upper part of the Var valley (the Daluis gorge) at the western margin of the Barrot Dome. In this ore deposit, the cupriferous mineralisation is hosted in a gangue formed by dolomite, calcite and aragonite, and consists of native copper, cuprite, domeykite, algodonite, koutekite, native gold and native silver. Detailed mineralogical study of this ore deposit produced several secondary, rare and unknown mineral species (SARP *et al.*, 1994, 1995, 1996, 1999). The new mineral described here occurs in small geodes of cuprite in association with olivenite, cornubite, clinotyrolite, connelitte, brochantite, malachite, trippkeite, pharmacosiderite, strashimirite, gilmarite (SARP & ČERNÝ, 1999), native copper, cuprite, algodonite and domeykite.

PHYSICAL AND OPTICAL PROPERTIES

Theoparacelsite occurs as aggregates found in geodes of cuprite (1 mm diameter) which are formed by: xenomorph crystals of maximum size 0.2 x 0.1 x 0.05 mm, rectangular elongated crystals of maximum size 90 x 10 x 5 μm , perfect little rectangular crystals (10 x 7 x 2 μm), equidimensional crystals blunted at their extremities ($\sim 20 \mu\text{m}$), pseudomorphs after thin acicular crystals of olivenite (Fig. 1) and finally in powder. The rectangular crystals are elongated parallel to b, flattened on {001}, and have one perfect {001} cleavage; they are not twinned. The most developed forms are {001}, {010}, {100}, {110} and {101}. The crystals are dark pistachio green, translucent, with vitreous to adamantine lustre and yellowish green streak. The mineral is brittle with conchoidal fracture. The Moh's hardness could not be measured. The density could not be determined owing to the small quantity of the mineral. It sinks rapidly in Clerici solution. The calculated density is 4.72(1) g/cm^3 based on the ideal formula. The mineral is soluble in HCl. It is nonfluorescent and has medium pleochroism: γ = dark green pistachio; β = olive green; α = light olive green. Theoparacelsite is biaxial

