Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Fluorination-dependent Molecular Orbital Occupancy in Ring-shaped Perfluorocarbons

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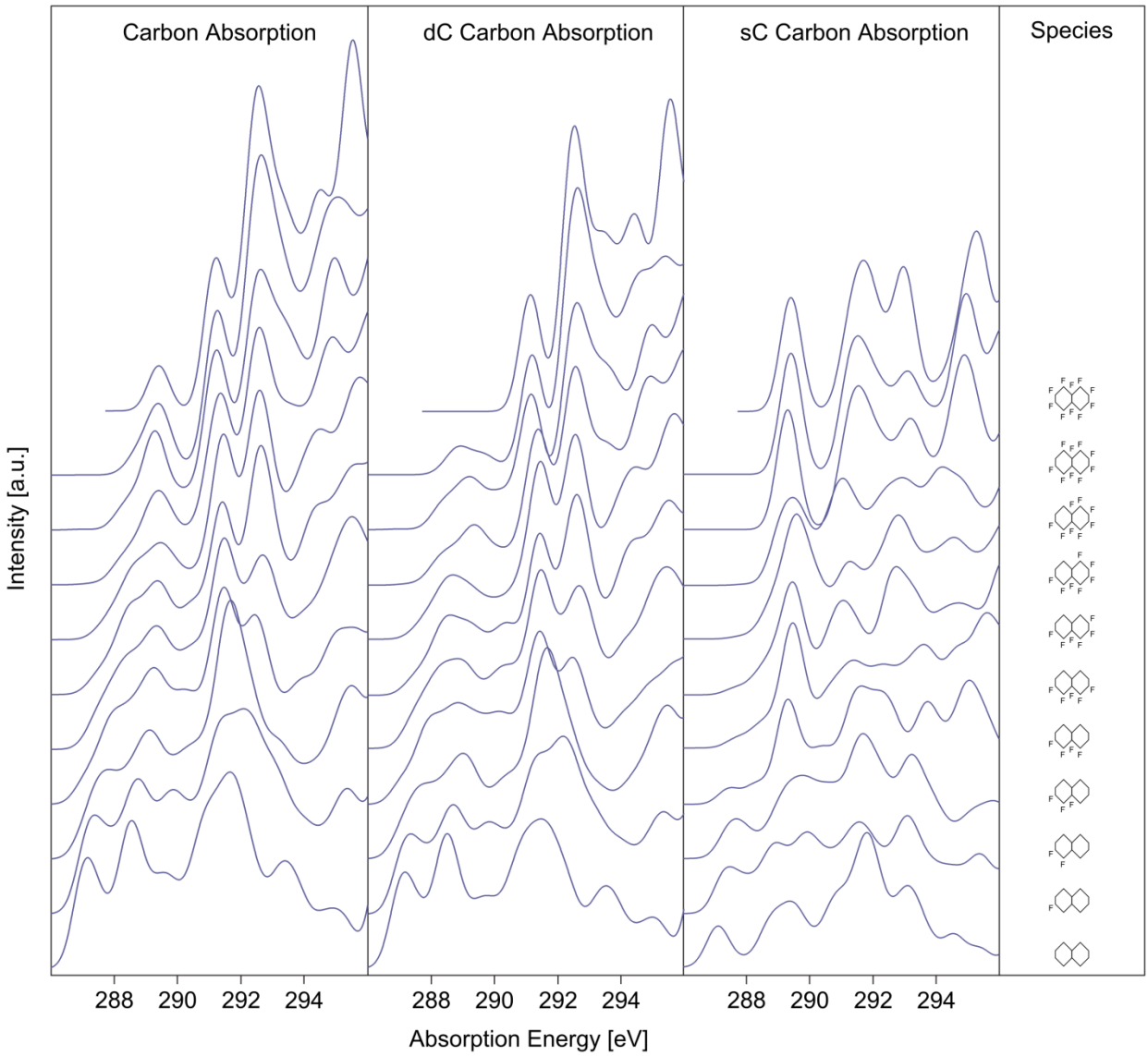
