

PANASQUEIRAITE, A NEW MINERAL: THE OH-EQUIVALENT OF ISOKITE*

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ABSTRACT

Panasqueiraite is a new mineral that occurs as a massive, fine grained pink mineral in specimens from the hydrothermal vein system at Panasqueira, Portugal. It is similar to thadeuite in association and paragenesis. Panasqueiraite is the hydroxyl analogue of isokite and has the ideal formula $\text{CaMgPO}_4(\text{OH},\text{F})$. It is optically biaxial, positive, α 1.590(2), β 1.596(2), γ 1.616(2), $2V$ 51(2)°, $b = Z$, $X\Lambda c$ +22°. Panasqueiraite is monoclinic, a 6.535(3), b 8.753(4), c 6.919(4) Å, β 112.33(4)°, V 366.1(6) Å³, with space group Cc or $C2/c$, $Z = 4$. The strongest five lines in the X-ray powder-diffraction pattern [d in Å (1) (hkl)] are 3.20(67) (002), 3.02(86)(200), 2.783(31)(20 $\bar{2}$), 2.626(100)(130), 2.584(45)(13 $\bar{1}$,022), 1.722(33)(24 $\bar{2}$,222), 1.658(30)(330). The density of panasqueiraite is 3.22 g cm⁻³ (calc.) and 3.27(1) g cm⁻³ (obs.). Isokite and panasqueiraite are isostructural on the basis of similar chemistries and powder patterns. In the literature, the isokite cell has been described as body-centred instead of C-centred as required by the systematic extinctions we observed.

Keywords: isokite, new mineral description, Panasqueira, Portugal, panasqueiraite, thadeuite.

SOMMAIRE

La panasqueiraite, nouvelle espèce minérale, se présente sous forme massive; elle est rose, finement grenue dans des échantillons recueillis dans le système de filons hydrothermaux de Panasqueira (Portugal). Elle ressemble à la thadeuite par ses minéraux associés et sa paragenèse. De formule idéale $\text{CaMgPO}_4(\text{OH},\text{F})$, elle est l'analogue hydroxylé de l'isokite. Biaxe positive, α 1.590(2), β 1.596(2), γ 1.616(2), $2V = 51(2)^\circ$, $b = Z$, $X\Lambda c = +22^\circ$. La panasqueiraite est monoclinique, a 6.535(3), b 8.753(4), c 6.919(4) Å, β 112.33(4)°, V 366.1(6) Å³, groupe spatial Cc ou $C2/c$, $Z = 4$. Les cinq raies les plus intenses du cliché de poudre [d en Å (1) (hkl)] sont

3.20(67)(002), 3.02(86)(200); 2.783(31)(20 $\bar{2}$), 2.626(100)(130), 2.584(45)(13 $\bar{1}$,022), 1.722(33)(24 $\bar{2}$,222), 1.658(30)(330). La densité de la panasqueiraite est de 3.22 (calc.), 3.27(1) (obs.). Isokite et panasqueiraite sont isostructurales, autant que puissent l'indiquer un même chimisme et des clichés de poudre semblables. Les travaux antérieurs ont attribué à la maille de l'isokite le mode "maille centrée" plutôt que "maille à face C centrée" qu'indiquent les extinctions systématiques observées.

(Traduit par la Rédaction)

Mots-clés: isokite, espèce minérale nouvelle, Panasqueira (Portugal), panasqueiraite, thadeuite.

INTRODUCTION

During the course of an electron-microprobe study of a suite of fluorine- and hydroxyl-bearing phosphate-rich specimens from the hydrothermal vein system at Panasqueira, Portugal, we encountered material that, on the basis of an energy-dispersion analysis, appeared to be isokite (CaMgPO_4F). Upon obtaining quantitative wavelength-dispersion analyses, we found that, as for several associated phosphates, this material is enriched in the hydroxyl ion and is the hydroxyl analogue of isokite. We have named this new mineral *panasqueiraite* after the type locality. The mineral and the name have been approved by the I.M.A. Commission on New Minerals and Mineral Names. Type material is present in the collections of the Department of Geological Sciences, the University of Michigan and the Smithsonian Institution (N.M.N.H. 144521).

The general geological setting of the Panasqueira tin-tungsten deposits is described by Thadeu (1951) and Conde *et al.* (1971), and the general mineralogy of the veins is summarized by d'Orey (1967), Gaines & Thadeu (1971) and Kelly & Rye (1979). The association and paragenesis of panasqueiraite are identical with those of thadeuite (Isaacs *et al.* 1979). Both panasqueiraite and thadeuite are found in the vein selvages, sharing a localized phosphate-rich assemblage comprised largely of

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fluorapatite, wolfeite, topaz, muscovite, sphalerite, quartz, chalcopyrite, pyrrhotite, siderite, arsenopyrite, minor chlorite and rare vivianite and althausite.

