Spectroscopy, Monte Carlo, and Electronic Structure Studies of Benzene-Derivative Solvation Clusters

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- R2PI spectra of benzene (B), 1,3,5-trifluorobenzene (T), the BT dimer, and the B₂T trimer measured at 1 cm⁻¹ resolution. Spectral shifts are relative to the forbidden T A'₂ ← A'₁ 0₀₀ origin at 38527 cm⁻¹.

- BT Dimer spectral features are generally sharp with no apparent indications of van der Waals progressions. The B₂T trimer spectrum also contains sharp features within broader underlying features.

- The sharp features may indicate relatively few isomeric forms and that electronic excitations are localized in the dimer, and to a lesser extent in B₂T.