Taprobanite, a new mineral of the taaffeite-group

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Abstract

Taprobanite, $BeMg_3Al_8O_{16}$ from Sri Lanka is hexagonal, $P6_3mc$ with $a = 5.684(1)$ Å and $c = 18.332(7)$ Å, $Z = 2$. The strongest reflections in the X-ray diffraction pattern are (d in Å, intensity, hkl) 4.58 (50)(004); 2.595 (60)(106); 2.415 (100)(114); 2.043 (60)(205); 1.469 (50)(2.0.10); 1.421 (50)(220).

Taprobanite is red; the Mohs' hardness is approximately 8. Measured density is 3.605(5) g/cm³, calculated density 3.588 g/cm³. No cleavage can be observed; fluorescence in ultraviolet radiation is very weak. Optically, taprobanite is uniaxial (–) with refractive indices $\varepsilon = 1.717(2)$ and $\omega = 1.721(2)$.

The empirical formula, calculated on the basis of 32 oxygens, is $Be_{1.94}Mg_{5.92}Fe_{0.19}Al_{15.94}Cr_{0.02}O_{32}$ or ideally $BeMg_3Al_8O_{16}$.

The crystal structure has been determined from 903 counter-measured intensity data. The final R-value is 0.092. Taprobanite represents a link between the spinel and taaffeite structures. The space group $P6_3mc$ allows only ordered Be:Mg ratios of 3:1, 1:1 and 1:3. The structure analysis corresponds to the latter case. Consequently taprobanite is a discrete mineral species with well-defined cation ordering.

INTRODUCTION

The new mineral described in this paper was acquired by Mr. A. G. B. Amarasinghe, Ratnapura, Sri Lanka as a hexagonal-prismatic crystal from a local gem prospector. The crystal was then cut as a gemstone of 204 mg and sold as red taaffeite to Dr. E. Gübelin, Switzerland. The physical properties were nearly identical with taaffeite but, due to the unusual color, Dr. E. Gübelin asked the two other authors for a more detailed investigation. There was also doubt about the true space group, as ANDERSON et al. (1951) gave $P6_322$ and PENG and WANG (1963) $P6_3mc$. As will be shown in the section on X-ray structure analysis, the space group determined by ANDERSON et al. (1951) was found to be er-

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roneous; furthermore the investigated material turned out to be a new mineral species closely related to taaffeite and spinel.

The new mineral is named according to the old Greek name for the Island of Sri Lanka, Taprobane. Holotype material is deposited at the Mineralogical-Petrographical Collection of the Swiss Federal Institute of Technology, Zürich. The mineral and the name have been approved by the IMA Commission on New Minerals and Mineral Names.

CHEMISTRY

Taprobanite was chemically investigated by two methods. Mg, Al, Fe, Mn and Cr were analysed with an ARL-EMX electron microprobe using an operating voltage of 15 kV and a sample current of 0.01 μA. The data were corrected online for X-ray absorption, fluorescence and atomic number with the aid of a modified MAGIC IV program fitting the CDC 6500 computer system at the ETH-Zürich. The standards used were: synthetic spinel (Al, Mg), Mn-pyrite (Fe, Mn) and Cr-pyroxene (Cr). Be and again Al and Mg were analysed by atomic absorption spectroscopy using a Perkin Elmer 420 spectrometer, a nitrose oxide-acetylene-flame and standard solutions of Al, Mg and Be (Table 1).

Table 1   Microprobe and AAS analysis of taprobanite.

Oxide	(1)	(2)	(3)
Al_2O_3	73.63	72	73.64
MgO	21.64	21	21.84
BeO	3.33*	4.4	4.52
FeO (tot)	1.24		
MnO	0.04		
Cr_2O_3	0.12		
Total	100.00	97.4	100.00

* by difference

(1) Microprobe analysis

(2) AAS analysis

(3) Theoretical composition for $BeMg_3Al_8O_{16}$

Using for the calculation the values of the microprobe analysis and Be of the AAS analysis, the empirical formula on the basis of 32 oxygens is $Be_{1.94}Mg_{5.92}Fe_{0.19}Al_{15.94}Cr_{0.02}O_{21.932}$ and the idealized formula is $BeMg_3Al_8O_{16}$.

