

INVESTIGATING INTERMOLECULAR INTERACTIONS WITHIN NAPHTHOL DIMERS USING BROADBAND ROTATIONAL SPECTROSCOPY

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Present in a variety of chemical systems, π - π stacking and hydrogen bonding are intermolecular forces critical to the formation and stabilization of various chemical structures. Within DNA these two forces work in unison to stabilize the infamous double helix structure;¹ however, these forces do not always act cooperatively and often compete with each other. This competition is clearly exhibited within the phenol dimer structure, where a predominance of hydrogen bonding over π - π stacking is observed.² However, it was unclear how the competition between of hydrogen bonding and π - π stacking would change as the size of the aromatic subunit increases. We use 1-naphthol and 2-naphthol, which can be considered analogues of phenol, as a tool to further understand the complex interplay between π - π stacking and hydrogen bonding. Using chirped-pulse Fourier transform microwave spectroscopy, we detected pure rotational transitions of two conformers for both 1-naphthol and 2-naphthol. We additionally observed and subsequently assigned the dimers of 1-naphthol and 2-naphthol. The experimental identifications of the observed dimers were supplemented with a conformer search enabled by dispersion corrected DFT³ and the CREST sampling program.⁴ Through this study we find, somewhat surprisingly, that the structures of 1-naphthol and 2-naphthol are dictated mainly by π - π stacking, unlike the case of the phenol dimer. Furthermore, the dominance of the π - π stacking interactions not only provides information about 1-naphthol and 2-naphthol like structures, but also insights into the complicated and intricate dynamics of these intermolecular forces and the fine balance between them.

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