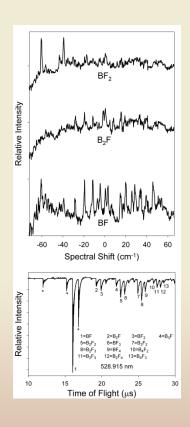
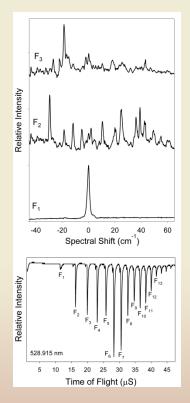
Spectroscopy, Monte Carlo, and Electronic Structure Studies of Benzene-Derivative Solvation Clusters

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R2PI spectra of mixed benzene-fluorobenzene (left) and neat fluorobenzene (right) dimers and trimers. Spectral shifts are relative to fluorobenzene's $B_2 \leftarrow A_1 \ 0^0_0$ origin at 37813 cm⁻¹. The time-of-flight mass spectrum is shown below each set of ultraviolet spectra

All spectra through the trimer show a limited number of reproducible sharp features. After correcting for fragmentation of F_3 , the F_2 spectrum reveals evidence of four van der progressions at 4.1, 6.1, 14.6, and 16.2 cm⁻¹.

MP2 calculations are under way to determine structures and van der Waals frequencies consistent with the spectra.

