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From Small Substituted Heteroaromatic Rings to Highly Flexible Macrocycles: How Intermolecular and Intramolecular Interactions influence Conformation

Monday 15 September 2025 14:30 (30 minutes)

Intermolecular and intramolecular non-covalent interactions play a crucial role in the conformational preferences of flexible molecules, which are key in chemical and biochemical processes. Rotational spectroscopy is a powerful technique for the precise determination of molecular structure and when aided by quantum chemical calculations can reveal the intricate interplay of non-covalent interactions present within molecules and complexes. In this talk, we will discuss the flexibility and conformational choices of two different molecular systems. We will show that the isomers *N*-ethylimidazole and 2-ethylimidazole behave differently upon hydration. While *N*-ethylimidazole retains its lowest-energy conformation, optimising hydrogen bonding drives a change in the lowest-energy conformation of 2-ethylimidazole. Secondly, we will focus on the rich conformational landscape of macrocyclic musks, widely used in the perfume industry, and their interactions with odorant receptors. Understanding the relationship between musk conformation and smell is important for the development of new and sustainable musks. We will comment on the non-covalent interactions governing musk conformation and the preliminary results of molecular docking simulations to the human musk receptor will be presented.

Keywords

Weak, medium and strong hydrogen bonds, gas phase

This abstract is submitted for....

Early-career researchers´ workshop

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