HIGH-RESOLUTION INFRARED SPECTROSCOPY OF CUBANE, C₈H₈

VINCENT BOUDON, Laboratoire ICB, CNRS/Université de Bourgogne, DIJON, France; OLIVIER PIRALI, SÉBASTIEN GRUET, AILES beamline, Synchrotron SOLEIL, Saint Aubin, France; LUCIA D’ACCOLTI, CATERINA FUSCO, COSIMO ANNESE, Dipartimento di Chimica, Università di Bari A. Moro, Bari, Italy.

Carbon-cage molecules have generated a considerable interest from both experimental and theoretical point of views. We recently performed a high-resolution study of adamantane (C₁₀H₁₆), the smallest hydrocarbon cage belonging to the diamandoid family. There exist another family of hydrocarbon cages with additional interesting chemical properties: the so-called Platonic hydrocarbons that comprise dodecahedrane (C₂₀H₂₀) and cubane (C₈H₈). Both possess C–C bond angles that deviate from the tetrahedral angle (109.8°) of the sp³ hybridized form of carbon. This generates a considerable strain in the molecule. Cubane itself has the highest density of all hydrocarbons (1.29 g/cm³). This makes it able to store large amounts of energy, although the molecule is fully stable. Up to now, only one high-resolution study of cubane has been performed on a few bands [2].

We report here a new wide-range high-resolution study of the infrared spectrum of cubane. The sample was synthesized in Bari upon decarboxylation of 1,4-cubanedicarboxylic acid thanks to the improved synthesis of literature [3]; its ¹H and ¹³C NMR, FTIR, and mass spectrometry agreed with reported data [4]. Several spectra have been recorded at the AILES beamline of the SOLEIL French synchrotron facility. They cover the 800 to 3100 cm⁻¹ region. Besides the three infrared-active fundamentals (ν₁₀, ν₁₁ and ν₁₂), we could record many combination bands, all of them displaying a well-resolved octahedral rotational structure. We present here a preliminary analysis of some of the recorded bands, performed thanks the SPVIEW and XTDS software, based on the tensorial formalism developed in the Dijon group [5].