

## Spectroscopic studies of molecules and molecular ions using helium nanodroplets

Andrew Ellis, University of Leicester, UK

Recent work on the spectroscopy of molecules, clusters and complexes within, or originating from, liquid helium nanodroplets, will be described. There will be a deliberate bias towards work done in our laboratory, and a sizeable proportion of the work I will present is currently unpublished. After a brief overview of helium droplets and how spectroscopy can be performed in this environment, some studies on neutral molecules will be presented, including solute-solvent complexes.<sup>1</sup> Particular emphasis will be placed on how helium droplets allow access to parts of potential energy surfaces that are difficult or impossible to reach using other methods,<sup>2,3</sup> and I will include examples where remarkably clean production of structural isomers/conformers are formed which are way above the global energy minimum. The talk will then switch to describe some of our recent work on helium-tagged ions, produced by electron ionization of molecule-doped helium droplets.<sup>4,5</sup> This provides a means to explore the spectroscopy of the bare ion, assuming perturbation by helium is small, but also allows the role of the helium tag to be assessed by recording IR photodissociation spectra as a function of the number of attached helium atoms. Examples will be shown for a number of ions drawn from organic and inorganic chemistry, including the ubiquitous  $\text{H}_3\text{O}^+$  ion.

1. "IR spectroscopy of the cesium iodide-water complex", J. A. Davies, M. Mugglestone, S. Yang, A. M. Ellis, *J. Phys. Chem. A* **124**, 6528- 6535 (2020).
2. "Dimers of acetic acid in helium nanodroplets", J. A. Davies, M W. D. Hanson-Heine, N A. Besley, A. Y. Shirley, J. Trowers, S. Yang, A. M. Ellis, *Phys. Chem. Chem. Phys.* **121**, 13950-13958 (2019).
3. "Shifting formic acid dimers into perspective: vibrational scrutiny in helium nanodroplets" K. A. E. Meyer, J. A. Davies, A. M. Ellis, *Phys. Chem. Chem. Phys.* **22**, 9637- 9646 (2020).
4. "Probing elusive cations: infrared spectroscopy of protonated acetic acid", J. A. Davies, N. A. Besley, S. Yang, A. M. Ellis, *J. Phys. Chem. Lett.* **10**, 2108-2112 (2019).
5. "Infrared spectroscopy of a small ion solvated by helium: OH stretching region of  $\text{He}_N\text{-HOCO}^+$ ", J. A. Davies, N. A. Besley, S. Yang, A. M. Ellis, *J. Chem. Phys.* **151**, 194307 (2019).