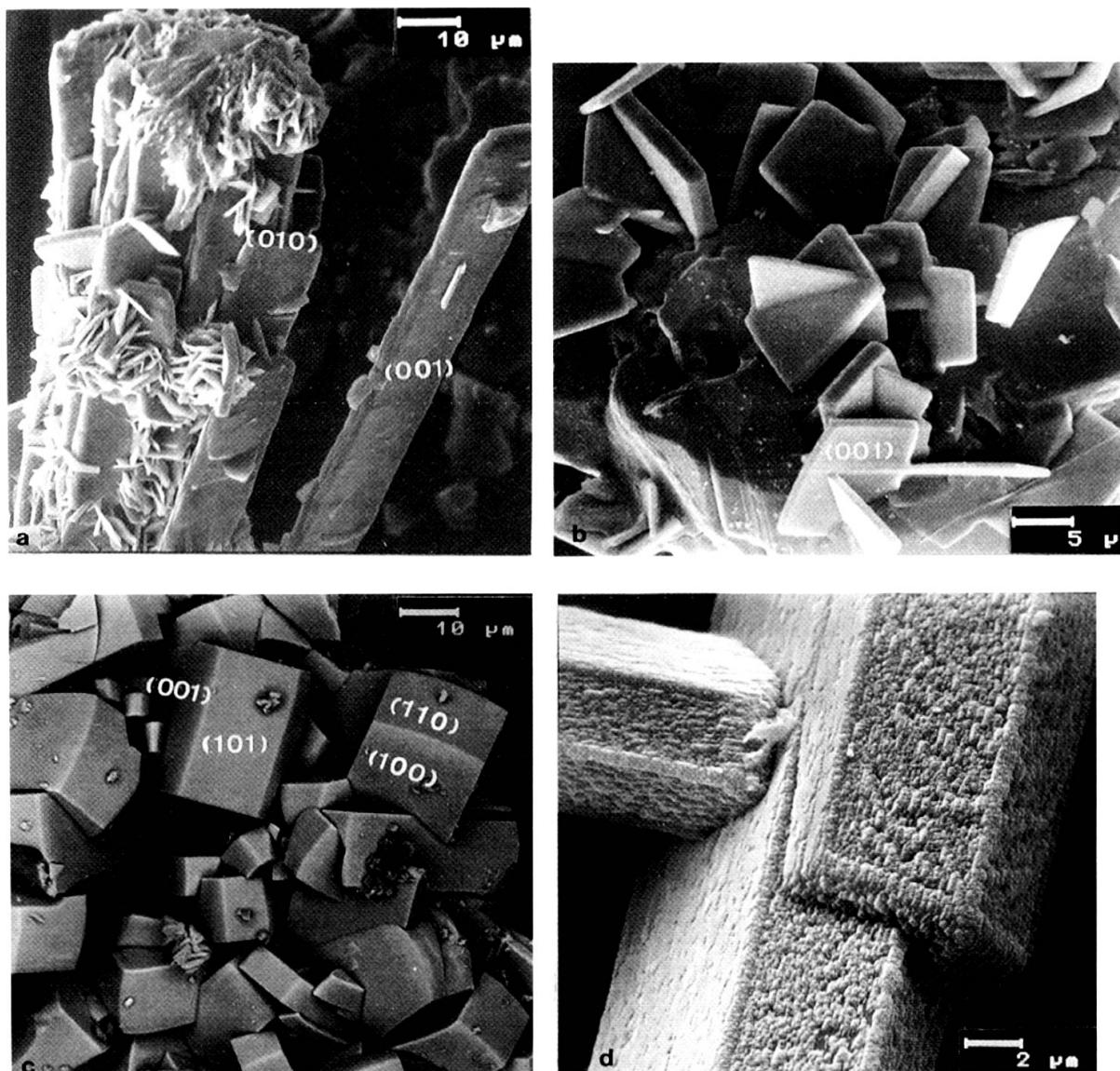


FIG. 1.

SEM images of the different morphologies of theoparacelsite crystals, a) rectangular crystals elongated in the b axis direction; aggregates of small crystals are cornubite, b) perfect little rectangular crystals, c) equidimensional crystals blunted at their extremities, d) pseudomorphs after olivenite crystals.

positive, with $\alpha = 1.81(1)$, $\beta = 1.82(1)$, $\gamma = 1.86(1)$ (determined at 589 nm), $2V_{\text{obs}} = 57(3)^\circ$ and $2V_{\text{calc}} = 54(1)^\circ$. The index of refraction was to be measured rapidly due to the fact that the mineral is attacked by Cargille's liquids of refractive index > 1.80 . The dispersion ($r > v$) is moderate. The optical orientation is: $\alpha = a$, $\beta = c$, $\gamma = b$.

CHEMICAL COMPOSITION

Theoparacelsite was chemically analyzed with a Cameca electron microprobe, using a beam size of $10 \mu\text{m}$, operating voltage of 5kV, and a beam current of 11 nA. Qualitative examination showed only Cu and As. For quantitative analysis, trippkeite

(Cu, As), arsenic metal (As) and copper metal (Cu) were used as standards. The results are given in Table I. The H_2O content was estimated by difference due to insufficient quantity of the material. The empirical formula based on 9 oxygen atoms is: $\text{Cu}_{2.99}\text{As}_{2.02}\text{H}_{1.92}\text{O}_9$ and the idealized formula, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, was confirmed by structure determination. The Gladstone-Dale constants of MANDARINO (1981) along with the oxide proportions, determined from the electron-microprobe data and from the crystal structure, lead to K_c values of 0.172 and 0.170, respectively. The value of K_p (MANDARINO, 1981), calculated using the average index of refraction (1.83), and the calculated density from the empirical formula, is 0.175. For the same average index of refraction and the calculated density from the idealized formula, K_p is 0.204. The compatibility index is -0.017 for the empirical formula, and -0.035 for the idealized formula, indicating superior and excellent compatibility (MANDARINO, 1981) between the physical and chemical data.

TABLE I. Chemical analysis [wt.%] of theoparacelsite.