PHYSICAL PROPERTIES

Taprobanite is reported to have been discovered as a hexagonal crystal. The investigated material originated from a cut gemstone and it is undoubtedly of natural origin. The color of the mineral is a bright red, according to the standard color-card DIN 6164; the values vary between 8:4:2 and 8:5:2 and the color norm values are X_c 35.8 and 32.6; Y_c 23.8 and 20.1 and Z_c 14.8 and 10.7. Dichroism varies between yellow-rose (ε) and clear carmin red (ω). Taprobanite is uniaxial negative; the refractive indices being $\varepsilon = 1.717(2)$ and $\omega = 1.721(2)$. Ultraviolet radiation in both short and long wave lengths is a very

Table 2 X-ray diffraction data for taprobanite.

d(obs)	d(calc)	hkl	I/I_0	d(obs)	d(calc)	hkl	I/I_0
9.12	9.16	002	5	1.678	1.677	208	10
4.94	4.92	100	5	1.659	1.659	215	10
4.76	4.75	101	10	1.638	1.641	300	10
4.58	4.58	004	50	1.588	1.589	216	30
4.34	4.34	102	40	1.568	1.569	209	10
3.83	3.83	103	10	1.544	1.545	304	20
3.35	3.35	104	20	1.529	1.528	0,0,12	10
2.941	2.940	105	30	1.516	1.517	217	30
2.842	2.842	110	30	1.499	1.498	305	5
2.722	2.714	112	5	1.469	1.470	2,0,10	50
2.595	2.596	106	60	1.421	1.421	220	50
2.444	2.439	201	5	1.380	1.380	2,0,11	30
2.415	2.415	114	100	1.357	1.357	224	10
2.378	2.377	202	40	1.246	1.246	316	10
2.312	2.312	107	20	1.219	1.220	402	5
2.281	2.283	203 / 008	10	1.209	1.208	228 / 317	5
2.167	2.168	204	40	1.187	1.188	404	5
2.043	2.043	205	60	1.167	1.167	405	5
1.917	1.917	206	40	1.142	1.141	406	5
1.718	1.718	1,0,10	5				

weak red. In the absorption spectrometer, one absorption line at 685.2 nm can be observed.

The Mohs' hardness of the mineral is approximately 8; no cleavage is present; fracture is conchoidal.

The density, determined by heavy-liquid techniques is $3.605(5)$ g/cm³, agreeing satisfactorily with the calculated density $3.588(4)$ g/cm³ (value for ideal composition).

X-RAY CRYSTALLOGRAPHY

X-ray diffraction pattern data of Table 2 were obtained from a single crystal with a Gandolfi camera (114,6 mm), using CuK_α radiation (Ni filter) and silicon as an internal standard. The intensities are visually estimated.

X-RAY STRUCTURE ANALYSIS

Preliminary investigation

The investigated sample was a piece broken off from the facetted sample with dimensions of about 0.1 x 0.1 x 0.15 mm. Initially, Laue and precession

Table 3 Crystal data for taprobanite.

Formula	$BeMg_3Al_8O_{16}$
Formula weight	553.79
Crystal system	hexagonal
Crystal class	C_{6v} – 6mm
Space group	$P6_3mc$
Selection rule	(hhl) : l = 2n
Lattice parameters **	a = 5.684(1) Å
	c = 18.332(7) Å
	V = 512.8(4) Å³
	c/a = 3.225(2)
Density	D(calc) = 3.588 g/cm³
	D(meas) = 3.605 g/cm³
Molecules per unit cell	Z = 2

* all values for pure composition of $BeMg_3Al_8O_{16}$

** from refinement of Gandolfi data

photographs were used to confirm that it was a single crystal with hexagonal symmetry and the possible space groups $P6_3mc$, $P\bar{6}2c$, $P6_3/mmc$ or (with special positions only) $P6_322$, and with approximate cell dimensions $a = 5.7$ Å and $c = 18.3$ Å. Using McKie's (1962) nomenclature, a 4H-polytype seemed possible (see also Grey and Gatehouse [1979]).

Intensity data collection

For the intensity data collection the crystal was remounted on an automatic Syntex $P2_1$ single crystal diffractometer. For the refinement of lattice parameters, 25 strong, unambiguous, carefully centered reflections with relatively high 2θ-angles were used. The refinement was carried out with the XTL-program (1976) for the diffractometer integrated computer (Nova 1200 from Data General). Intensities were collected with graphite monochromated MoK_α radiation. Intensities were measured for one quarter of the sphere of reflection, up to $2\theta = 90°$ ($h \geq 0$, k, $l \geq 0$, 4277 reflections). After absorption and Lp correction ($\mu = 10.1$ cm^{-1}) and averaging the intensities of equivalent reflections, a unique set of 969 resulted, 903 of which had $F^2 \geq 3\sigma$ [F^2]; these were used in the structure refinement. Data reduction, normalizing of structure factors and least-squares refinements were calculated on a CDC computer of the 7000 series, using the programs of the X-ray system (1972). Scattering factor curves of Cromer and Mann (1968) for Al, Be and Mg, and of Suzuki (1960) for O-atoms have been used.

Structure determination

A close-packed eight-layer structure can have only two possible stacking sequences if a c-glide plane or a 6_3-screw axis is assumed.

Notation of position parameters: (0 , 0 ; ......) = C
(1/3,2/3; ......) = A
(2/3,1/3; ......) = B

The only two stacking sequences are C A B A C B A B ...
and C A C A C B C B ...

