

The T - X dependence of the isosymmetric displacive phase transition in synthetic Fe^{3+} -Al zoisite: A temperature-dependent infrared spectroscopy study

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ABSTRACT

We have studied three synthetic Al- Fe^{3+} zoisites with variable Fe^{3+} -contents [$X_{\text{ps}} = 0.0, 0.035$ (12), and 0.062 (23)] by means of temperature-dependent infrared powder spectroscopy. Spectra were recorded from -150 to 170 °C in steps of 20 °C in the lattice vibrational range 400 to 1200 cm^{-1} . At -150 °C, a total of 34 bands could be identified in all samples. With increasing temperature, the bands broaden and generally shift smoothly to lower wave numbers. The maxima of bands at ~ 620 and ~ 909 cm^{-1} as well as the autocorrelation analysis of the spectral region 820 to 1050 cm^{-1} display linear but different temperature dependencies of the spectral properties at low and high temperatures. These changes in temperature dependence of the spectral properties marks the isosymmetric displacive phase transition between zoisite I and II. The transition temperatures T_{tr} are about 45 °C for $X_{\text{ps}} = 0.0$ and $= 0.035$ (12), and about -35 °C for $X_{\text{ps}} = 0.062$ (23) and suggest a negative correlation between T_{tr} and X_{ps} . A combination with literature data yields a positive slope of 9.4 ± 2.0 MPa/K and a ΔS of 0.5 ± 0.1 J/(K·mol) for the zoisite I \rightarrow zoisite II transition for a composition of about $X_{\text{ps}} = 0.035$.