

FOUR EXPERIMENTAL SYSTEMS THAT TEST DISPERSION INTERACTIONS IN LARGE MOLECULES

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Non-covalent interactions have been proposed to play a large role in organic and organometallic chemistry, with the magnitude of the interactions increasing rapidly with the number of atoms. Detailed experimental tests of the proposition in the gas phase focus on small molecules, for a variety of technical reasons. For small molecules, though, the magnitude of the interactions is small, which introduces its own suite of technical constraints. We report four different experimental systems, examined with a range of gas-phase, physical techniques ranging from energy-resolved collision-induced dissociation cross-sections to ion spectroscopy by cryogenic ion vibrational predissociation spectroscopy or IRMPD, of electrosprayed molecular ions, in which the non-covalent interactions become large enough that the experiments can provide hard benchmarks against which theory can be tested. We find that the present generation of dispersion-corrected DFT methods appear to overestimate the attractive component of the interaction, at least for certain interaction geometries.