

Al-Fe disorder in synthetic epidotes: A single-crystal X-ray diffraction study

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ABSTRACT

Synthetic epidotes were produced using a Tuttle type hydrothermal vessel in the temperature range from 500 to 700 °C and at 4.5 to 5.0 kbars pressure. Single-crystal X-ray diffraction structure refinements yielded intracrystalline cation distributions for two crystals grown at 600 °C (0.68 and 0.73 Fe apfu) and five crystals grown at 700 °C (0.88 to 1.08 Fe apfu). The resulting Fe occupancies were compared with those calculated according to a thermodynamic model: The samples formed at 700 °C display a Fe distribution between M3 and M1 sites that match the calculation; nevertheless, we found the presence of a small but appreciable amount of Fe in the M2 sites that increases with the total Fe content (up to 0.08 Fe apfu). The crystals formed at 600 °C show a much higher disorder than expected, but have no Fe in the M2 site. Crystal-chemical features of the samples studied were compared with those of a previously published set of natural epidotes displaying a much lower Fe disorder: In particular, the unit-cell volume vs. Fe content relationship is not affected by the intracrystalline Fe distribution. This relation suggests that the Al-Fe intracrystalline distribution is independent of pressure.