# THE ROTATIONAL SPECTRUM AND CONFORMATIONAL STRUCTURES OF METHYL VALERATE

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Methyl valerate, $C_4H_9COOCH_3$, belongs to the class of fruit esters, which play an important role in nature as odorants of different fruits, flowers, and wines. A sufficient explanation for the structure–odor relation of is not available. It is known that predicting the odor of a substance is not possible by knowing only its chemical formula. A typical example is the blueberry- or pine apple-like odor of ethyl isovalerate while its isomers ethyl valerate and isoamyl acetate smell like green apple and banana, respectively. Obviously, not only the composition but also the molecular structures are not negligible by determining the odor of a substance. Gas phase structures of fruit esters are thus important for a first step towards the determination of structure–odor relation since the sense of smell starts from gas phase molecules.

For this purpose, a combination of microwave spectroscopy and quantum chemical calculations (QCCs) is an excellent tool. Small esters often have sufficient vapor pressure to be transferred easily in the gas phase for a rotational study but already contain a large number of atoms which makes them too big for classical structure determination by isotopic substitution and requires nowadays a comparison with the structures optimized by QCCs. On the other hand, the results from QCCs have to be validated by the experimental values.

About the internal dynamics, the methoxy methyl group -$COOCH_3$ of methyl acetate shows internal rotation with a barrier of 424.581(56) $\mathrm{cm}^{-1}$. A similar barrier height of 429.324(23) $\mathrm{cm}^{-1}$was found in methyl propionate, where the acetyl group is extended to the propionyl group. The investigation on methyl valerate fits well in this series of methyl alkynoates. In this talk, the structure of the most energetic favorable conformer as well as the internal rotation shown by the methoxy methyl group will be reported. It could be confirmed that the internal rotation barrier of the methoxy methyl group remains by longer alkyl chain.