PHYSICAL PROPERTIES

Panasqueiraite occurs as a massive, fine grained pink mineral in aggregates commonly several centimetres in diameter. No crystal faces are observed in any of our material, which consists of randomly intergrown grains typically about a millimetre in size. Panasqueiraite has a poor {010} cleavage, vitreous lustre, white streak and a Mohs hardness of 5. Although it does not fluoresce under ultraviolet radiation, it does exhibit a blue cathodoluminescence in an electron beam at a 12 kV potential. It is optically biaxial, positive, nonpleochroic, α 1.590(2), β 1.596(2), γ 1.616(2), $2V$ 51(2)° (obs.), $b = Z$, $X:c + 22^\circ$. The density of panasqueiraite is 3.22 g cm⁻³ (calc.) and 3.27(1) g cm⁻³ (obs.), as determined by suspension in

a solution of methylene iodide and acetone; the density of the matching liquid was determined by pycnometer.

CRYSTALLOGRAPHY AND STRUCTURE

Cell dimensions and symmetry were determined using precession single-crystal X-ray-diffraction techniques on two individual crystals. Panasqueiraite is monoclinic; extinctions are consistent with two space groups, *Cc* and *C2/c*. Unit-cell parameters, obtained by least-squares refinement of 25 uniquely indexed powder-diffraction data, are a 6.535(3), b 8.753(4), c 6.919(4) Å, β 112.33(4)°. Powder-diffraction data for panasqueiraite are presented in Table 1 along with selected powder-diffraction data for isokite.

It is likely that panasqueiraite and isokite are isostructural, on the basis of their similar chemistries and the similarity of the diffraction data for the two minerals, given in Table 1. The cell dimensions reported for isokite, how-

TABLE 1. POWDER-DIFFRACTION DATA FOR PANASQUEIRAITE AND SELECTED POWDER-DIFFRACTION DATA FOR ISOKITE

$d_{(obs.)pana.}^*$	I/I_0	$d_{(calc.)}$	hkl	$d_{(obs.)iso.}^{**}$	$d_{(obs.)pana.}$	I/I_0	$d_{(calc.)}$	hkl	$d_{(obs.)iso.}$
4.36	5	4.38	020	4.38					
3.61	2	3.61	021	3.62	1.722	33	1.722	24 $\bar{2}$	1.740
3.43	5	3.44	111	3.45			1.720	22 $\bar{2}$	1.720
3.20	67	3.20	002	3.185	1.706	14	1.708	20 $\bar{4}$	1.705
							1.706	33 $\bar{2}$	
3.02	86	3.02	200	3.023					1.684
				2.887					
2.783	31	2.789	20 $\bar{2}$	2.784	1.671	9	1.670	15 $\bar{1}$	1.671
2.626	100	2.628	130	2.630	1.658	30	1.658	330	1.656
2.584	45	2.585	13 $\bar{1}$	2.586	1.599	2	1.600	004	1.602
		2.583	022		1.559	13	1.558	15 $\bar{2}$	1.557
				2.487	1.543	6	1.543	24 $\bar{3}$	1.539
				2.301	1.523	5	1.524	42 $\bar{2}$	1.522
2.229	18	2.229	11 $\bar{3}$		1.512	5	1.511	400	1.510
2.220	18	2.218	13 $\bar{2}$	2.222	1.496	2	1.496	203	1.495
2.106	20	2.109	31 $\bar{1}$	2.105			1.496	331	
		2.106	221		1.481	11	1.479	13 $\bar{4}$	1.479
2.072	14	2.071	041	2.069					1.453
2.041	16	2.045	31 $\bar{2}$	2.041	1.430	6	1.429	420	
1.963	6	1.964	310	1.962	1.426	5	1.428	15 $\bar{2}$	1.428
1.948	5	1.948	22 $\bar{3}$	1.946	1.394	20	1.395	404	1.392
1.880	6	1.884	132	1.886			1.394	153	
					1.873	7	1.871	202	1.388
				1.872	1.346	7	1.346	24 $\bar{4}$	1.344
				1.837			1.346	35 $\bar{2}$	
1.821	9	1.819	31 $\bar{3}$				1.345	11 $\bar{5}$	
1.808	7	1.809	13 $\bar{3}$	1.807					1.313
		1.806	042						1.303
1.771	2	1.772	240						

*Panasqueiraite data obtained using a powder diffractometer, CuK α radiation, a graphite monochromator, and quartz as an internal standard. Calculated d-values corresponding to panasqueiraite observed values.

