

Discerning rotamers of fluorinated stilbenes via transient absorption and femtosecond-stimulated Raman spectroscopy

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“Rotational isomerism” refers to distinguishable torsional conformations around a single bond. We consider rotational isomers (rotamers) of *trans*-1,2-diaryl-ethylenes where rotational axes exist between the central ethylene and the outer aromatic moieties^[1]. In particular, for *ortho*- and *meta*-substituted fluoro-stilbenes an equilibrated mixture of three rotamers exists in the electronic ground state S_0 as shown in Fig. 1. The rotamers have different rates for electronic relaxation $S_1 \rightarrow S_0$. Using Transient Absorption (TA) and Femtosecond-Stimulated Raman (FSR) spectroscopies, we obtain the species-associated TA & FSR spectra of each rotamer together with the ground state population ratios. Qualitative agreement exists with theoretically derived S_0 population ratios and calculated excited-state Raman frequencies.

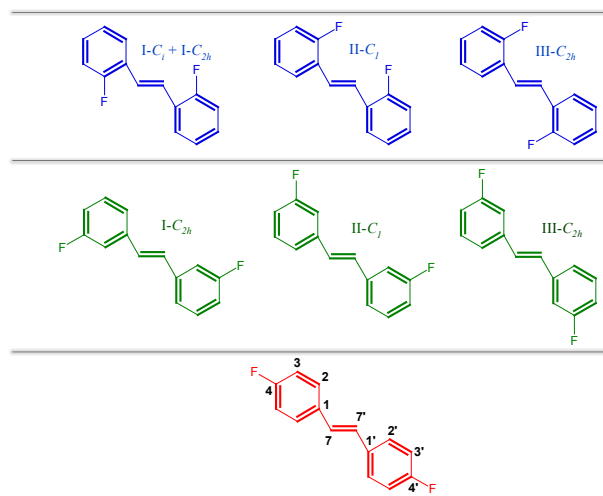


Figure 1. Stilbene is substituted with fluorine atoms in the *ortho*-, *meta*- and *para*-position, respectively. Three rotamers exist for stilbene in the cases of *ortho*- and *meta*-substitution. Only one rotamer is present for F4 which therefore serves as a reference.

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References:

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