Supporting Information

A Near-Edge X-ray Absorption Fine Structure Investigation of the Quasi-One Dimensional Organic Conductor $(TMTSF)_2PF_6$

K. Medjanik[†,*], A. Chernenkaya[‡,§], X. Kozina[‡], S. A. Nepijko[‡], G. Öhrwall[†], P. Foury-Leylekian[⊥], P. Alemany[‖], G. Schönhense[‡], E. Canadell[#] and J.-P. Pouget[⊥]

[†] Lund University, MAX IV Laboratory, 22100 Lund, Sweden

[‡] Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany

[§] Graduate School Materials Science in Mainz, 55128 Mainz, Germany

[⊥] Laboratoire de Physique des Solides, Université Paris-Sud, CNRS UMR 8502, 91405 Orsay, France

[‖] Departament de Ciència de Materials i Química Física and Institut de Química Teórica i Computacional (IQTCUB), Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain

[#] Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de la UAB, 08193 Bellaterra, Spain

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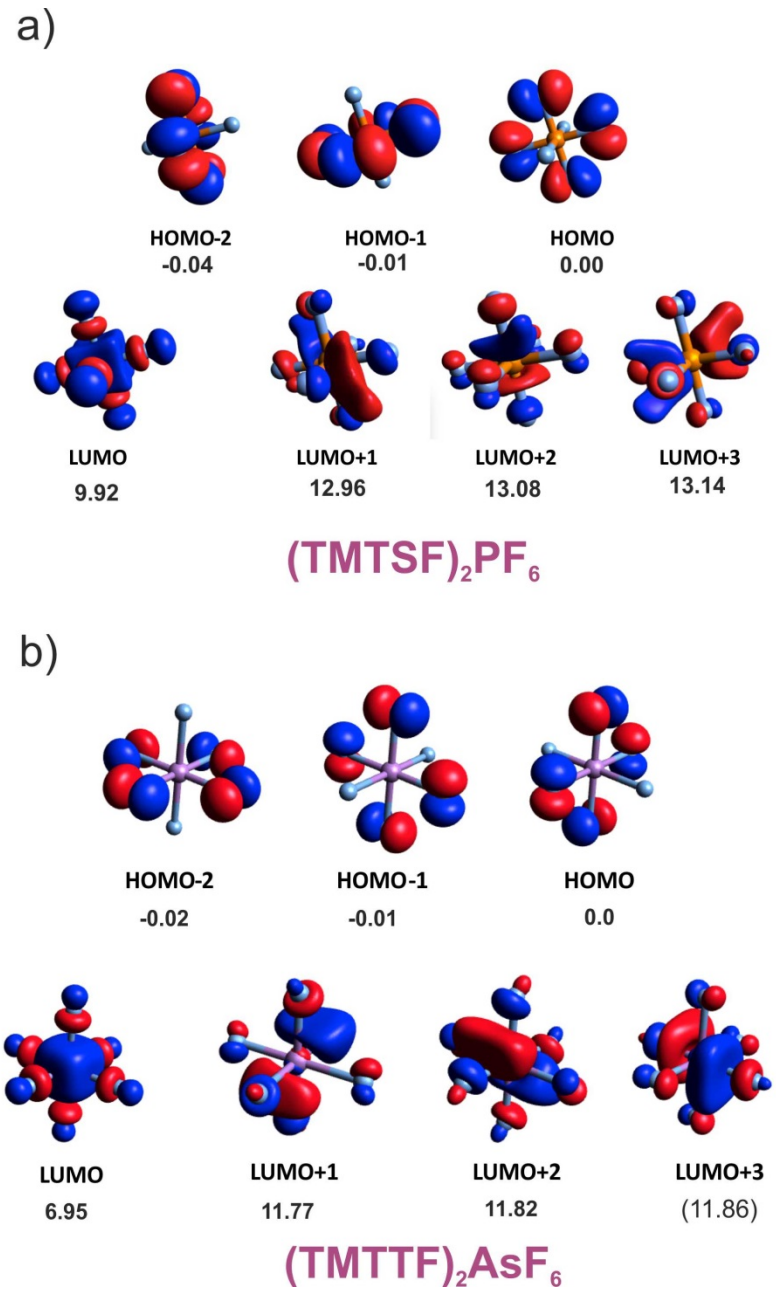

Figure S1. Comparison of the anion molecular orbitals relevant for the analysis of the NEXAFS spectra of $(TMTSF)_2PF_6$ (a) and $(TMTTF)_2AsF_6$[12] (b). Energy values (in eV) are given with respect to the energy of the HOMO.

