HYDROGEN-BONDING AND HYDROPHOBIC INTERACTIONS IN THE ETHANOL-WATER DIMER

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The conformational energy landscape of the ethanol-water dimer is determined by the relative hydrogen-bond donor and acceptor strengths of the two molecules, as well as weaker hydrophobic interactions between the water and the ethyl group. Using a combination of *ab initio* calculations and chirped-pulse Fourier transform microwave spectroscopy, we have recorded the first rotationally-resolved, jet-cooled spectrum of the ethanol-water dimer between 8-18.5 GHz and identified two water-donor ethanol-acceptor conformers. The lowest energy conformer is chiral, has ethanol in the gauche configuration, and is consistent with previous raman and infrared results.[a] The second conformer corresponds to the trans-ethanol configuration, and exhibits a significant splitting.

[a]Nedić, Marija, et al. PCCP 13.31 (2011): 14050-14063.