The similar features of the powder patterns of taprobanite, taaffeite and spinel show that there is a close similarity between these three structures (JCPDS index) which is corroborated along c by comparing a model with a one-dimensional Fourier synthesis. It is reasonable to assume, that in taprobanite as in taaffeite and spinel, Al-atoms fill octahedral sites and Be- and/or

Mg-atoms are dispersed in tetrahedral sites of a hexagonal closest-packed oxygen matrix. Considering the symmetry of the Be site, only space group $P6_3mc$ has equipoints of acceptable symmetry and rank. The space group for taaffeite found by ANDERSON et al. (1951) must be wrong, because a spinel-like metal-distribution in a hexagonal closest-packed eight-layer structure is incompatible with the space group $P6_322$. PENG and WANG (1963) determined the structure of taaffeite, and they too found the space group $P6_3mc$. The variable coordinates referred to special values, so we solved the problem by the «trial and error» method. For each of the two possible oxygen stacking sequences structure factors were calculated. After one cycle of least-squares refinement the R-value was calculated. The stacking sequence C A B A C B A B... brought a significantly better result. Furthermore, in the implication diagram for z = 0.5

Table 4   Atomic position parameters.

atom	number of positions	point symm.	x	y	z
O(1)	2	3m	0.0(r)	0.0(r)	0.0(r)
O(2)	6	m	-0.0454(r)	0.4773(6)	-0.0100(7)
O(3)	2	3m	2/3(r)	1/3(r)	0.1057(9)
O(4)	6	m	0.1622(7)	0.3243(r)	0.1092(7)
O(5)	2	3m	1/3(r)	2/3(r)	0.2388(9)
O(6)	6	m	0.3779(r)	0.1890(7)	0.2389(7)
O(7)	2	3m	2/3(r)	1/3(r)	0.3524(9)
O(8)	6	m	0.1869(6)	0.3737(r)	0.3567(7)
Al(1)	6	m	0.3331(r)	0.1665(4)	0.0525(7)
Al(2)	2	3m	0.0(r)	0.0(r)	0.1900(8)
Al(3)	6	m	-0.0057(r)	0.4972(4)	0.2971(6)
Al(4)	2	3m	1/3(r)	2/3(r)	0.4222(7)
Mg(1)	2	3m	1/3(r)	2/3(r)	0.1410(7)
Mg(2)	2	3m	0.0(r)	0.0(r)	0.3903(7)
Mg(3)	2	3m	2/3(r)	1/3(r)	0.4573(7)
Be	2	3m	2/3(r)	1/3(r)	0.196(5)

(r) restricted

no high peaks were found, as should be the case for the other possibility. There are two possibilities for arranging the Al-atoms relative to symmetry constraints:

1) half of the layers: all octahedral holes filled
   half of the layers: all octahedral holes empty
2) half of the layers: 3/4 of the octahedral holes filled
   half of the layers: 1/4 of the octahedral holes filled

By using the spinel- and taaffeite-like distribution (2) of the Al-atoms the R-value immediately decreased to 0.2. GREY and GATEHOUSE (1979) describe this arrangement as O T_2O T_2O T_2O T_2... (no distinction between Be- and Mg-occupancy). An electron density Fourier synthesis showed only three occupied tetrahedral sites interpreted to correspond to magnesium positions. The electron density at the fourth tetrahedral site was equal to that of the other unoccupied sites. Refinement was carried out with beryllium at this site, therefore, as consistent with the symmetry restraints described above.

By refining position parameters, isotropic and anisotropic temperature parameters, the R-value decreased to 0.092. Refined atom coordinates are listed in Table 4. A list of all calculated and observed structure factors and a list of the temperature parameters can be obtained from R. Moor.

Structure description

The structure is based on a closest-packed oxygen framework with an eight-layer stacking sequence C A B A C B A B... One can achieve the taprobanite- and taaffeite-like eight-layer packing easily by four-layer rearrangements of the cubic-closest-packed sequence of spinel. For fixed positions of A,
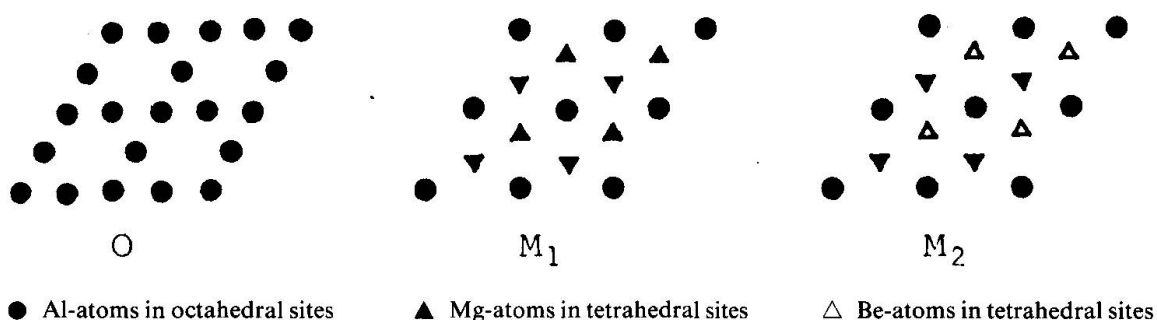