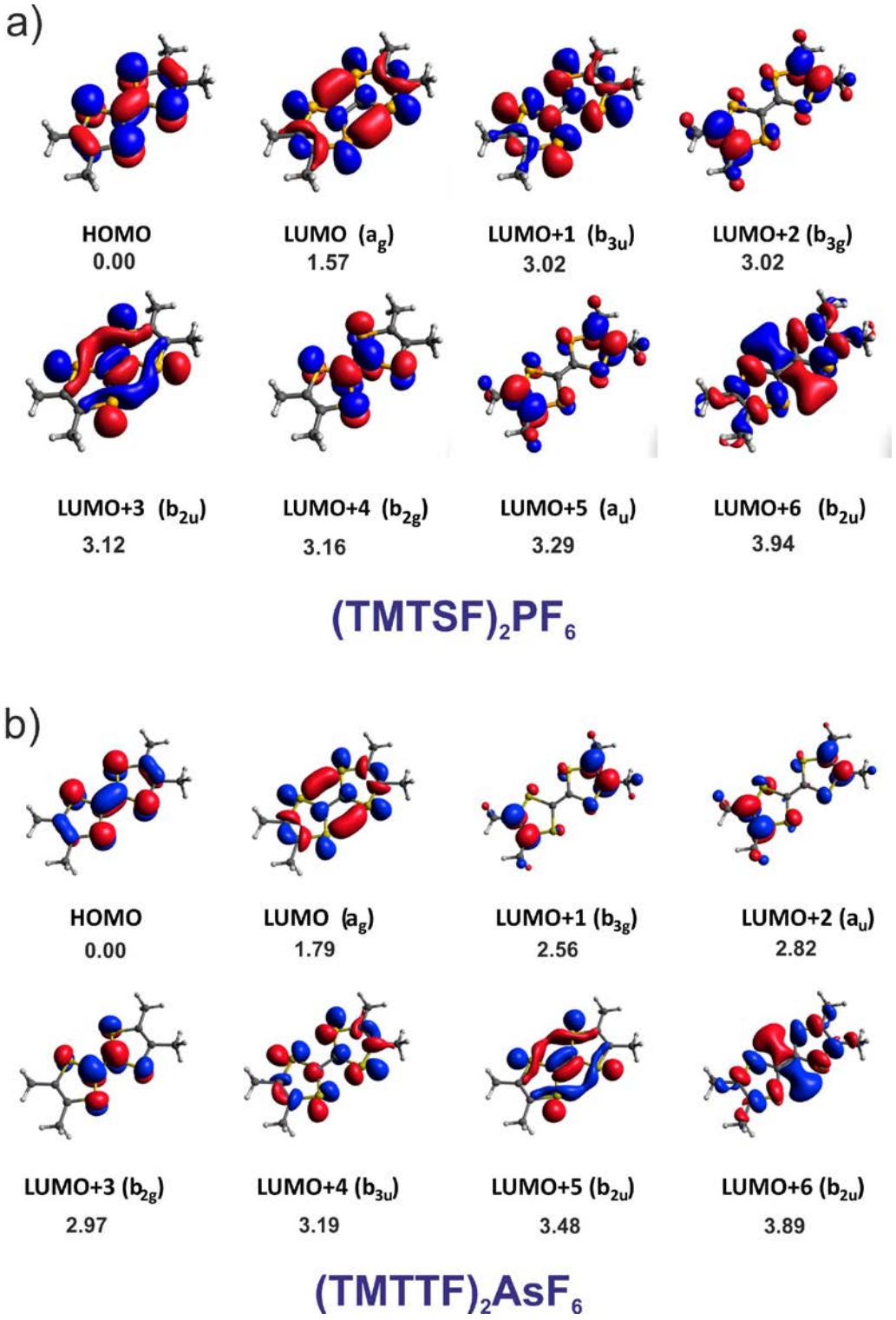

Figure S2. Comparison of the TMT(S/T)F molecular orbitals relevant for the analysis of the NEXAFS spectra of $(TMTSF)_2PF_6$ (a) and $(TMTTF)_2AsF_6$[12] (b). The geometry of TMTSF is based on the 4 K crystal structure of $(TMTSF)_2PF_6$ where the TMTSF donors where symmetrized so as to possess D_{2h} symmetry. Energy values (in eV) are given with respect to the energy of the HOMO.