**Isokite data are those of Deans & McConnell (1955) with $d > 1.3$ Å.

ever, are a 6.52, b 8.75, c 7.91 Å, β 121.47° (Deans & McConnell 1955), quite different from those of panasqueiraite. In the original description of isokite, Deans & McConnell supplied 60 powder lines with relative intensities, but did not index the data. In examining their tabulation, we found that none of the major powder lines given could be indexed using the lattice parameters that they had determined. However, we found that by using the panasqueiraite lattice parameters, we were able to index all of the powder lines for isokite with intensities reported as "moderate" or stronger, as well as the d values that we determined for panasqueiraite. Using the C-centring axial transformation (100/010/ $\bar{1}$ 0 $\bar{1}$) on a body-centred isokite cell, we obtained the parameters a 6.52, b 8.75, c 7.16 Å, β 109.50°, which are approximately those reported for panasqueiraite. Deans & McConnell (1955) have therefore reported the space group $C2/c$ for isokite and apparently have given the unit-cell dimensions based on an I-centred cell. The ability to index isokite using the panasqueiraite cell dimensions is consistent with the isostructural nature of the two minerals. The following discussion of structures is based on this premise.

Povarennykh (1972) described isokite as isostructural with titanite, *i.e.*, it is a structure dominated by chains of vertex-sharing MgO₆ octahedra parallel to a . The chains are cross-linked by PO₄ groups, resulting (by analogy with the description of the titanite structure of Speer & Gibbs 1976) in a (MgOPO₄) framework with large cavities enclosing the seven-fold-coordinated Ca. Fluorine occupies the same site in isokite as does the nontetrahedral oxygen in titanite.

In reporting their refinement of the structure of tilasite, Bladh *et al.* (1972) noted that this mineral, which is the As-analogue of isokite and is also isostructural with titanite, is slightly noncentric, with space group Cc . The explanation supplied for this is that the F and Ca sites are displaced from the pseudo-2₁ axis in space group Cc ; the latter displacement was determined unambiguously. The resulting structural distortion, combined with a slight rotation of the arsenate group, requires the lowering of the symmetry of the cell.

The tilasite, isokite and panasqueiraite structures all have at least Cc symmetry. The structure of tilasite has been shown to be of no higher symmetry, but the isokite structure has been postulated to have a $C2/c$ cell on the basis of a negative result in a test for pyroelectricity

(Deans & McConnell 1955). The higher space-group symmetry is apparently dependent principally on the substitution of the smaller P ion for As in the tetrahedral site in tilasite. On this basis we infer that the panasqueiraite structure probably has space group $C2/c$.

CHEMISTRY

Electron-microprobe analyses (Table 2) were carried out using an ARL-EMX instrument with three wavelength-dispersion spectrometers using LiF, PET and TAP crystals. Standards used were apatite for Ca, P and F, clinopyroxene for Fe and Mg, and synthetic tephroite for Mn. The analyses were made with a 0.015 μ A specimen current and 12 kV excitation potential; drift, atomic number, fluorescence and absorption corrections were applied to the raw data using the program EMPADR VII (Rucklidge & Gasparini 1969).

The cell contents were calculated using the results of the chemical analysis, measured density and refined cell parameters. The results indicated that there are four P *per* unit cell, consistent with the isokite structure; we therefore normalized the atomic ratios to four P atoms (Table 2). The ideal formula of panasqueiraite, with $Z = 4$, is CaMgPO₄(OH,F), OH > F, with trace amounts of iron substituting

TABLE 2. ELECTRON-MICROPROBE ANALYSIS OF PANASQUEIRAITE

	Wt. %	Atoms/Ce11
CaO	31.0	3.95
MnO	0.0	0.00
FeO	0.4	0.04
MgO	22.9	4.06
P ₂ O ₅	39.6	3.98
F	3.1	1.17
OH*	6.7	2.82
	103.7	
Less 0 for F, OH:	4.4	
	99.3	

*OH calculated assuming P:(OH+F) = 1:1.

for magnesium on the octahedral site. No Cl was observed in any of the energy-dispersion spectra obtained.

Whereas all the specimens of panasqueiraite from the Panasqueira vein system studied here were found to have $\text{OH} > \text{F}$, samples from other areas of the district have $\text{F} > \text{OH}$ and are therefore isokite. In none of our material did the two phases coexist; however, it appears that the presence of one or the other mineral is a function of the local activities of OH^- and F^- in the vein-forming solutions. Associated wolfeite, also with $\text{OH} > \text{F}$, was found to contain $< 0.1\%$ Ca by weight and a Fe:Mn ratio of 1:2. No As was detected in any of the phosphates in this assemblage.

ACKNOWLEDGEMENTS

We are grateful to Dr. J.A. Mandarino for his careful review of and valuable suggestions regarding this manuscript.

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Received February 1981, revised manuscript accepted April 1981.