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Bridging Non-Covalent Interactions in Diverse Cyclic Systems: Insights from Rotational Spectroscopy and Quantum Chemistry Calculations

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The conformational behaviour of biologically relevant cyclic molecules raises fundamental questions from a physicochemical perspective, as their structural and energetic features are closely linked to physicochemical properties and biological function. These systems are often classified by ring size into small (3–7 members), medium (8–11), and large (>12). However, as molecular flexibility increases, identifying energetic minima becomes challenging due to the interplay of weak and competing intramolecular interactions.[1]

Despite their relevance, conformational studies—particularly on larger rings and their hydrated complexes[2]—remain scarce. This work summarises key findings from recent years on non-covalent interactions that govern structural preferences, the role of functional group modifications, and the effects of microsolvation on a series of cyclic systems of increasing size, including their water complexes. These studies employ high-resolution rotational spectroscopy combined with quantum chemical calculations, showing this approach is a powerful tool for elucidating the subtle but crucial structural and interaction features that define the behaviour of these systems.

[1] V. W. Tsoi, E. Burevschi, S. Saxena and M. E. Sanz, J. Phys. Chem. A, 2022, 126, 6185–6193.
[2] C. Pérez, J. C. Lopez, S. Blanco and M. Schnell, J. Phys. Chem. Lett., 2016, 7, 4053–4058

Keywords

Non-covalent interactions, rotational spectroscopy, microsolvation

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