PROBING THE METHYL TORSIONAL BARRIERS OF THE *E* AND *Z* ISOMERS OF BUTADIENYL ACETATE BY MICROWAVE SPECTROSCOPY

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The Fourier transform microwave spectra of the *E* and the *Z* isomer of butadienyl acetate have been measured in the frequency range from 2 to 26.5 GHz under molecular beam conditions. The most stable conformer of each isomer, in which all heavy atoms are located in a symmetry plane, was identified after analyzing the spectrum by comparison with results from quantum chemical calculations. The barrier to internal rotation of the acetyl methyl group was found to be 149.1822(20) cm^{-1} and 150.2128(48) cm^{-1} for the *E* and the *Z* isomer, respectively, which are similar to that of vinyl acetate [a,b]. A comparison between two theoretical approaches treating internal rotations, the rho axis method (using the program *BELGI-C_s*) and combined axis method (using the program *XIAM*), is also performed.

Since several years we study the barriers to internal rotation of the acetyl methyl group in acetates, CH_3-COOR. Currently, we assume that all acetates can be divided into three classes. Class I contains α,β saturated acetates, where the torsional barrier is always close to 100 cm^{-1}. Examples are a series of alkyl acetates such as methyl acetate and ethyl acetate. Class II contains α,β-unsaturated acetates where the C=C double bond is located in the COO plane. This is the case of vinyl acetate and butadienyl acetate. Finally, in class III with isopropenyl acetate and phenyl acetate as two representatives, α,β-unsaturated acetates, in which the double bond is not located in the COO plane, are collected. There, we observed a barrier height around 135 cm^{-1}. This observation will be discussed in details.

[a] B. Velino, A. Maris, S. Melandri, W. Caminati, J. Mol. Spectrosc. 2009, 256, 228

[b] H. V. L. Nguyen, A. Jabri, V. Van, and W. Stahl, J. Phys. Chem. A, 2014, 118, 12130