Supplementary Information for:

Phonon Bottleneck and Long-Lived Excited States in π-Conjugated Pyrene Hoop

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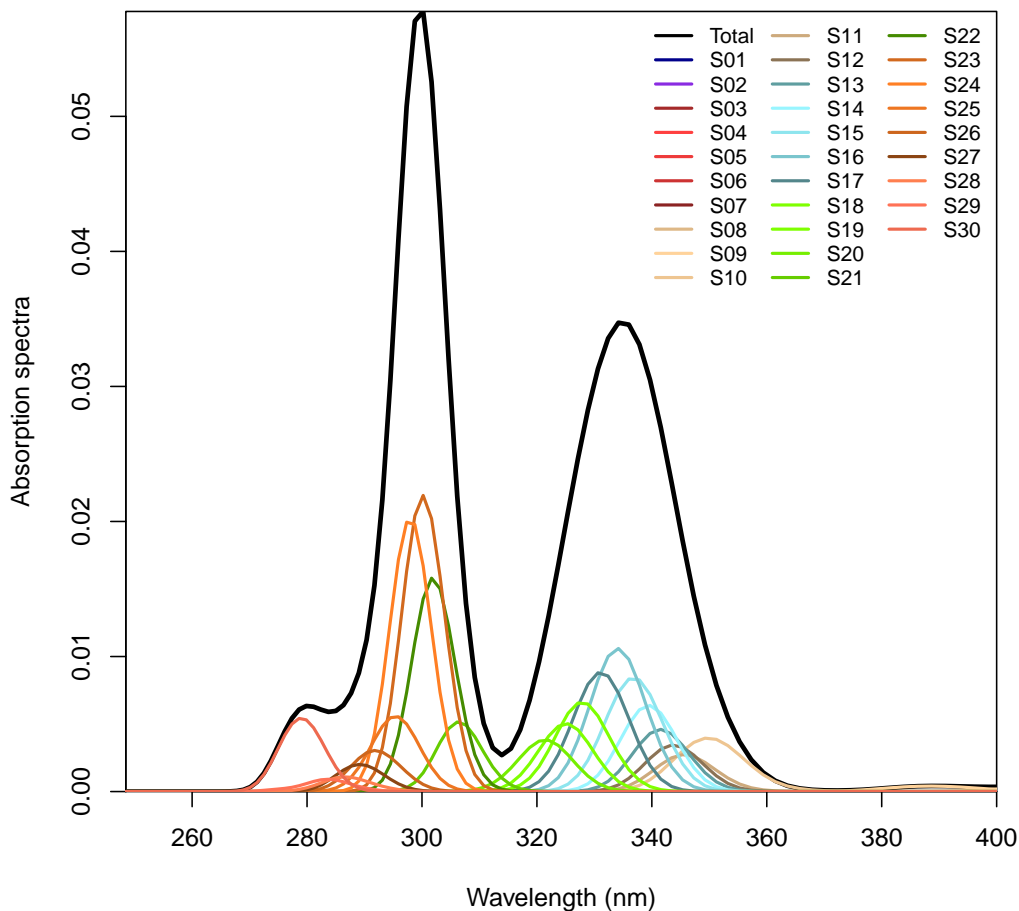[‡]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

Figure S 1: Individual contributions from 30 electronic excited states to the calculated total equilibrated absorption spectrum for [4]CPY at 300 K. The absorption maximum at 300 nm contains contributions mainly from states S_{22} to S_{25}, while contributions to the lower energy peak at 340 nm are mainly from states S_5 to S_9. Accordingly, our simulated laser pulse centered at 300 nm leads to a distribution of initial electronic populations relating to the relative oscillator strengths of contributing states within the specified full width at half maximum (FWHM) of 100 fs. We obtain 25% on S_{22}, 34% on S_{23}, 27% on S_{24}, 9% on S_{25}, and minor contributions from S_{21}, S_{26} and S_{28}.