Structural Studies of biologically active compounds in different states of aggregations

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Regardless of their chemical composition, odorants have to meet at least two requirements: They must be sufficiently volatile to achieve a discernible concentration in the gas phase, and they must interact with a receptor. The former condition makes odorants candidates for gas-phase studies, while the latter explicitly suggests that one investigates the structure of odorants in the condensed phase, especially with respect to their soft degrees of freedom.

To perform conformational studies of such biologically active molecules in the gas phase, molecular beam Fourier transform microwave spectroscopy is the ideal tool, as it allows to observe only the lowest energy conformers due to rotational temperatures of approximately 5 K. This is especially interesting, when the molecules of interest possess large amplitude motions, which may cause difficulties for the prediction of theoretical geometries at different levels of theory. The method then yields highly accurate barriers to internal rotation of the methyl groups. The experimental results can be directly used to validate the quantum chemical calculations.

To study the conformations in the solid phase, structural information may be obtained by either analyzing inclusion compounds of the target molecule with large host molecules (e.g., cholic acid) or by directly comparing structures of crystalline derivatives.