



ESRF

**Experiment title: Study of electronic and structural phase transition in Rb<sub>1</sub>C<sub>60</sub>**

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**Report:**

In solid C<sub>60</sub> and in most of its compounds, the intermolecular separation is mainly determined by van der Waals interactions and the center to center distance of C<sub>60</sub> molecules is typically 10Å. Recently some exceptions have been found in which C<sub>60</sub> molecules are linked by covalent bonds. M<sub>1</sub>C<sub>60</sub> compounds (M=K or Rb) have a polymeric form at room temperature with an orthorhombic crystal structure in which C<sub>60</sub> ions form chains. There is evidence of covalent bonds between C<sub>60</sub> molecules both from powder x-rays diffraction and <sup>13</sup>C NMR resonances. The intermolecular separation along the chain is unusually short (an interfullerene C-C distance of about 1.6Å,<sup>6</sup> instead of the usual 3.3Å) and supports the model of a quasi-one-dimensional electronic conductor. Electron-spin-resonance data support a metal-insulator transition of the polymeric Rb<sub>1</sub>C<sub>60</sub> at 50K, in contradiction with the expected metallic character due to the filling of the first empty energy-bands of C<sub>60</sub>. This phase transition is

said to be a consequence of the formation of spin- and charge-density waves that doubles the unit cell and opens a gap at the Fermi level. In contradiction, a recent model developed by S. Erwin to describe the electronic states in the low temperature phase of  $M_1C_{60}$  shows that the electronic properties of even this polymerized phase remain strongly 3-D, without a zero density of states at Fermi level. **Our first aim** is to test the waves functions of S. Erwin comparing the experimental compton profiles with the theoretical profiles. Theoretical profiles are obtained using the plane wave expansion of wave functions from an ab-initio self-consistent field calculation (SCF) of the energy band-structure. The linear combination of atomic orbitals (LCAO) method within the local-density-approximation has been employed for this calculation.

Recently, a not polymeric (fcc) $M_1C_{60}$  compounds (M=K or Rb) has been also synthesized. **Our second aim** is to compare the electron momentum distribution of the polymeric phase with its covalent inter balls bonds with the fcc not polymeric phase.

Experiments on polymeric and not polymeric  $M_1C_{60}$  have been performed at ESRF, using the scanning mode spectrometer of beam line ID15B. Synchrotron radiation have been monochromatized at 55.8 keV. The photons are back-scattered by a sample of  $M_1C_{60}$  powder under argon atmosphere and analysed by a Ge(440) curved analysing crystal.

The scattered photons spectrum is measured at the scattering angle of  $160^\circ$ . The resolution is determined from the full width at half maximum of the thermal diffuse scattering peak, which is 0.3 a.u., when expressed in terms of the electron momentum scale.

For comparison, the Compton profile of a powder of  $C_{60}$  has been measured, using exactly the same experimental conditions as for  $M_1C_{60}$ .

Difference of profiles obtained on the two solids is used in order to eliminate effects of systematic experimental errors.