Zodacite, the Mn analogue of montgomeryite, from Mangualde, Portugal

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ABSTRACT

Zodacite is a new Mn-dominant member of the montgomeryite group. Microprobe analysis yielded MgO 0.2, MnO 4.8, CaO 18.0, Al_2O_3 7.7, Fe_2O_3 14.1, P_2O_5 34.8, H_2O (by difference) 20.4, total = 100.0 wt%. The idealized formula is $Ca_4MnFe_2^{3+}(PO_4)_6(OH)_4 \cdot 12H_2O$. Zodacite is monoclinic, $C2/c$ or Cc, with $a = 10.152(8)$, $b = 24.14(3)$, $c = 6.308(6)$ Å, $\beta = 91.14(7)°$, and $Z = 2$. The strongest diffractions in the powder pattern are $[d_{obs}, I_{obs}, hkl]$ 5.18(10)(111), 12.00(6)(020), 2.907(5)($\bar{1}$71), 3.150(4)(002,260), and 2.656(4)(202). Zodacite occurs as individual yellow crystals and as aggregates of radiating crystals, with a density of 2.68 g/cm³ (meas.) and 2.65 g/cm³ (calc.). It is biaxial, negative, $2V = 83°$, with $\alpha = 1.598$, $\beta = 1.601$, and $\gamma = 1.602$. Pleochroism is weak: Y = very pale green and Z = pale green; orientation is $X = \mathbf{b}$, $Y \wedge \mathbf{c} = 24°$, $Z \wedge \mathbf{a} = 23°$. Zodacite is found associated with a Mn-rich jahnsite-group mineral, phosphosiderite, and hureaulite, on a specimen from the Mangualde pegmatite in Portugal. The name honors the late Peter Zodac, who inspired generations of mineralogists.

INTRODUCTION

During an investigation of jahnsite-group minerals from various localities, we noted some bright yellow crystals associated with Mn-rich jahnsite from Mangualde, Portugal. X-ray data indicated that they belonged to the montgomeryite group, and because the assemblage is a Mn-dominant one, we investigated the Mn content of these crystals and found them to be a new species, the Mn and Fe^{3+} analogue of montgomeryite.

We have named this new mineral *zodacite* in honor of the late Peter Zodac (1894–1967), founder and long-time editor of *Rocks and Minerals* magazine and mentor to many mineralogists and thousands of mineral collectors. His influence was truly pervasive and positive, as noted by Mitchell (1987). The new mineral and the name were approved by the Commission on New Minerals and Mineral Names, IMA. Type material is deposited in the Smithsonian Institution under catalogue no. NMNH 149953 and in the National Museum of Natural Sciences, Ottawa, under catalogue no. NMNS no. 53452.

DESCRIPTION AND PHYSICAL PROPERTIES

Zodacite is light to medium yellow; tiny crystals may appear colorless. The streak is light yellow to white, and the luster is vitreous. The hardness (Mohs') is approximately 4; cleavage was not observed but is presumably present and parallel to {010} by analogy with montgomeryite. The density, measured with heavy liquids, is 2.68 g/cm³, compared with the calculated value of 2.65 g/cm³.

Zodacite forms radial aggregates of 0.1–0.2-mm crystals, which form flattened sprays (Fig. 1).

Optically, zodacite is biaxial, negative, $2V = 83(1)°$ (meas.) (EXCALIBR program; Bloss, 1981), and 60° (calc.), with $\alpha = 1.598$, $\beta = 1.601$, and $\gamma = 1.602$ (all ± 0.001), measured in Na light. Dispersion was not observed; pleochroism is very weak: Y = very pale green, and Z = pale green. The orientation is $X = \mathbf{b}$, $Y \wedge \mathbf{c} = 24°$, $Z \wedge \mathbf{a} = 23°$; absorption is $Y < Z$. There is no discernible response to ultraviolet radiation.

X-RAY CRYSTALLOGRAPHY

X-ray precession photographs show zodacite to be monoclinic with possible space groups $C2/c$ and Cc. Diffraction spots on photographs show considerable mosaic spread in the $\mathbf{a}^*$-$\mathbf{c}^*$ plane. Unit-cell dimensions were refined from X-ray powder-diffraction data obtained using a 114.6-mm-diameter Gandolfi camera with $CuK\alpha$ radiation and NBS Si as an internal standard (Table 1). The refined cell parameters (Appleman and Evans, 1973) are $a = 10.152(8)$, $b = 24.14(3)$, $c = 6.308(6)$ Å, $\beta = 91.14(7)°$, $V = 1545(2)$ Å³, with $Z = 2$.

CHEMICAL COMPOSITION

Zodacite was chemically analyzed using an ARL-SEMQ electron microprobe operated at 15 kV, with a sample current of 0.025 μA, measured on brass. The standards used for analysis were montgomeryite (Mg, Ca, Al, P), manganite (Mn), and maricite (Fe). The data were cor-
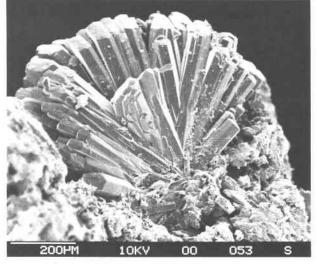
Fig. 1.   Zodacite crystals in a divergent spray.

rected using a modified version of the MAGIC-4 program. A wavelength-dispersive microprobe scan indicated the absence of elements with atomic number greater than nine, except those reported here. Water was calculated by difference owing to the extreme paucity of material. The resultant analysis yielded MgO 0.2, CaO 18.0, MnO 4.8, Al_2O_3 7.7, Fe_2O_3 14.1, P_2O_5 34.8, H_2O (by difference 20.4,

sum = 100.0 wt%. The chemical formula, calculated on the basis of 40 oxygen atoms, is $Ca_{3.96}(Fe^{3+}_{2.18}Al_{1.86})_{\Sigma 4.04}(Mn_{0.83}Mg_{0.06})_{\Sigma 0.89}(PO_4)_{6.05}(OH)_{3.67}\cdot 12.13H_2O$. This is idealized as $Ca_4(Fe^{3+}, Al)_4Mn(PO_4)_6(OH)_4\cdot 12H_2O$ with Z = 2.