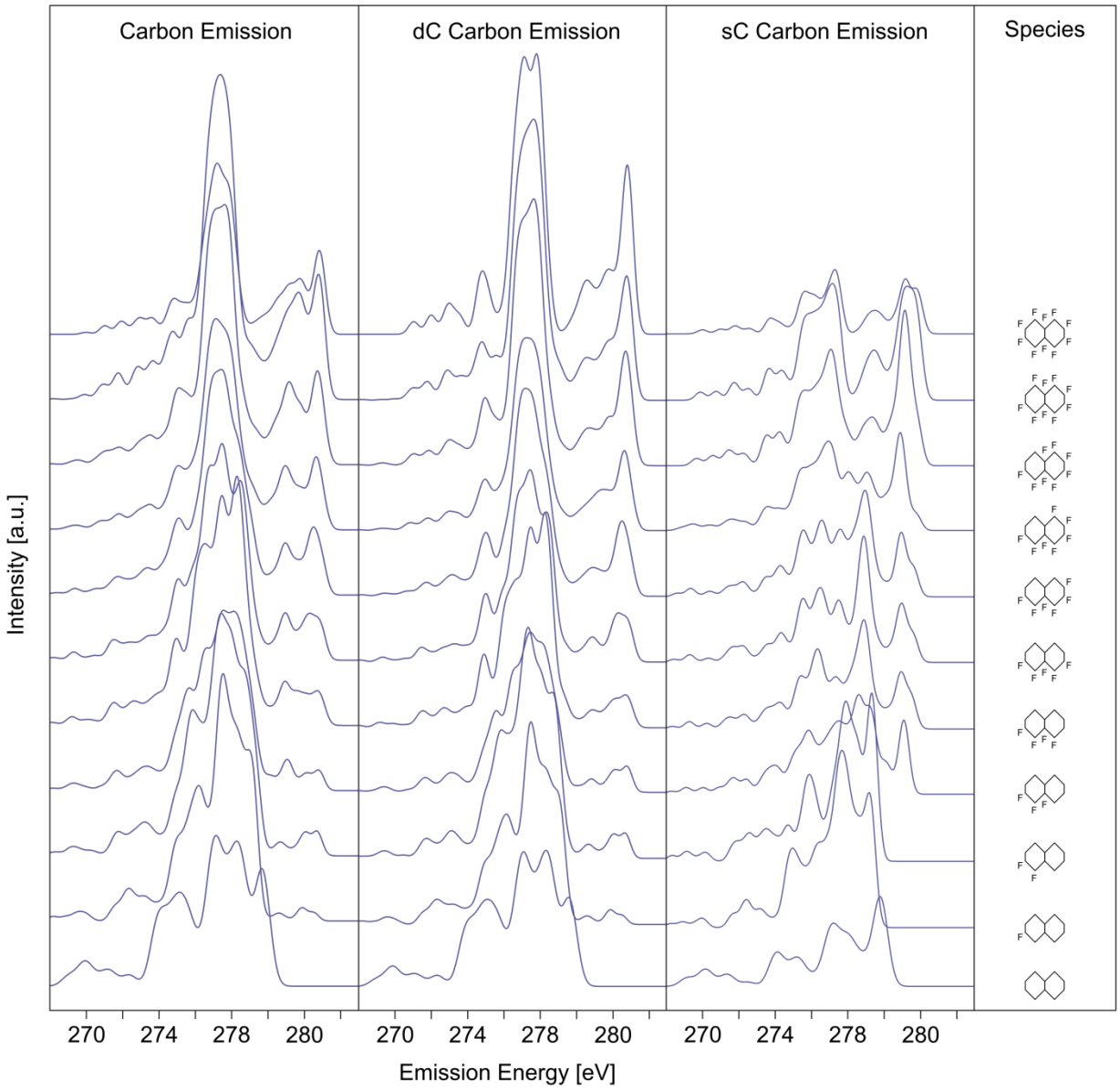
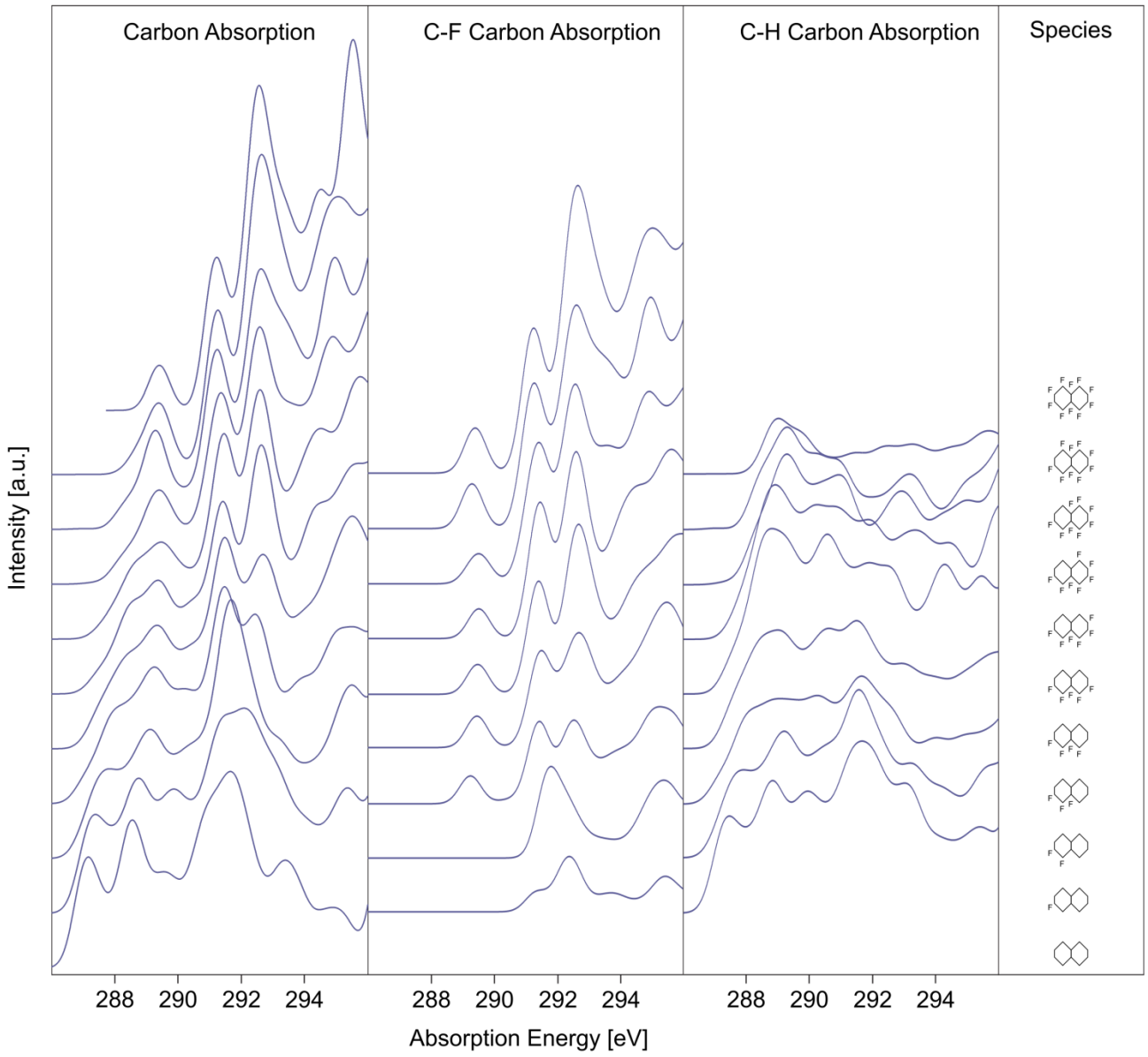


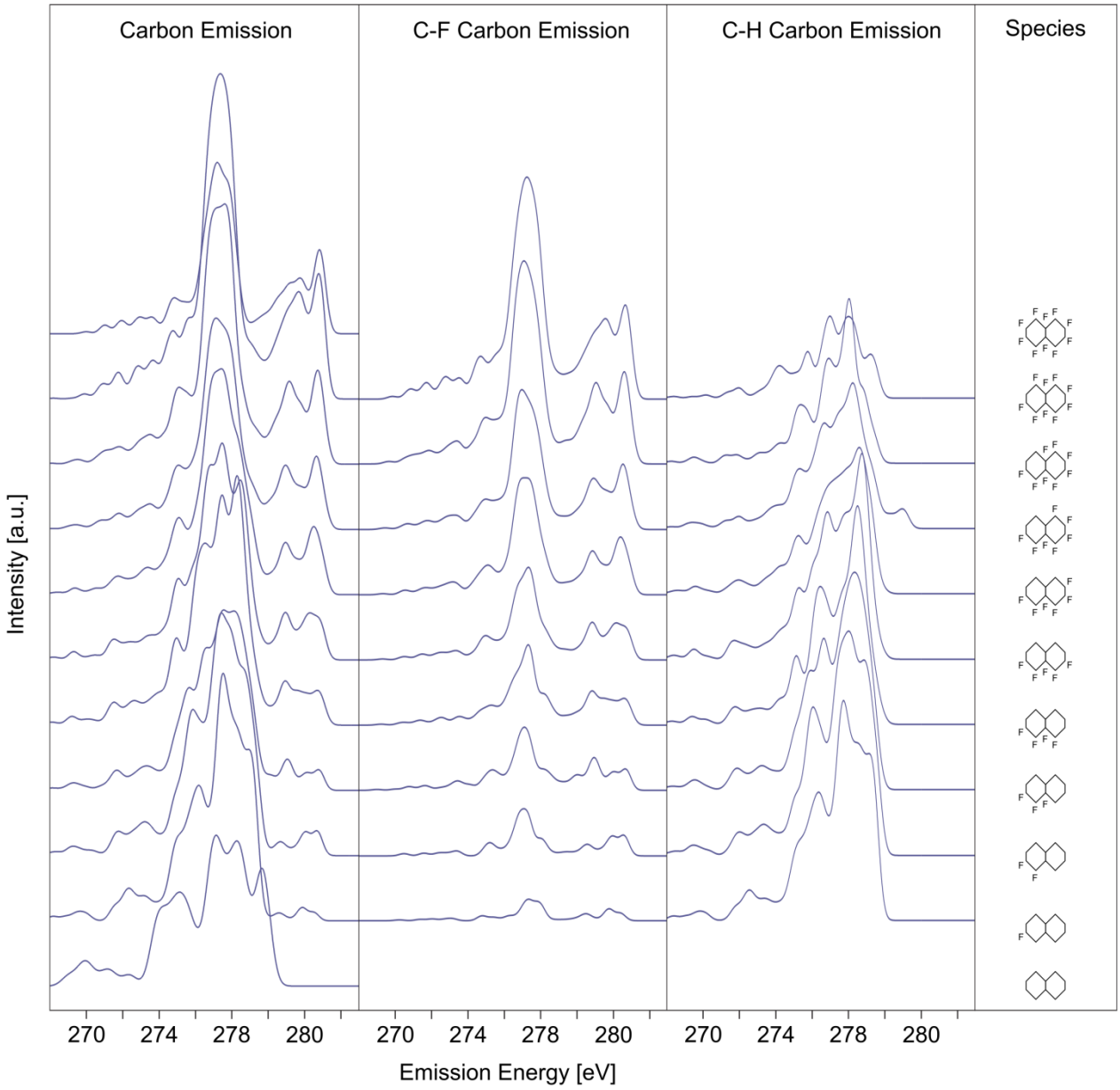
Sup 1. Carbon K absorption calculations for all fluorination stages between decalin and PFD.



