STRUCTURE AND ROTATIONAL DYNAMICS OF ISOAMYL ACETATE AND METHYL PROPIONATE STUDIED BY MICROWAVE SPECTROSCOPY

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The microwave spectra of a number of organic aliphatic esters have been recorded for the first time in the 3-26.5 GHz frequency range, using the molecular beam Fourier-transform microwave (MB-FTMW) spectrometer in Aachen, with an instrumental uncertainty of a few kHz for unblended lines. The combined use of *ab initio* quantum chemical calculations and spectral analysis allowed us to determine the spectroscopic parameters and potential barriers to internal rotation of the methyl groups for the lowest energy conformers.
We will compare here the results from *ab initio* calculations and from two different hamiltonian methods (the XIAM and BELGI codes) for isoamyl acetate H_3C-COO-(CH$_2$)$_2$-CH(CH$_3$)$_2$, an one-top internal rotor molecule with a C_1 symmetry and for methyl propionate CH_3CH_2COOCH_3 containing two inequivalent methyl tops (C_{3v}), with different barrier heights.
This study is part of a larger project which aims at determining the structures of the lowest energy conformers for a serie of organic esters and ketones which are of interest for flavour or perfume applications.