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The quantitative analysis of H_2O and CO_2 in cordierite using single-crystal polarized-light FTIR microspectroscopy

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We relate here a microchemical and microspectroscopic FTIR (Fourier-transform infrared) study of a set of cordierite samples from different occurrence and with different H_2O/CO_2 content. The specimens were fully characterized by a combination of techniques including optical microscopy, single-crystal X-ray diffraction, EMPA (electron micro probe analysis), SIMS (secondary ion mass spectrometry), and FTIR spectroscopy. All cordierites are orthorhombic *Ccmm*. According to the EMPA data, the Si:Al ratio is always close to 5:4; X_{Mg} ranges from 76.31 to 96.63 and additional octahedral constituents occur in very weak amounts. Extraframework K and Ca are negligible, with Na up to 0.84 apfu. SIMS shows H_2O up to 1.52 and CO_2 up to 1.11 wt%.

Optically transparent single-crystals were oriented using the spindle-stage and examined by FTIR microspectroscopy under polarized light. On the basis of the polarizing behaviour, the observed bands were assigned to water molecules in two different orientations, and to CO_2 molecules in the structural channels. Prior to the quantitative analyses, the samples were examined for their water and carbon dioxide distribution using a focal-plane-array (FPA) of detectors. The evidence was that at the μm-scale the distribution of H and C in cordierite may be significantly inhomogeneous, particularly for H_2O, whose zoning within the crystal can be strongly affected by the geological history of the mineral after its formation.

Refined integrated molar absorption coefficients were calibrated for the quantitative microanalysis of both H_2O and CO_2 in cordierite based on single-crystal polarized-light FTIR spectroscopy. For H_2O the integrated molar coefficients for type I and type II water molecules were calculated separately and turned out to be $^{[I]}\varepsilon$ = 5000 ± 1000 l•mol^{-1}•cm^{-2} and $^{[II]}\varepsilon$ = 13200 ± 500 l•mol^{-1}•cm^{-2}, respectively. For CO_2 the integrated coefficient is ε_{CO2}= 19000± 1000 l•mol^{-1}•cm^{-2}.