EXPLORING THE HYPERFINE STRUCTURE OF MOLECULAR HYDROGEN INTERACTING WITH SMALL AROMATIC SYSTEMS THROUGH ROTATIONAL SPECTROSCOPY

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Non-covalent interactions play a key role in the formation of molecular complexes and reactivity. In previous works only interactions of small molecules with hydrogen have been investigated by rotational spectroscopy while interactions of molecular hydrogen with aromatic systems are unexplored.

In this work, the bond of hydrogen to the π-system of halogenated benzaldehydes is investigated. These volatile systems possess a large dipole moment and have multiple non-covalent binding sites to investigate selectivity. By introducing quadrupolar nuclei the complexity of the system is increased, the quadrupolar nucleus acts as a spectroscopic probe for the electronic field gradient and provides insights into the long-range dispersive interactions. Of particular interest are the differences observed for the rotational spectrum of *ortho*- and *para*-hydrogen and its structural impact investigated by isotopic substitution. The two spin isotopes show significant differences in rotational constants which demonstrate that there are significant differences in binding strength of o-H_2 and p-H_2 to the π-system, which are experimentally observable. Broadband rotational spectra are presented which are supplemented with cavity data to resolve the additional hyperfine splitting caused by the spin-spin coupling of o-H_2. We present elements of the spin-spin coupling tensor and draw experimental conclusions about hydrogen bond distance and the orientation of the o-H_2 with respect to the benzaldehyde plane.