

## BRIDGING THE GAP: ROTATIONAL STUDY OF H<sub>2</sub> IN COMPLEXES WITH SMALL AROMATIC MOLECULES

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Molecular hydrogen plays a key role in our efforts to shift our energy production to renewable resources. Hydrogen is an important energy storage molecule which in the future may replace our fossilized fuels as a transportable energy source. To appropriately model hydrogen storage materials, an understanding of the fundamental binding to organic systems is required. In previous works only a few inorganic and metallic complexes with hydrogen have been investigated by rotational spectroscopy.<sup>a,b</sup> This work aims to bridge the gap to large covalent organic frameworks (COF) by focusing on the microwave structure of hydrogen heterodimers with small aromatic ring systems.<sup>c</sup>

In this work the binding sites of hydrogen to halogen benzaldehydes which serve as mimics COF monomers, specifically boronic ester based COFs, are studied. These volatile systems possess a large dipole moment and provide a method of increasing the complexity of the system by the introduction of quadrupolar nuclei to finally look at small boronic esters in hydrogen complexes. 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 significant differences between these two species demonstrate there are significant differences in binding strength of *o*-H<sub>2</sub> and *p*-H<sub>2</sub> which are experimentally observable. Broadband rotational spectra are presented, are supplemented with cavity Fourier transform microwave spectroscopy data to resolve the additional hyperfine splitting of *o*-H<sub>2</sub> ( $j = 1$ ). These experimental results can be directly compared to a number of quantum chemical predictions to provide a foundation for the simulation of large scale covalent organic frameworks.

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<sup>a</sup>Jäger, W. et al., *J. Chem. Phys.*, **127** 054305, 2007, DOI: 10.1063/1.2756534

<sup>b</sup>Obenchain, D., Frank, H., Pickett, H., Novik, S., *J. Chem. Phys.*, **146** 204302, 2017, DOI:10.1063/1.4983042

<sup>c</sup>Geng, K., He, T., Liu, R. et al., *Chem. Rev.*, **120** 8814, 2020, DOI: 10.1021/acs.chemrev.9b00550