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Orientational diffusion of methyl groups in crystalline CH3F: An infrared study

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Abstract

The mid-infrared (4000-400 cm-1) spectra of polycrystalline methyl fluoride have been investigated at temperatures between 8 and 85 K. Least-squares band fitting was performed for all fundamental bands belonging to symmetric and asymmetric vibrations of the methyl group, and the contributions of inhomogeneous broadening and vibrational and orientational relaxation to the bandwidths have been evaluated. From the temperature dependence of the bandwidths, using the modified Rakov approach, the activation enthalpy, ΔH*, and activation entropy, ΔS*, for orientational diffusion of the methyl groups have been determined to be ΔH* = 0.85(7) kJ mol-1 and ΔS* = -7(1) J mol-1 K-1.