MICROHYDRATION ON MULTICONFORMATIONAL LARGE MOLECULES: INTRA- AND INTERMOLECULAR INTERACTIONS OF MACROLACTONES WITH WATER

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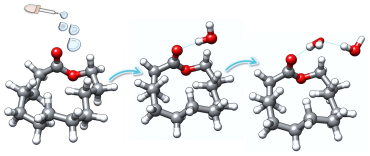

Exploring the conformational landscape of multi-conformational systems, such as macrolactones, can be challenging, as their great flexibility leads to small structural changes that result in a large number of energy minima. High-resolution gas-phase microwave spectroscopy has proven to be unique technique, being able to isolate and discern conformers or clusters unambiguously without masking effects. Macrolactones are considered "privileged scaffolds" within the medicinal chemistry community, because their study led to the discovery of bioactive compounds. However, gas-phase studies on the changes in structure and intra/intermolecular interactions after solvation of these biomolecules are very scarce. Based on the previous rotational study of oxacyclotridecan-2-one (C12) and 16-hexadecanolide (C15),[a] in this work we have studied the structural behaviour of these molecular systems after the addition of individual water (W) molecules.

Using broadband chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy, five conformers have been observed so far for the C12···W complex and the global minimum for C15···W. This study has once again challenged the limits of rotational spectroscopy and quantum chemical calculation due to the structural complexity of these complexes. These results are the initial steps for future microsolvation studies with different solvents.

[a] M. Parra-Santamaria, I. Usabiaga, A. Insausti, E. R. Alonso, F. J. Basterretxea, C. Calabrese, E.J. Cocinero, HRMS2022, Prague (Czech Republic), 2022.