

Rb₄C₆₀ Equation of States and Electronic Density Study by Compton Scattering

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In the family of compounds A_nC₆₀ (A=K, Rb and Cs; n=1,3,4 and 6), Rb₄C₆₀ exhibits an unusual behavior : it is a non-magnetic insulator at ambient pressure, whereas expected as a conductor, even a superconductor (cf. Rb₃C₆₀), by theory [1]. Furthermore Rb₄C₆₀ undergo an insulator to metal transition under pressure around 0.8 GPa, as observed by NMR study of Rb₄C₆₀ [2].

We have performed combined Compton scattering (ID15B) and diffraction experiments at ESRF (ID-30), at pressures below and above the insulator-metal transition. Our diffraction experiment exhibits, for the first time, an abrupt jump in compressibility between 0.5 GPa and 0.8 GPa. We attributed this jump to a structural phase transition preserving the initial tetragonal symmetry [3]. By *ab-initio* calculations we reproduced the experimental phase transition and studied the pressure dependence of internal coordinates. Going further, the comparison with *ab-initio* LDA calculations allowed us to quantitatively evaluate contributions due to contraction of the unit cell as well as an unexpected contraction of the C₆₀ molecule itself, evidenced by Compton measurements. In fact, this C₆₀ molecule contraction leads to a major effect on electronic density of Rb₄C₆₀ compound [5].

[1] Erwin S.C., *Buckminsterfullerenes*, ed. W. E. Billups M. A. Ciufolini, VCH, New York, 1993, 217. [2] Kerkoud R. *et al*, *J. Phys. Solids*, 1996, **57**, 143. [3] Sabouri-Dodaran A.A. *et al.*, *Phys. Rev.*, 2004, **B70**, 174114.

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