Mott transition to Superconductivity in Fulleride Cs₃C₆₀ compounds: an NMR study

Y. Ihara¹, H. Alloul¹, P. Wzietek¹, D. Pontiroli², M. Mazzani² and M. Riccò²

¹Physique des Solides, UMR 8502 CNRS, Université Paris-Sud 91405, Orsay (France) ² Dipartimento di Fisica, Università di Parma , 43100, Parma, (Italy)

The variation with *n* of the electronic properties of cubic A_nC_{60} compounds, where A is an alkali, cannot be explained by a simple progressive band filling of the C_{60} six-fold degenerate t_{1u} molecular level. This has been ascribed to the influence of electron correlations and Jahn-Teller Distortions (JTD) of the C_{60} ball, which energetically favour evenly charged C_{60} molecules[1].

This approach is supported by the detection by NMR of a small spin-gap in Na₂C₆₀ and K₄C₆₀ which is ascribed to a transition from a fundamental spin singlet state of C_{60}^{2+} or C_{60}^{4+} to an excited spin triplet state [2]. Similarly, a charge disproportionation in the low *T* quenched cubic phase of Cs C₆₀ [3], with a sizable fraction of the C₆₀ balls in a doubly charged C_{60}^{2+} singlet ground state also confirms that Hund's rule is disfavoured by the JTD in such compounds.

More recently it has been discovered that the expanded A15 fulleride Cs_3C_{60} displays a Mott transition to superconductivity (SC) driven by an applied pressure [4]. This system has a phase diagram where dome shaped superconductivity appears in the vicinity of a Mott insulating phase, a common situation encountered nowadays in correlated electron systems.

We report here an NMR and magnetisation study on Cs_3C_{60} in both its A15 and face centered cubic structures [5]. NMR allowed us to evidence that both exhibit a similar first-order Mott transition to a SC which occur at distinct critical pressures p_c and temperatures T_c . Though the ground state magnetism of the Mott phases differs, their high T paramagnetic and SC properties are found similar, and the phase diagrams versus unit volume per C_{60} are superimposed. Thus, as expected for a strongly correlated system, the inter-ball distance is the relevant parameter driving the electronic behavior and quantum transitions of these systems. Our detailed NMR results allow us to demonstrate that, although the high temperature superconductivity found so far in the A_3C_{60} compounds admittedly results from an electronphonon mechanism, the incidence of electron correlations has an importance on the electronic properties, as had been anticipated from DMFT calculations [6].

[1] M. Capone, M. Fabrizio, P. Giannozzi and E. Tosatti, Phys. Rev. B 62,7619 (2000).

[2] V. Brouet, H. Alloul, T.N Le, S. Garaj and L. Forro, Phys. Rev. Lett. 86, 4680 (2001);

V. Brouet, H. Alloul et al, Phys. Rev. B 66, 155122(2002)

[3] V. Brouet, H. Alloul et al Phys. Rev. Lett. 82, 2131 (1999); Phys. Rev. B 66, 155123 (2002).

[4] Y. Takabayashi et al Science 323, 1585 (2009).

[5] Y. Ihara , H. Alloul, P. Wzietek, D. Pontiroli, M. Mazzani and M. Riccò, Phys. Rev. Lett. 104, 256402 (2010)

[6] M. Cappone, M. Fabrizio, C. Castellani and E. Tosatti, Rev. Modern Physics, 81, 943 (2009).