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

J.-M. FLAUD, *Laboratoire de Photophysique Moléculaire, C.N.R.S., Bât. 350, Université Paris-Sud, 91405 Orsay Cedex, France*; W. J. LAFFERTY, *Optical Tech. Division, NIST, Gaithersburg, MD 20899-8440, USA*; M. HERMAN, *Lab. de Chimie Physique Moléculaire, Université Libre de Bruxelles, 50 Av. Roosevelt, 1050-Brussels, Belgium.*

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 5×10^{-3} 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 $\tilde{\nu_0}(\nu_{19}) = 1338.965$ cm^{-1}, $\tilde{\nu_0}(\nu_{18}) = 1376.850$ cm^{-1}, $\tilde{\nu_0}(\nu_{24}) = 1471.874$ cm^{-1} and $\tilde{\nu_0}(\nu_4) = 1476.710$ 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.