American Mineralogist, Volume 96, pages 1568–1574, 2011

Quantum-mechanical calculations of the Raman spectra of Mg- and Fe-cordierite†

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Abstract

Quantum-mechanical calculations with a hybrid HF/DFT Hamiltonian (B3LYP) model yielded the Raman-active vibrational modes of the Mg- and Fe-cordierite structure. Maximum and mean deviation between experimentally derived bands and calculated modes of synthetic Mg- and natural Fe-rich cordierite are ±19 and 7 cm^{-1}. Most of the observed bands could be related to specific vibrational modes of tetrahedral and octahedral sites of the cordierite structure, although the large number of Raman-active modes (87) prevents a complete assignment. Atomic motions in cordierite are compared with those of the structurally similar mineral beryl. The calculations enable more accurate interpretation of the Raman spectra with respect to structural changes of cordierite, in particular Al-Si ordering and Mg-Fe exchange.

Keywords: Raman spectroscopy, cordierite, quantum-mechanical calculations, band assignment, Al-Si ordering, Mg-Fe exchange.