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

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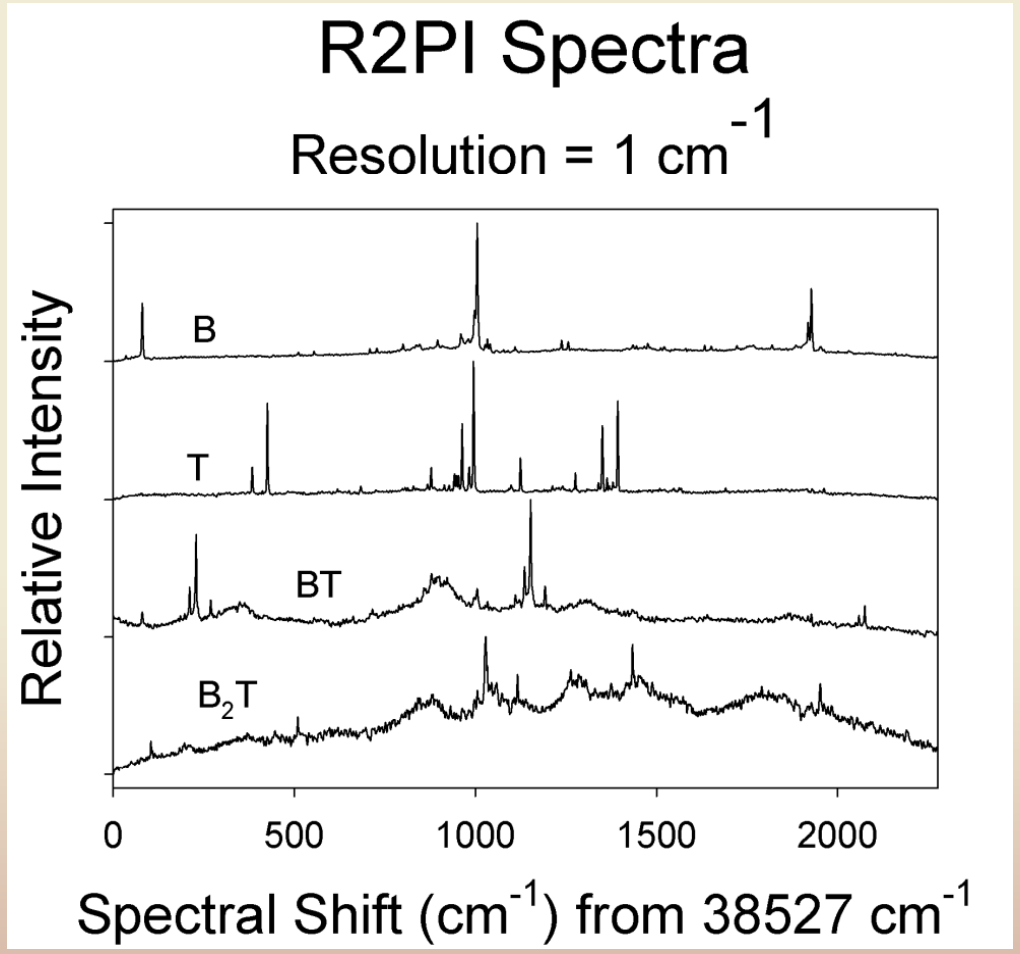

- *R2PI* spectra of benzene (*B*), 1,3,5-trifluorobenzene (*T*), the *BT* dimer, and the B_2T trimer measured at 1 cm^{-1} resolution. Spectral shifts are relative to the forbidden $T\ A'_2 \leftarrow A'_1\ 0^0_0$ origin at 38527 cm^{-1}.
- *BT* Dimer spectral features are generally sharp with no apparent indications of van der Waals progressions. The B_2T 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 B_2T.

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