● Al-atoms in octahedral sites   ▲ Mg-atoms in tetrahedral sites   △ Be-atoms in tetrahedral sites

Fig. 1 Metal atom arrangements between close-packed oxygen layers for octahedral sites only (O), octahedral and tetrahedral sites occupied by Al and Mg only (M_1) and octahedral and tetrahedral sites occupied by Al, Mg and Be (M_2).
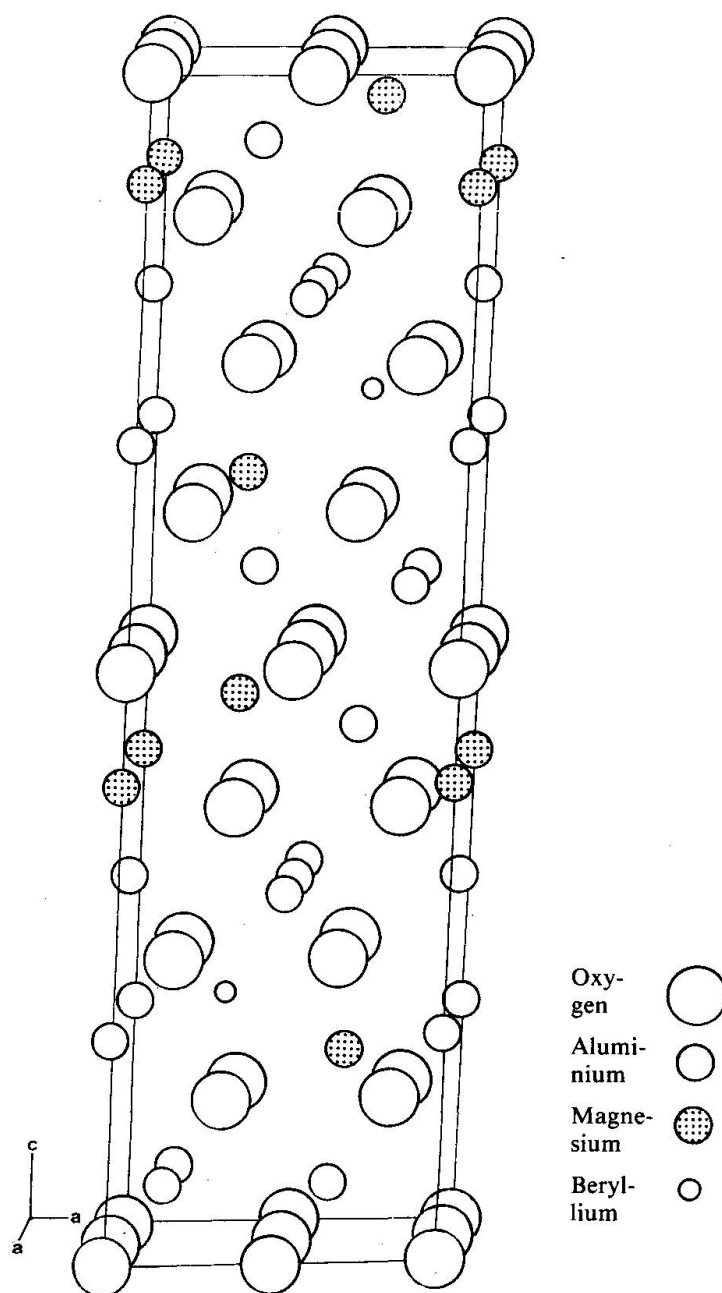
Fig. 2 Idealized taprobanite structure, hexagonal cell.

B and C there are two possibilities for stacking: P_1: ABCÁBCAB́CABC, P_2: CBACB́ACBÁCBA. The taprobanite stacking sequence results from combination of these. In taprobanite there are three different arrangements of metal atoms between the layers (Fig. 1).

The three closely related structures may be described in very similar ways:

	stacking sequence of oxygen atoms	arrangement of metal atoms
Spinel	C A B C A B...	O M_1O M_1O M_1...
Taaffeite	C A B A C B A B...	O M_2O M_2O M_2O M_2...
Taprobanite	C A B A C B A B...	O M_1O M_2O M_1O M_2...

Knowledge of the stacking sequence, the occupation of the voids with metal atoms and the space group lead to an idealized structure (Fig. 2).

Acknowledgments

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