ROTATIONAL SPECTROSCOPIC BENCHMARK FOR π INTERATION

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A great deal of attention has been given to noncovalent interactions involving π systems because of their widespread presence in biology as well as materials, where they are pivotal in determining the three-dimensional structures of, e.g., proteins and polymers or the selectivity of molecular affinity. Despite dramatic advances in our understanding over past decades, many aspects of π interactions have only recently been discovered, with many questions remaining. Rotational spectroscopy is arguably the most accurate high resolution molecular spectroscopic technique due to its high sensitivity to mass distributions of molecules and molecular complexes. Since the interaction sites and the relative arrangement of moieties can be determined without environmental bias, rotational spectroscopy allows describing the intermolecular forces at play and enables testing of quantum chemical methods. In this talk, with the recent rotational spectroscopic results we have obtained on π interactions, the comparisons between experimental and computaional data will be discussed.