

## DOUBLY HYDROGEN BONDED BIS-(4-HYDROXYPHENYL)METHANE DIMERS.

CHIRANTHA P. RODRIGO, WILLIAM H. JAMES III, TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907-2084.*

Single-conformation spectroscopic methods were used to investigate the jet-cooled dimers of the bichromophore bis-(4-hydroxyphenyl) methane (B4HPM). This study serves as an extension of our previous studies on the B4HPM monomer, which revealed two stable monomer conformations in the jet expansion. Here, resonant two-photon ionization, IR-UV holeburning, and resonant ion-dip infrared spectroscopy were used to record the conformation-specific IR and UV spectra of two distinguishable dimer conformations. The first conformer possessed a strong  $S_0-S_1$  origin transition at  $34899\text{ cm}^{-1}$  with little vibronic activity, whereas the second conformer exhibits long progressions in several low frequency modes without a clear origin band. The  $S_0-S_1$  origin transitions of the dimer conformations are shifted  $-285\text{ cm}^{-1}$  from the monomer  $S_0-S_1$  origins, similar to the shift observed between  $S_0-S_1$  origins of *para*-cresol monomer and dimer<sup>a</sup> ( $-328\text{ cm}^{-1}$ ). Furthermore, single-conformation IR spectra show that both dimer conformers have two hydroxyl groups H-bonded. The dimer OH stretches are shifted from the B4HPM monomer values by  $(-11/-144)$  and  $(-17/-144)\text{ cm}^{-1}$ . These shifts are comparable to those of phenol dimer, relative to phenol monomer hydroxyl group stretching frequency.<sup>b</sup> Finally, theoretical predictions provide evidence for two low energy structures. The lowest energy structure consists of monomers in which each molecule acts simultaneously as donor and acceptor. In the second lowest energy structure, however, the two monomers are distinguishable, with one acting as double-donor and the other as double acceptor. This talk will discuss the comparison of the experimental results with the predicted structures and their properties as flexible tetrachromophores.

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<sup>a</sup>K. Song and J. M. Hayes, *J. Mol. Spectrosc.*, **1989**,134,82.

<sup>b</sup>T. Ebata, T. Watanabe and N. Mikami, *J. Phys. Chem.*, **1995**,99,5761.