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Site disorder revealed through Raman spectra from oriented single crystals: A case study on karooite ($MgTi_2O_5$)

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ABSTRACT

Raman spectroscopic data were collected from five oriented single crystals of karroite ($MgTi_2O_5$) with different ordering states obtained by quenching crystals from 600, 700, 800, 1000, and 1400 °C. The Raman spectra were normalized and treated as vectors. The inner products among the Raman spectra are shown to correlate linearly with the ordered state of the crystals, suggesting that such an analysis of Raman spectra can, in principle, be used to rapidly estimate the ordering state of a mineral, and thus many other crystal properties related to the atomic order-disorder.

Keywords: Raman spectroscopy, cation ordering state, karooite, pseudobrookite