



Experiment title:

3D mapping of electronic density of C₆₀

Experiment number:

HC 83

Beamline:

BL2

Date of Experiment:

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Shifts:

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Report:

Compton profile measurements of a C₆₀ single crystal were carried out on the BL2 (ID11).

On the main arm of the κ diffractometer, we have setup a dispersive analysing device : photons scattered by the sample at an angle of 135° are energy analysed and focused by a Cauchois curved crystal on a sensitive detector. Compton profiles for 8 different directions of the scattering vector **K**, with respect of crystallographic directions, were measured at 2 different temperatures below and above the structural transition, i.e. at room and liquid nitrogen temperatures.

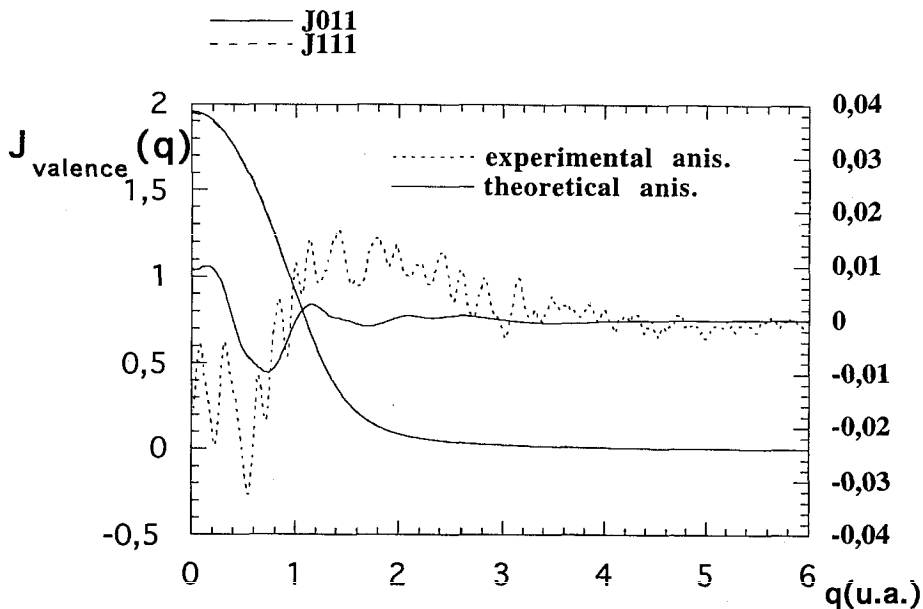
Energy of the beam delivered by the ID 11 monochromator was equal to 16.38keV.

After background subtraction, the data were corrected for sample, analyser and detector absorption. The core profile calculated, beyond the Impulse approximation and using the QSCF method¹, is removed, leading to valence profiles normalized to 4, number of electrons per carbon atom.

a) Preliminary results have been presented at the 1995 ESRF Users' Meeting : *Sample housing for high energy Compton measurements : application to C₆₀*, Ch. Benin, J. Frouin, M. Marangolo and G. Loupias.

b) Data analysis is now finished, and we got a paper accepted in Acts Physics Polonica : *Investigation of electronic density in C₆₀ by Compton scattering*, Ch. Benin, M. Marangolo, J. Moscovici, G. Loupias, S. Rabbii and S. Erwin.

The difference between the two C_{60} profiles measured at room and low temperatures is no larger than the statistical error bar for any value of q , indicating the weakness of interball bonds. The Figure below shows the tight anisotropies obtained by both theory (LDA calculations, collaboration with S. Rabii, Philadelphia and S. Erwin, NRL Washington DC) and experiment :



Even if the details of the experimental features are not well described by theory, we can notice that the orders of magnitude are similar, supporting the fact that solid effect is surprisingly weak in C_{60} .

The last step is to reconstruct the 3D map of the electronic density in momentum space. Because we have no way to experimentally discriminate the photons scattered more than one time, both elastically and inelastically, this parasitic Compton profile is simulated by the Monte-Carlo method (collaboration with J. Felsteiner, Israel).

This map is under construction, using the method of spherical harmonics.