

The infra-red spectrum of painite

THE mineral painite was discovered in 1952 in material from one of the ruby mines at Mogok in Upper Burma and first described by Claringbull *et al.* (1957). Its crystal structure was found by Moore and Araki (1976) to be related to that of eremeevite and fluoborite and in the course of the same investigation the chemical composition was re-determined to give a modified formula of $\text{CaZrB}(\text{Al}_9\text{O}_{18})$.

In the present contribution these results have been confirmed by infra-red spectroscopy carried out on a small fragment of the original specimen (Reg. no. BM 1954, 192). The spectrum was recorded on a UR-20 spectrophotometer (Carl Zeiss, DDR), using KBr in compressed discs as the dispersion medium.

formed into pairs with one common edge and grouped around the hexagonal channels in which the calcium ions are situated in sixfold coordination (Moore and Araki, 1976, fig. 2). The strengths of the different Al-O bonds in the AlO_6 octahedra are unequal because these octahedra are held in the structure in different ways. Around the shared edges of the AlO_6 octahedra these bonds are of shorter length (1.82-1.88 Å) and consequently the bond is strengthened, corresponding to the most intense absorption band with the maximum of 652 cm^{-1} . Where the bonds form the common vertices they are a little longer (1.89-1.95 Å) and less strong, corresponding to the absorption band of 596 cm^{-1} .

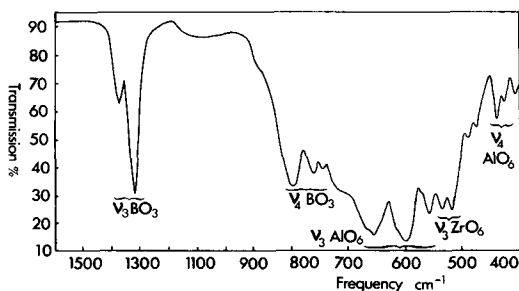


FIG. 1. Infra-red absorption spectrum of painite.

The spectrum (fig. 1 and Table I) shows a narrow intense absorption band in the high-frequency part of the spectrum ($1360\text{--}1310\text{ cm}^{-1}$) corresponding to the stretching vibrations ν_3 of B-O bonds in the $(\text{BO}_3)^{3-}$ radical, which, allowing for the additional maximum at 1360 cm^{-1} , has the shape of a slightly deformed scalene triangle. The absorption bands in the $800\text{--}750\text{ cm}^{-1}$ region with maxima at 792 and 760 cm^{-1} belong to the deformation vibrations ν_4 of the B-O bonds in the $(\text{BO}_3)^{3-}$ radical, which, along with the ν_3 vibrations, are at a slightly higher frequency than is observed in most metaborates (Moenke, 1962, 1966).

The two most intense and broad absorption bands with maxima at 652 and 596 cm^{-1} belong to the bond stretching vibrations of the slightly distorted AlO_6 octahedra. These octahedra are

TABLE I. Data for IR-absorption spectrum of painite

ν (cm^{-1})	Assignments	Interatomic distances (Å)
1360 } 1310 }	ν_3 B-O ₃	1.38
792 } 760 } 740 }	ν_4 B-O ₃	1.38
652 } 596 } 554 }	ν_3 Al-O ₆	{ 1.82-1.88 1.89-1.95 2.03-2.09
526 } 513 }	ν_3 Zr-O ₆	2.13
432 } 420 }	ν_4 Al-O ₆	1.82-1.88

A less intense absorption band at 554 cm^{-1} probably corresponds to ν_3 vibrations of Al-O bonds of length $2.03\text{--}2.09\text{ Å}$, there being less than half the number of these bonds compared to the shorter bonds in the AlO_6 octahedra (Moore and Araki, 1976, p. 93). The two weak bands in the IR spectrum with maxima at 526 and 513 cm^{-1} belong, apparently, to the stretching vibrations of Zr-O bonds, the low intensity being related to the

number of zirconium atoms in the painite unit cell. The double band with maxima at 432 and 420 cm^{-1} probably belongs to the deformation vibrations ν_4 of the bonds of the AlO_6 octahedra, corresponding to the first band of stretching vibrations ν_3 at 652 cm^{-1} .

Taking into consideration the extremely high vibration frequency of the $(\text{BO})^{3-}$ radical in painite it seems logical to write its formula as $\text{CaAl}_9\text{ZrO}_{15}(\text{BO}_3)$.

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[Manuscript received 4 July 1978]

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