MICROWAVE SPECTRUM OF THE ETHANOL-METHANOL DIMER

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The hydrogen bond donor/acceptor competition in mixed alcohol clusters remains a fundamental question in physical chemistry. Previous theoretical work on the prototype ethanol-methanol dimer has been inconclusive in predicting the energetically preferred structure. Here, we report the microwave spectrum of the ethanol-methanol dimer between 8-18 GHz, using a chirped pulse Fourier transform microwave spectrometer. With the aid of ab initio calculations, 36 transitions have been fit and assigned to a t-ethanol-acceptor, methanol-donor structure in an argon-backed expansion. In a helium-backed expansion, a second excited conformer has been observed, and tentatively assigned to a g-ethanol-acceptor, methanol-donor structure. No ethanol-donor, methanol-acceptor structures have been found, suggesting such structures are energetically disfavored.