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Aliphatic hydrocarbons in structural channels of cordierite: A first evidence from polarized single-crystal IR-absorption spectroscopy

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ABSTRACT

Polarized IR-absorption spectra were measured on inclusion-free spots, 50 μm in diameter of (100)-, (010)-, and (001)-oriented single-crystal plates of orthorhombic cordierites extracted from anatectic granitoids and their pegmatite from the western part of the Ukrainian shield. In the range 3100–2700 cm^{-1}, the spectra display four weak ($\alpha_{lin} \leq$ ca. 7 cm^{-1}) and sharp ($\Delta\nu_{1/2} \cong 20$ cm^{-1}) bands typical of the antisymmetric and symmetric stretching modes of CH_3^- and $-CH_2^-$ groups of aliphatic hydrocarbons, C_nH_{2n+2} ($\nu_{as,CH3}$ at 2951–2959 cm^{-1}, $\nu_{as,CH2}$ at 2920–2923 cm^{-1}, $\nu_{sym,CH3}$ at 2871–2874 cm^{-1}, $\nu_{sym,CH2}$ at 2850–2851). All bands are polarized in the *ac*-plane of orthorhombic cordierite. In the temperature range $123 \leq T$ (K) ≤ 573, the degree of polarization decreases as temperature increases. The band polarizations and their temperature dependence ensure that the hydrocarbons are incorporated in the cordierite matrix, i.e., in the ca. 5.8 Å wide cavities of the c-parallel channels of the crystal structure. The concentrations of alkanes, C_nH_{2n+2} from band intensities, are between about 20 and about 100 ppm, corresponding to about $0.7 \cdot 10^{-3}$ and about $2.3 \cdot 10^{-3}$ molecules per formula unit cordieriite. Evaluation of the averaged intensities of the antisymmetric as well as symmetric C-H stretching vibrations of either species, CH_3^- and $-CH_2^-$, yields a ratio of 1:1 between them consistent with n = 4 only, realized in butane C_4H_{10} or in a butane-rich mixture with n = 4 on average and concentrations between 0.7×10^{-3} to 2.3×10^{-3} molecule pfu. Polarizations as well as molecular and cordierite-cavity sizes are consistent with an allocation of butane molecules in the channel cavities of the cordierite structure, with the molecular axes of butane predominantly parallel to **b**.