## Supporting information for 'The Electronic Structure of Perfluorodecalin studied by Soft X-ray Spectroscopy and Electronic Structure Calculations'

T. Brandenburg<sup>*a,b*</sup>, M. Agåker<sup>*c*</sup>, K. Atak<sup>*a,b*</sup>, M. Pflüger<sup>*a,b*</sup>, C. Schwanke<sup>*a*</sup>, T. Petit<sup>*a*</sup>, K. M. Lange<sup>*a*</sup>, J.-E. Rubensson<sup>*c*,†</sup> and E. F. Aziz<sup>*a,b,d*,††</sup>

<sup>a</sup> Institute of Methods for Material Development, Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Straße 15, 12489 Berlin, Germany

<sup>b</sup> Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

<sup>c</sup> Department of Physics and Astronomy, Uppsala University, Box 516, SE 751 20 Uppsala, Sweden

<sup>d</sup> Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan

† jan-erik.rubensson@physics.uu.se

<sup>††</sup> emad.aziz@helmholtz-berlin.de



**Sup 1:** Perfluorodecalin carbon and fluorine K emission compared to gas phase reference data of fluoromethanes<sup>1</sup>. The reference data was shifted by 2.3 eV to fit with the experimental features. Comparison shows striking resemblance between reference and experimental data.

1. P. Glans, R. E. L. Villa, Y. Luo, H. Agren, and J. Nordgren, J. Phys. B At. Mol. Opt. Phys., 1994, 27, 3399.



**Sup 2:** Perfluorodecalin carbon K absorption compared to theoretical data of trans- and cis-PFD (see Fig.1). Both isomers exhibit similar spectra concerning peak positions and intensity. Subsequently, a discussion of the influence of either isomer is not needed.



**Sup 2:** Perfluorodecalin carbon K absorption compared to theoretical calculations of monomer and trimer configurations. Both configurations exhibit similar spectra concerning peak positions and intensity.