EXPLORING THE DIFFERENCES IN *ORTHO*- AND *PARA*-H_2-FLUOROBENZALDEHYDE COMPLEXES USING FTMW METHODS

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Understanding the intermolecular binding of molecular hydrogen to other compounds is a basic requirement for the design of possible H_2 storage materials. Nevertheless, studies on H_2 van der Waals complexes with e.g. H_2O,[1] OCS[2], HCN[3], and AgCl[4] show that to date, there are still gaps in the comprehension especially concerning differences in the binding of *ortho*- and *para*-H_2 to a specific host molecule. Our group investigates the structure of bimolecular *ortho*- and *para*-H_2 complexes with 2-, 3-, and 4-fluorobenzaldehyde, applying chirped pulse and high-resolution cavity Fourier-transform microwave (FTMW) spectroscopy. Rotational and centrifugal distortion constants were determined, supported by DFT-based predictions. Furthermore, the cavity FTMW measurements, taken with a Fabry-Pérot spectrometer, enabled us to resolve the nuclear spin-spin interaction for complexed *ortho*-H_2. The measured rotational constants were used to fit the intermolecular distance. We found that the H_2's center of mass distance to the aromatic plane is 0.36 – 0.37 nm for *ortho*-H_2 and 0.34 – 0.35 nm for *para*-H_2 complexes. This result is surprising since the mentioned studies encourage the conclusion that *ortho*-H_2 generally binds more strongly to a host molecule than *para*-H_2. A possible explanation could be a coupling distortion of the *ortho*-H_2's rotational energy levels due to internal rotation of the H_2 group, which we investigate here. DFT-predicted rotational barriers are between 16 and 32 cm^{-1}.

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