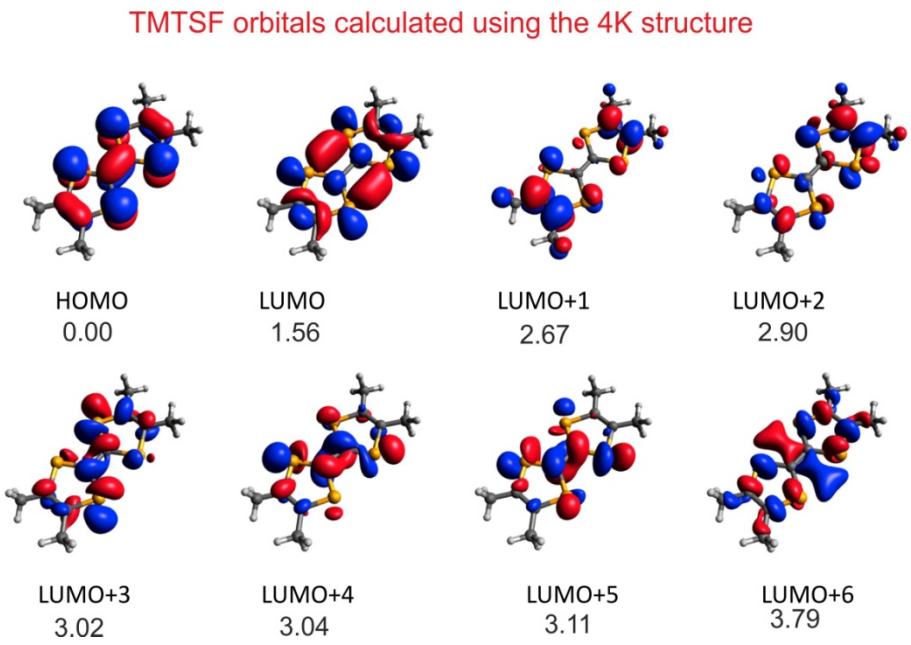

Figure S3. TMTSF molecular orbitals calculated using the 4K crystal structure[14] of $(TMTSF)_2PF_6$. Energy values (in eV) are given with respect to the energy of the HOMO.

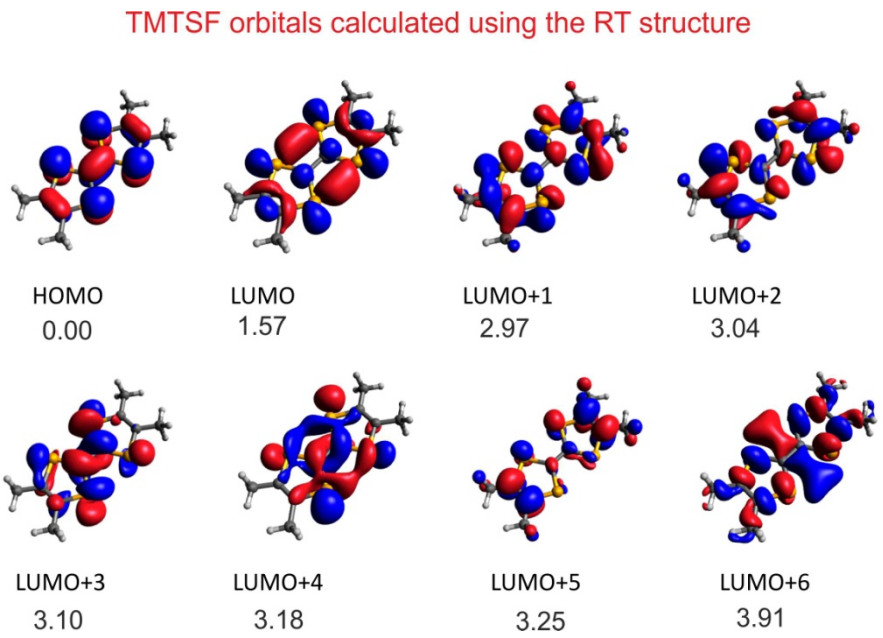

Figure S4. TMTSF molecular orbitals calculated using the room temperature crystal structure[21] of $(TMTSF)_2PF_6$. Energy values (in eV) are given with respect to the energy of the HOMO.

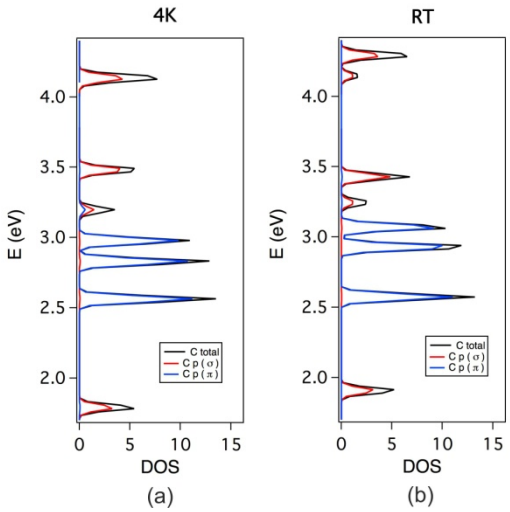

Figure S5. Projection of the σ (red) and π (blue) contributions of the 2p orbitals of C to the ”DOS” of discrete TMTTF levels calculated using the crystal structure of $(TMTTF)_2AsF_6$ at 4 K (a) and room temperature (b). Energies (in eV) are given with respect to the energy of the HOMO.