

MENTHYL ACETATE. A NEW LINK IN THE CHAIN OF ACETATES STUDIED WITH ROTATIONAL SPECTROSCOPY

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Natural essential oils have nowadays a vast range of applications in different areas, from medicine and pharmacology, to food industry and cosmetics. They are composed of several, structurally often similar constituents. Due to the high relevance of essential oils in our everyday life it is of interest to obtain detailed structural and conformational information on their main constituents, to widen our knowledge of their unique properties. Rotational spectroscopy is a powerful technique to address these important questions in an accurate and precise manner.

Here we present a comprehensive conformational analysis of menthyl acetate, one of the constituents of peppermint oil (*Mentha x piperita*). Two conformers of menthyl acetate were observed in the broadband rotational spectrum in the 2-12 GHz frequency range. The structure of the lowest energy conformer was obtained experimentally, based on the assignment of the singly-substituted ^{13}C -isotopologues. Additionally, the internal rotation of the methyl top of the acetyl side group was characterized. The experimentally determined low barrier height is in line with previous rotational spectroscopy results for other acetates, for which barrier heights on the order of 1 kJ/mol were reported. A comparison to the other acetates will be discussed in the scope of this talk.