	Average of 5 analyses	Range of 8 analyses	Standard deviation	Ideal formula
CuO	48.77	47.90-49.69	0.6	49.05
As_2O_5	47.68	46.43-49.57	1.0	47.25
H_2O^*	3.55			3.70

*By difference

X-RAY CRYSTALLOGRAPHY

Powder-diffraction data (Table II) were obtained using a Gandolfi camera (114.6 mm diameter, Ni-filtered $\text{CuK}\alpha$ radiation). The relative intensities of the reflections were estimated visually. A single-crystal of theoparacelsite 0.083 x 0.083 x 0.035 mm in size was examined by the precession method (Ni-filtered $\text{Cu K}\alpha$) and the same crystal was measured on a Philips PW1100 diffractometer with monochromatized Mo $\text{K}\alpha$ radiation in $\Theta/2\Theta$ scanning-mode with limits $-11 < h < 11$, $-4 < k < 4$, $-6 < l < 6$. A total of 1548 reflections was measured up to $\Theta = 30^\circ$. Lattice parameters were refined on the basis of 23 reflections with $6.6^\circ < \Theta < 24^\circ$ using a program LATCON from the *Xtal3.2* package (HALL *et al.*, 1992): $a = 8.3212(8)$, $b = 2.9377(3)$, $c = 4.6644(5)$ Å, $V = 114.02(2)$ Å³, $a : b : c = 1 : 0.3530 : 0.5605$. Data reduction was done using the programs REFCAL and SORTRF and analytical absorption correction using LSABS from the *Xtal3.2* package. The structure was solved in the space group *Pmma* by direct methods with program GENTAN from the *Xtal3.2* package. The structure (without hydrogen atoms) was refined on F2 with program LSLS from the *Xtal3.2* package using all 207 observed unique reflections ($R_{int} = 0.074$) weighted $1/\sigma^2$. The occupancy of the As site was refined to 2/3 and fixed to that value in the final refinement. The secondary-extinction correction was done according to BECKER & COPPENS (1974) with the extinction parameter $g = 381(67)$. The refinement converged to $R = 0.063$, $R_w = 0.064$ and

TABLE II. X-ray powder diffraction data for theoparacelsite (d in Å)

(hkl)	d(calc.)	d(obs.)	I(vis.)	(hkl)	d(calc.)	d(obs.)	I(vis)
001	4.660	4.658	5	411	1.595	1.596	25
200	4.161	4.162	5	003	1.553	1	
101	4.066	4.065	15			}	1.552
201	3.104	3.104	100	402	1.552	1	10
010	2.938	2.940	<5	103	1.527	1	
011	2.485	2.486	70			}	1.526
210	2.400	2.400	25	312	1.525	1	<5
301	2.384	1		020	1.469	1.470	<5
		}	2.384	10	203	1.455	1.455
111	2.381	1		013	1.373	1	
002	2.330	2.330	15			}	1.372
211	2.134	2.136	<5	412	1.372	1	5
400	2.081	2.080	10	303	1.355	1	
012	1.826	1826	<5	113	1.355	1	<5
302	1.784	1		502	1.354	1	
		}	1.783	<5	601	1.329	1
112	1.783	1				}	1.330
410	1.698	1.699	<5	221	1.328	1	25
212	1.672	1.672	30	610	1.254	1.255	10

Goof = 1.99 with 20 parameters, including anisotropic-displacement parameters. The largest residuals in the Fourier-difference map are -1.28 and 1.23 e/Å³.

