WHAT MICROWAVE SPECTROSCOPY TELLS US ABOUT THE BENZENE DIMER

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The benzene dimer is a model system for investigating dispersive intermolecular interactions between aromatic molecules. Numerous theoretical and experimental studies exist. Infrared and Raman spectra show different signatures for the two benzene rings in the dimer from which it can be concluded that they are symmetrically inequivalent. Different theoretical calculations find two different minimum structures for the benzene dimer. One is a "parallel-displaced" structure, and the other a distorted $\mathcal{T}$-shaped one with "stem" and "top" benzene rings. The former structure has symmetrically equivalent rings, whereas the latter has symmetrically inequivalent rings in agreement with the Infrared and Raman studies.

We try to solve this conflict using microwave spectroscopy in the 3 to 6 GHz range. In agreement with the only previous microwave study[a] we find two subgroups of microwave transitions. One fits a symmetric top Hamiltonian with a quartet fine structure that has a characteristic intensity and splitting pattern. To explore the origin of the quartet splitting we have studied the microwave spectrum of the $(C_6H_6)_2$ and C_6H_6-C_6D_6 isotopomers. The other subgroup of lines is presumably due to a different state. Our first experimental results will be presented and discussed in the light of the nuclear spin statistics.

[a] E. Arunan and H. S. Gutowsky, *J. Chem. Phys.*, **98**, 4294 (1993)