

WATER BINDING TO KETONES: CYCLOOCTANONE · · (H₂O)₃₋₇ COMPLEXES

VALERIE W. Y. TSOI, ECATERINA BUREVSCHI, M. EUGENIA SANZ, *Department of Chemistry, King's College London, London, United Kingdom.*

Understanding the first interaction stages of water with organic molecules is of great interest given the ubiquity of water in nature. Here we explore the microsolvation of the eight-membered cyclic ketone cyclooctanone (CYO) using chirped pulse Fourier transform microwave spectroscopy. We previously assigned three conformers of CYO monomer and complexes of CYO · · (H₂O)_{1,2}[1,2]. Cyclooctanone hydrates with higher number of water molecules, CYO · · (H₂O)₃₋₇, have now been observed and identified with the aid of ab initio and DFT methods. Most of the complexes show several arrangements, highlighting the versatility of water molecules in their interactions with an organic solute. Binding preferences and relevant interactions will be discussed.

[1] E. Burevschi, I. Peña, M. E. Sanz, *Phys. Chem. Chem. Phys.* **2019**, *21*, 4331-4338.

[2] E. Burevschi, I. Peña, M. E. Sanz, *J. Phys. Chem. Lett.* **2021**, *12*, 12419-12425.