FIRST HIGH-RESOLUTION STUDY OF VIBRATIONALLY EXCITED STATES ν_{17} AND ν_{12} OF PROPYLENE OXIDE

KAREL VÁVRA, EILEEN DÖRING, JAN JAKOB, GUIDO W. FUCHS, PASCAL STAHL, ARNE VEREI-JKEN, MARCEL SCHLESAG, THOMAS GIESEN, *Institute of Physics, University of Kassel, Kassel, Germany.*

Propylene oxide, $CH_3C_2H_3O$, is a stable chiral molecule that gained new attention through its recent radio astronomical discovery in the interstellar medium toward the galactic center^{*a*}. Subsequently, extensive laboratory data on rotational transitions in the ground state and in the lowest vibrationally excited ν_{24} torsion state were published^{*b,c*}. Previously, only the 3 μ m spectral range of the four C-H stretching vibration modes was measured with high spectral resolution at mid-infrared wavelength^{*d*}.

In the present study we used two quantum cascade laser spectrometers at 8 and 10 μ m to record ro-vibrational spectra of the ν_{17} fundamental mode (CH₂ rock) at 1023 cm⁻¹ and the ν_{12} ring breathing mode at 1266 cm⁻¹. The spectra were measured in a static cell at room temperature and in a supersonic jet expansion at low temperatures. The room temperature measurement allowed a quick assignment via graphical techniques (Loomis-Wood diagram) and determination of the molecular parameters using the SPFIT/SPCAT program package^e. In the supersonic jet spectrum line splittings could be observed for certain transitions. The combination of measurements at low temperature (30K) and at room temperature conditions led to an assignment of hundreds of transitions of the very dense infrared spectrum and covers quantum numbers from lowest J and K up to J = 55 and K_a = 36.

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