CRYSTAL STRUCTURE

Atom coordinates, standardized by the program STRUCTURE TIDY (GELATO & PARTHÉ, 1987), and equivalent isotropic-displacement parameters for non-hydrogen atoms are given in Table III, and a list of selected interatomic distances is given in Table IV. Atom coordination was analyzed by the program IVTON (BALIC ŽUNIĆ & VICKOVIĆ, 1996). The structure of theoparacelsite is disordered. There is one Cu and one As site in the structure. Cu is coordinated by a distorted octahedron, which forms *trans*[CuO₄] chains parallel to b. The chains are cross-linked by apical vertices with other chains and form (001) sheets of CuO₃. The site of As is coordinated by a slightly distorted tetrahedron. The tetrahedra AsO₄ are cross-linked with other tetrahedra by sharing the oxygen O₂ and form chains parallel to b. However, the As site is occupied only by 2/3. The As_{2/3}O₃ chains cross-link the CuO₃ sheets in the c-axis direction. The partial occupancy of the As site and high values of all displacement parameters *U* means that the structure is disordered. A possible inversion twinning in the non-centro-symmetric sub-groups was checked and excluded (using the inversion-distinguishing power of As and MoK α radiation). By a careful inspection of the precession photographs *hk0* and *0kl* very weak lines of diffuse intensity were observed at *k* = 2/3, 5/3. It means probably a local ordering on the As site occupied in our model by 2/3. No long range order showing a superstructure peaks was, however, observed. Further investi-

TABLE III. Atom positions and displacement parameters for theoparacelsite.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq} (\AA^2)	<i>Occ.</i>
Cu	0	0	0	0.0197(2)	1
As	1/4	1/2	0.5443(2)	0.0263(3)	2/3
O1	0.0876(3)	1/2	0.7798(5)	0.0212(7)	1
O2	1/4	0	0.368(2)	0.102(3)	1

The equivalent isotropic atomic displacement parameters are expressed as

$$U_{\text{eq}} = (1/3) \sum i \sum j U_{ij} \alpha i^* \alpha j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

TABLE IV. Selected interactomic distances (\AA) for theoparacelsite.

Cu-O1 (x 4)	1.935(2)	As-O2 (* 2)	1.684(4)
Cu-O2 (x 2)	2.697(5)	As-O1 (* 2)	1.742(3)
Range of edges within			
CuO ₆ octahedron:		2.519(3) - 3.244(3)	
Range of edges within			
AsO ₄ tetrahedron:		2.703(4) - 2.9377(7)	

gation of the diffuse intensity is currently undergone.

No hydrogen atoms were detected in the Fourier-difference map. For this reason and, because of the disordered structure, we have not performed the calculations of the bond valence sums.

DISCUSSION OF THE STRUCTURE

The sum formula of theoparacelsite, $\text{CuAs}_{2/3}\text{O}_3$, corresponds to $Z = 2$. If we suppose the usual cationic charges As^{5+} and Cu^{2+} , the charge equilibrium needs 2/3 of a hydrogen atom giving so a probable formula $\text{CuO}_{1/3}[\text{AsO}_3\text{OH}]_{2/3}$. To get a stoichiometric formula we need to suppose $Z = 2/3$ and the formula becomes $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$. It indicates a probable 3-fold superstructure if the structure were ordered. This corresponds to the observed diffuse intensity in the reciprocal space with $k = 2/3, 5/3$. The final conclusion about the stoichiometric formula can be done, however, only after the complete analysis of the diffuse intensity.

The structure of theoparacelsite, $\text{CuO}_{1/3}[\text{AsO}_3\text{OH}]_{2/3}$, (see Fig. 2) belongs to the group of M=M-T framework structures according to the classification of EBY & HAWTHORNE (1993). The arrangement of the CuO₄ and AsO₃ chains resembles that in olivenite, $\text{Cu}_2\text{AsO}_4(\text{OH})$ (TOMAN, 1977). However, in olivenite the AsO₄ tetrahedra do not form chains, but they are isolated, because each second tetrahedron is missing. Consequently each second CuO₄ chain is replaced by isolated pairs of trigonal bipyramidal Cu₂O₈.

