ROTATIONAL SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS OF A FRUIT ESTER: THE MICROWAVE SPECTRUM OF n-BUTYL ACETATE

T. ATTIG, L.W. SUTIKDJA, R. KANNENGIEßER, W. STAHL, *Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, D-52074 Aachen, Germany*; I. KLEINER, *Laboratoire Interuniversitaire des Systèmes Atmosphériques, CNRS et Universités Paris Diderot et Paris Est, 61 av. Général de Gaulle, 94010, Créteil, France*.

In the course of our studies on a number of aliphatic ester molecules and natural substances, the rotational spectrum of n-butyl acetate (CH_3-COO-C_4H_9) has been recorded for the first time in the 10-13.5 GHz frequency range, using the MB-FTMW spectrometer in Aachen, with an instrumental uncertainty of a few kHz for unblended lines.
Three conformers were observed. The main conformer with C_1 symmetry has a strong spectrum. The other two conformers have C_s and C_1 symmetries. Their intensities are considerably weaker. The quantum chemical calculations of specific conformers were carried out at the MP2/6-311++G(d,p) level, and for the main conformer different levels of theory were calculated. To analyze the internal rotation of the acetyl methyl groups the codes XIAM (based on the Combined Axis Method) and BELGI (based on the Rho-Axis-Method) were used to model the large amplitude motion. The molecular structures of the three conformers were determined and the values of the experimental rotational constants were compared with those obtained by ab initio methods. For all conformers torsional barriers of approximately 100 cm^{-1} were found.
This study is part of a larger project which aims at determining the lowest energy conformers and their structures of organic esters and ketones which are of interest for flavour or perfume synthetic applications[a].

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