NEW INSIGHTS ON ODORANTS AND THEIR COMPLEXES BY ROTATIONAL SPECTROSCOPY

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Understanding the relationship between structure and smell is important to disentangle the molecular mechanisms involved in olfaction and to develop new odorants with scalable synthesis and higher biodegradability. However, the conformations of a large number of widely used odorants are unknown. Moreover, detailed information on the interactions between odorants and amino acid residues in the binding pockets of olfactory receptors is also lacking. Rotational spectroscopy, combined with quantum chemistry methods, is a powerful tool to obtain precise data on the conformations and interactions of a variety of molecular systems. In this talk we will present some of our recent results on the conformations of odorants and their complexes, and the interactions, namely hydrogen bonding and dispersion, driving them. The performance of several theoretical methods will be discussed in the context of the experimental observations.

p-number: p214 **Submitted on Fri, 16 Jun 2023 01:05:39 +0200**