

An FTIR study of tetrahedrally coordinated ferrous iron in the spinel-hercynite solid solution

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ABSTRACT

Room-temperature FTIR spectra of ten chemically and structurally well-characterized synthetic spinel-hercynite solid solution single crystals containing between 4 and 98 mol% hercynite component show that absorption in the range 2500–7000 cm^{-1} is linearly correlated ($R^2 = 0.995$) with ${}^{\text{IV}}\text{Fe}^{2+}$ concentration. The integral molar absorption coefficient for this absorption equals $1.49 \cdot 10^8$ cm/mol . In addition, the structure of the absorption envelope in this spectral region remains unchanged throughout the entire composition range. These two findings are consistent with assignments to a spin-allowed electronic $d-d$ transition (${}^5E \rightarrow {}^5T_2$) in ${}^{\text{IV}}\text{Fe}^{2+}$, split by the dynamic Jahn-Teller effect, and demonstrate that next-nearest interactions in Fe clusters have little or no effect on this absorption feature at ambient conditions.