

## **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  $\mu\text{m}$  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  $\text{cm}^{-1}$ , the spectra display four weak ( $\alpha_{\text{lin}} \leq \text{ca. } 7 \text{ cm}^{-1}$ ) and sharp ( $\Delta\nu_{1/2} \cong 20 \text{ cm}^{-1}$ ) bands typical of the antisymmetric and symmetric stretching modes of  $\text{CH}_3$  and  $-\text{CH}_2$  groups of aliphatic hydrocarbons,  $\text{C}_n\text{H}_{2n+2}$  ( $\nu_{\text{as,CH}_3}$  at 2951–2959  $\text{cm}^{-1}$ ,  $\nu_{\text{as,CH}_2}$  at 2920–2923  $\text{cm}^{-1}$ ,  $\nu_{\text{sym,CH}_3}$  at 2871–2874  $\text{cm}^{-1}$ ,  $\nu_{\text{sym,CH}_2}$  at 2850–2851). All bands are polarized in the *ac*-plane of orthorhombic cordierite. In the temperature range  $123 \leq T \text{ (K)} \leq 573$ , 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,  $\text{C}_n\text{H}_{2n+2}$  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 cordierite. Evaluation of the averaged intensities of the antisymmetric as well as symmetric C-H stretching vibrations of either species,  $\text{CH}_3$  and  $-\text{CH}_2$ , yields a ratio of 1:1 between them consistent with  $n = 4$  only, realized in butane  $\text{C}_4\text{H}_{10}$  or in a butane-rich mixture with  $n = 4$  on average and concentrations between  $0.7 \times 10^{-3}$  to  $2.3 \times 10^{-3}$  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**.