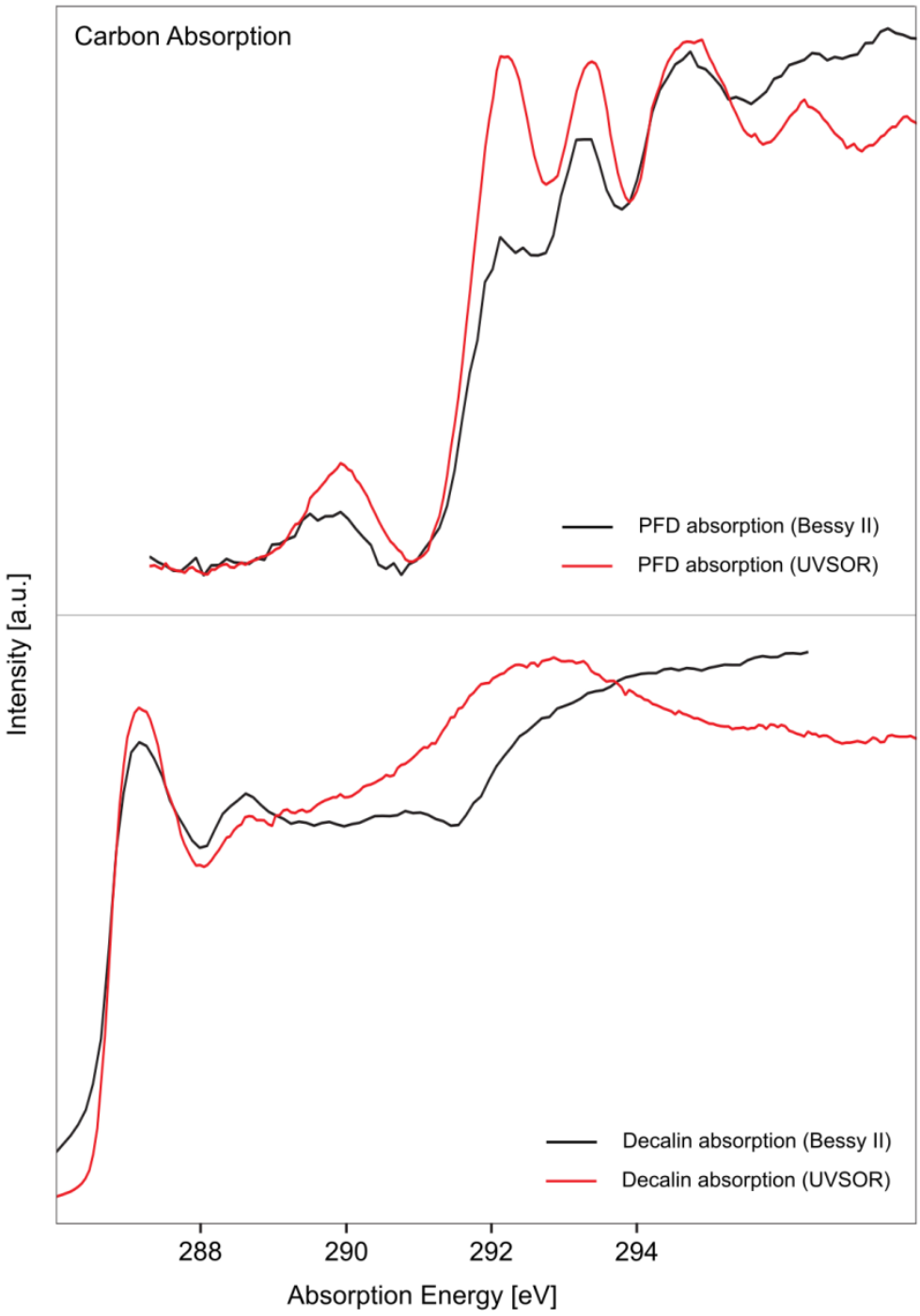
Sup 2. Carbon K emission calculations for all fluorination stages between decalin and PFD.



Sup 3. Carbon K absorption calculations for all fluorination stages between decalin and PFD, separated in absorption spectra of carbons with fluorine nearest neighbors and carbons with hydrogen nearest neighbors.



Sup 4. Carbon K emission calculations for all fluorination stages between decalin and PFD, separated in emission spectra of carbons with fluorine nearest neighbors and carbons with hydrogen nearest neighbors.



Sup 5. Comparison of absorption spectra obtained at both Synchrotron facilities (Bessy II and UVSOR). The spectra obtained at Bessy show clear effects of self-saturation, which result from the technique used to obtain these spectra (Total Fluorescence Yield). To circumvent this effect, another technique (Transmission) was employed where self-saturation effects do not occur.