ENERGY SPLITTING PATTERNS AND STATISTICAL WEIGHTS FOR THE BENZENE DIMER

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Based on recent *ab initio* results,[a] the benzene dimer is predicted to have a distorted $\mathcal{T}$-shaped equilibrium structure; one benzene ring forming the "stem" of the "$\mathcal{T}$" and the other forming the "cap." The barriers for several tunneling pathways, such as stem-bending, cap-torsion and stem-torsion, have been calculated. In this talk the energy splitting patterns, and nuclear spin statistical weights, that characterize such tunneling pathways will be discussed. Comparison with high resolution spectra will be made for $(C_6H_6)_2$, $(C_6D_6)_2$, and C_6H_6-C_6D_6.

[a]R. Podeszwa, R. Bukowski, and K. Szalewicz *J. Phys. Chem. A* **110,** 10345, (2006) and R. A. DiStasio Jr., G. von Helden, R. P. Steele, and M. Head-Gordon *Chem. Phys. Lett.* (2007), doi: 10.1016/j.cplett.2007.02.034.