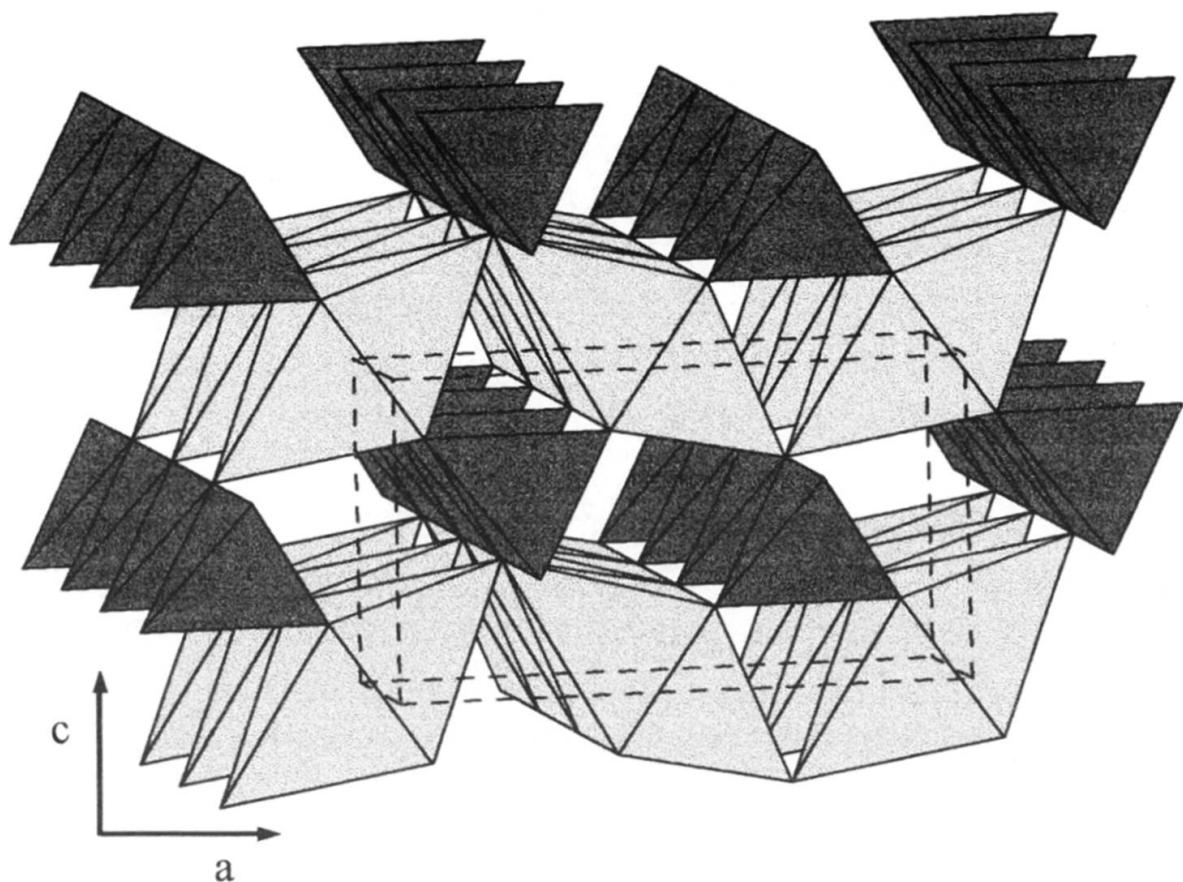


FIG. 2.

The structure of theoparacelsite viewed approximatively down [010]. The Cu octahedra are in light grey and the As tetrahedra are in dark grey.

RESUME

THEOPARACEL SITE, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, UN NOUVEAU MINÉRAL: SA DESCRIPTION ET SA STRUCTURE CRISTALLINE

Theoparacelsite, $\text{Cu}_3(\text{OH})_2\text{As}_2\text{O}_7$, un nouveau minéral, a été découvert dans les mines de cuivre de Roua (Alpes-Maritimes, France). Le minéral et son nom ont été homologués par la Commission internationale des nouveaux minéraux. Le minéral est orthorombique, son groupe d'espace est Pmma. Les paramètres de la maille élémentaire sont $a = 8,321(8)$, $b = 2,9377(3)$, $c = 4,6644(5)$ Å. Il est optiquement biaxe (+) avec $\alpha = 1,81(1)$, $\beta = 1,82(1)$, $\gamma = 1,86(1)$.

Mots-clés: theoparacelsite, nouveau minéral, diagramme de poudre, structure cristalline, arseniate, cuivre.

ACKNOWLEDGEMENTS

We thank C. de Jong Bozkurt for typing the manuscript and J. Wuest for the scanning electron microscope photographs.

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