

FIRST VIB-ROTATIONAL ANALYSIS OF PROPANE AROUND 7 μm USING JET SPECTRA

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The rotational structure of the ν_{19} (CH_2 -wagging, A-type band), ν_{18} (CH_3 -s-deformation, A-type band), ν_{24} (CH_3 -d-deformation, C-type band), and ν_4 (CH_3 -d-deformation, B-type band) vibrational fundamentals of propane, were recorded using a molecular beam coupled to a Fourier-transform spectrometer working at 0.005 cm^{-1} resolution. The analysis was performed using Watson Hamiltonians for the 19^1 and 18^1 states. However, to properly calculate the rotational levels of the 4^1 and 24^1 vibrational levels, it is necessary to include in the Hamiltonian matrix not only the strong A-type Coriolis interaction which couples them but also the various interactions (Coriolis or Fermi-type) which link them to the levels of the dark 5^1 and 17^1 vibrational states. It is then possible to calculate the upper-state levels to within an average uncertainty of 2 to $5 \times 10^{-3}\text{ cm}^{-1}$ depending on the state. These results are satisfactory given the fact that (i) possible perturbations with nearby combination states were not considered and (ii) several torsional splittings were not accounted for. The band centers derived from the fits are $\tilde{\nu}_0(\nu_{19}) = 1338.965\text{ cm}^{-1}$, $\tilde{\nu}_0(\nu_{18}) = 1376.850\text{ cm}^{-1}$, $\tilde{\nu}_0(\nu_{24}) = 1471.874\text{ cm}^{-1}$ and $\tilde{\nu}_0(\nu_4) = 1476.710\text{ cm}^{-1}$. The standard uncertainties of these values are estimated to be about 0.002 cm^{-1} , which includes the calibration errors as well as the statistical uncertainty of the fittings.