



ESRF

Experiment title:

Momentum electron density in Rb₄C₆₀

Experiment

number:

HE165

Beamline:

BL 25
(ID15)

Date of experiment:

from: 27.03.97 to:31.03.97

Date of report:

28/8/97

Shifts:

14

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Received at ESRF:

2 SEP. 1997

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Report:

Experimental

Experiments on Rb₄C₆₀ 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 R₄C₆₀ 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°. 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 C₆₀ has been measured, using exactly the same experimental conditions as for Rb₄C₆₀.

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

Results and discussion.

We have calculated the difference profile $\text{Rb}_4\text{C}_{60} - \text{C}_{60}$ and electron core profile, calculated within the Impulse Approximation .

In fig.1 the $\text{Rb}_4\text{C}_{60} - \text{C}_{60}$ profile is compared to $\text{K}_4\text{C}_{60} - \text{C}_{60}$ profile collected at 20 keV at LURE, Orsay. We note the great similarity to $\text{K}_4\text{C}_{60} - \text{C}_{60}$ and the marked effect of distortion at the same momentum range 1 to 1.6 a. u..

The difference profile is due to rubidium insertion effects:

a- charge transfer of the 5s Rb electron to C_{60} , b- presence of the initially Rb electrons c- distortion of the C_{60} electron density due to Rb^+ ions d- the structural transition (C_{60} cfc. ----> Rb_4C_{60} bct)

The electronic modifications of C_{60} host can be due to points b, c and d.

The remarkable effect in the presented spectra is that the difference profile is negative in the momentum range 1 to 1.6 a. u.. Such a fact, which is impossible in a rigid-band approach, evidences the modifications of C_{60} electron density in the R_4C_{60} compound.

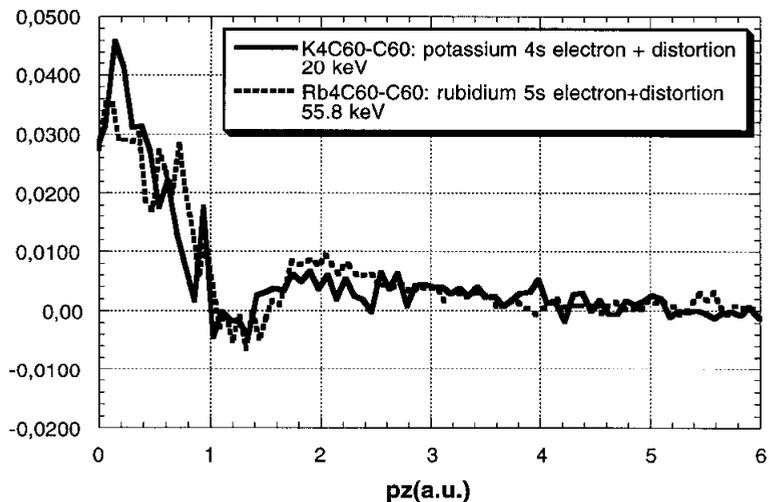


fig 1