A Soft X-ray Study of K_3C_{60}: Bulk Electronic Structure

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The alkali metal fulleride salts of composition A_3C_{60} (where A is an alkali metal) have attracted wide interest due to their metallic and superconducting properties (see, *e.g.* Refs. 1-4). We present C 1s absorption (XAS) and resonant inelastic X-ray scattering (RIXS) spectra from a single phase crystalline thin film of K_3C_{60}.

The experiments were performed on the Surface End-station of beamline I511 at MAX-Lab in Lund, Sweden. The energy resolution was 0.2 eV in the X-ray spectrometer and 0.1 eV in the excitation channel (the monochromator).

By comparing the absorption spectra from the K_3C_{60} and pristine C_{60} samples (see Fig. 1) it is seen that the lowest absorption resonance (corresponding to the LUMO of C_{60}) is broadened, compared to C_{60}, with the edge shifted slightly to lower energy. The next unoccupied energy levels have been lowered even further in energy, and broadened. The quite large modifications in the absorption spectrum have been a source of discussion considering even the assignment of the peaks. We have recorded RIXS spectra resulting from excitations to intermediate states of different parities (see Fig. 2), and used the inherent symmetry selectivity of the RIXS event in an attempt to identify the origin of the absorption peaks in terms of the C_{60}-derived electronic structure. The conclusion we can draw from these data is that it is correct to interpret the main features in the K_3C_{60} XAS as being directly analogous to those of pristine C_{60}.

The lines in the emission spectra are narrower than the corresponding valence band UPS-lines from K_3C_{60} (although the lines are broader than for C_{60} RIXS). As X-ray detection techniques are sensitive to the bulk of the material, and the electron detection techniques (UPS, and XPS) to a rather shallow surface layer, this points to differences in the bulk and surface electronic structure of K_3C_{60}.

References

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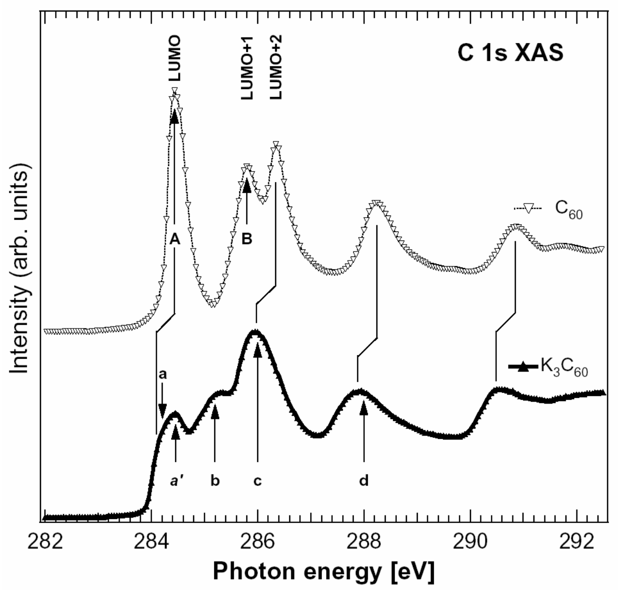

FIG. 1: X-ray absorption spectrum of K_3C_{60} at carbon K-edge (thick line), compared to the spectrum of C_{60} (thin line). Arrows indicate the excitation energies (*cf.* Fig. 2).

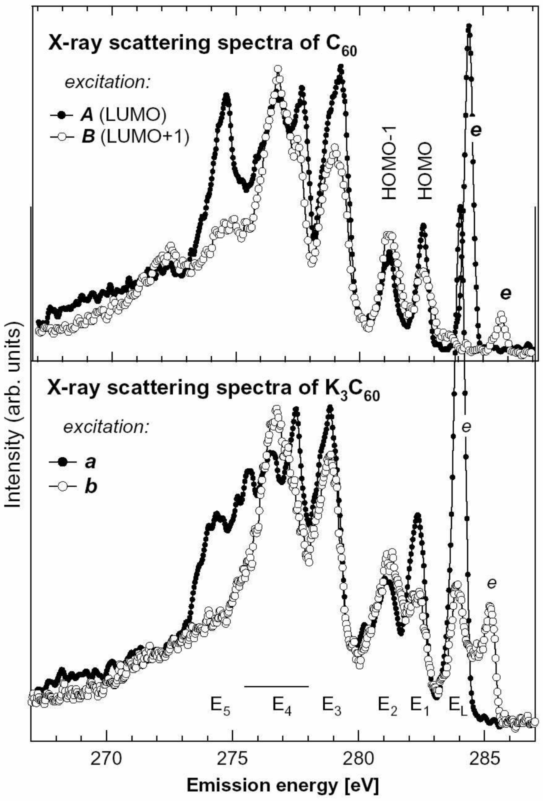

FIG. 2: Resonant inelastic scattering via the two lowest-energy absorption resonances. Excitation energies as marked in Fig.1 by ***a***, ***b*** (K_3C_{60}, lower panel), ***A*** and ***B*** (C_{60}, upper panel). The ***e*** in the spectra mark the elastic scattering peak at the incoming photon energy.