



ESRF	Experiment title: Momentum density of $\text{Rb}_2\text{CsC}_{60}$	Experiment number: HC320
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Report:

The aim of this project was :

- to study the electronic **density** of $\text{CsRb}_2\text{C}_{60}$, by comparison with C_{60} measurement
- to evidence possible effect on the momentum density when the temperature is decreased below the T_c .

For these purposes, we have measured Compton profiles of the 2 powdered samples, with same experimental conditions.

The experiments have been performed with scattering angle settled at 161° and the synchrotrons radiation beam has been monochromatized at 58 keV. Each sample was put in a sealed capillary of 1mm diameter, in order to obtain the best resolution of the set-up and also because of the high reactivity of the intercalated C_{60} with air.

On both samples, measurements have been performed at 3 different temperatures : room temperature and above and below the T_c of $\text{CsRb}_2\text{C}_{60}$, to take care of all the temperature effects, in particular the effect of rotations of the C_{60} molecules on interball bonding, i.e. solid state effect on the distribution of valence electrons.

The data sets have been corrected for energy dependent effects such as photoelectric absorption in the sample, the analyser and the air (photon path between analyser and detector) by using a local correction program (P. Fajardo, T. Buslaps, ESRF). Due to the flatness of the core profile in momentum space, it is easy to subtract its contribution, evaluated using the QSCF method (collaboration with A. Issolah, Tizi-Ouzou), from the total measured DCP in order to get the valence DCP of interest alone.

Results :

Comparison between CsRb₂C₆₀ measurements above and below T_c: we have not found any evidence for a budge effect, as already reported on high T_c compounds ¹.

Comparison between C₆₀ and CsRb₂C₆₀: even if the sample shape and volume are the same for both compounds, the difference in the absorption cross sections due to the large Z elements in the intercalated compound leads to carefull corrections in both photoabsorption and multiple scattering effect. In addition, the core profile has to be calculated beyond the impulse approximation for Cs and Rb atoms². These calculations are in progress.

On the other hand, in order to learn more about distortion of the C₆₀ density due to the presence of alkali atoms, a new all electron calculation is presently in progress don by Steve Erwin (NRL, Washington). The Compton profile will be calculated from the band-structure results in collaboration with S. Rabbii (Dept. of electrical engineering, Philadelphia)

A large distortion is evidenced due to the large size of the Cs atom (the largest which can be introduced in the initial FCC structure of solid C₆₀).

1 – G.D. Priftis, D.L. Anastassopoulos, A.A. Vradis and R. Suryanarayanan, Physics C 223, 106 (1994).

2 – A. Issolah, B. Lévy, A. Beswick and G. Loupías, Phys. Rev. A38, 4509 (1988) ; A. Issolah, Y. Garreau, B. Lévy and G. Loupías, Phys. Rev. A38, 4509 (1988).