Clearly, there is a series extending between a Ca-Fe^{3+}-Mn-member and a Ca-Al-Mn member of the montgomeryite group. Because Fe^{3+} is greater than Al in the type material, the name zodacite should be limited to those samples shown to have Fe^{3+} greater than Al, and Mn greater than Mg or Fe^{2+}. We also acknowledge the possibility of ordering of Fe^{3+} and Al in this mineral; definition of this possible relation will have to await the discovery of crystals of a quality suitable for crystal-structure investigations.

Zodacite extends the montgomeryite series to four minerals, assuming that calcioferrite is included (Table 2). There exists a potential for much solid solution among Mn, Fe^{2+}, Fe^{3+}, Al, and Mg, and some intermediate members exist, as noted by Dunn et al. (1983).

OCCURRENCE

Zodacite occurs in the Mangualde pegmatite, between Mangualde and Mesquitella, in Portugal. The specimen was found in the Smithsonian collection, and nothing is known of its geologic relations in the Mangualde deposit. The minerals found at Mangualde were listed by Gramaccioli (1981).

TABLE 1.   X-ray powder-diffraction data for zodacite

hkl	d_{calc}*	d_{obs}	I_{est}	hkl	d_{calc}*	d_{obs}	I_{est}
020	12.07	12.00	6	$\bar{2}81$	2.407	2.405	1
110	9.36	9.38	2	$\bar{1}91$	2.402		
130	6.30	6.31	3	440	2.339	2.334	<1
040	6.03	6.05	<1	$\bar{3}71$	2.266	2.264	1
021	5.59	5.59	2	172	2.261		
111	5.18	5.18	10	332	2.197	2.189	1
041	4.360	4.393	1	441	2.180		
150	4.359			460	2.146	2.150	<1
240	3.884	3.878	<1	1.11.0	2.145		
$\bar{2}21$	3.791	3.743	<1	390	2.102	2.103	1
221	3.725			023	2.071	2.067	<1
$\bar{1}51$	3.600	3.597	1	$\bar{2}.10.1$	2.066		
061	3.391	3.394	<1	$\bar{2}82$	2.013	2.012	<1
$\bar{2}41$	3.330	3.330	<1	0.12.0	2.011		
241	3.285	3.274	<1	133	1.987	1.986	<1
170	3.265			391	1.987		
002	3.154	3.150	4	043	1.985		
260	3.152			$\bar{2}23$	1.931	1.931	1
$\bar{3}11$	2.984	2.985	2	$\bar{3}72$	1.931		
$\bar{1}71$	2.907	2.907	5	$\bar{2}43$	1.861	1.854	1
$\bar{1}32$	2.834	2.830	<1	481	1.848		
$\bar{2}61$	2.834				1.793		<1
$\bar{2}02$	2.703	2.698	<1		1.757		<1
202	2.655	2.656	4		1.731		1
222	2.593	2.595	1		1.689		<1
190	2.593				1.666		1
152	2.545	2.543	<1		1.643		<1
400	2.538				1.581		1
420	2.483	2.477	<1		1.550		<1
062	2.482				1.501		<1
					1.475		1
					1.417		1

Note: CuKα radiation.
* Refined cell parameters: a = 10.152(8), b = 24.14(3), c = 6.308(6) Å, β = 91.14(7)°.

TABLE 2. The montgomeryite group

Species	Idealized formula	a (Å)	b (Å)	c (Å)	β (°)	Reference
Montgomeryite	$Ca_4MgAl_4(PO_4)_6(OH)_4 \cdot 12H_2O$	10.023	24.121	6.243	91.55	Moore and Araki (1974)
Kingsmountite	$Ca_4FeAl_4(PO_4)_6(OH)_4 \cdot 12H_2O$	10.029	24.46	6.258	91.16	Dunn et al. (1979)
Zodacite	$Ca_4MnFe_4^{3+}(PO_4)_6(OH)_4 \cdot 12H_2O$	10.152	24.14	6.308	91.14	Present study
Calcioferrite*	$Ca_4MgFe_4^{3+}(PO_4)_6(OH)_4 \cdot 12H_2O$					Dunn et al. (1983)

* Assumed to be isostructural; no single-crystal data exist.

Zodacite forms yellow isolated crystals and flattened, radial arrays of lustrous crystals, associated with a Mn-rich member of the jahnsite series, hureaulite, and phosphosiderite, on a specimen of altered varulite. Only one Mangualde zodacite specimen is known to us, and thus zodacite must be considered a rare mineral at present. The unnamed possible "kingsmountite," described by Dunn et al. (1983) from the Hagendorf pegmatite in Germany, has a composition now attributable, with some caution, to zodacite.

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