FIRST HIGH RESOLUTION ANALYSIS OF THE ν_{21} BAND OF PROPANE AT 921.4 cm^{-1}: EVIDENCE OF LARGE-AMPLITUDE-MOTION TUNNELLING EFFECTS

AGNES PERRIN, F. KWABIA TCHANA, JEAN-MARIE FLAUD, *LISA, CNRS, Universités Paris Est Créteil et Paris Diderot, Créteil, France*; LAURENT MANCERON, *Synchrotron SOLEIL, CNRS-MONARIS UMR 8233 and Beamline AILES, Saint Aubin, France*; JEAN DEMAISON, NATALJA VOGT, *Section of Chemical Information Systems, Universität Ulm, Ulm, Germany*; PETER GRONER, *Department of Chemistry, University of Missouri - Kansas City, Kansas City, MO, USA*; WALTER LAFFERTY, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD, USA*.

A high resolution (0.0015 cm^{-1}) IR spectrum of propane, C_3H_8, has been recorded with synchrotron radiation at the French light source facility at SOLEIL coupled to a Bruker IFS-125 Fourier transform spectrometer. A preliminary analysis of the ν_{21} fundamental band (B_1, CH_3 rock) near 921.4 cm^{-1}reveals that the rotational energy levels of 21_1 are split by interactions with the internal rotations of the methyl groups. Conventional analysis of this A-type band yielded band centers at 921.3724(38), 921.3821(33) and 921.3913(44) $\mathrm{cm}^{-1}$for the AA, EE and $AE + EA$ tunneling splitting components, respectively.[a] These torsional splittings most probably are due to anharmonic and/or Coriolis resonance coupling with nearby highly excited states of both internal rotations of the methyl groups. In addition, several vibrational-rotational resonances were observed that affect the torsional components in different ways. The analysis of the B-type band near 870 cm^{-1}(ν_8, sym. C-C stretch) which also contains split rovibrational transitions due to internal rotation is in progress. It is performed by using the effective rotational Hamiltonian method ERHAM[b] with a code that allows prediction and least-squares fitting of such vibration-rotation spectra.

[a] A. Perrin et al., submitted to $J.Mol.Spectrosc.$

[b] P Groner, $J.Chem.Phys.$ 107 (1997) 4483; $J.Mol.Spectrosc.$ 278 (2012) 52.