

Dynamic Jahn-Teller effect in the expanded fullerenes Cs₃C₆₀

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Katalin Kamarás, Gyöngyi Klupp and Péter Matus

Wigner Research Centre for Physics, Hungarian Academy of Sciences, P.O. Box 49, H 1525 Budapest, Hungary

Alexey I. Ganin, Alec McLennan and Matthew J. Rosseinsky

Department of Chemistry, University of Liverpool,

Liverpool L69 7ZD, UK

Yasuhiro Takabayashi, Martin T. McDonald and Kosmas Prassides

Department of Chemistry, Durham University, Durham DH1 3LE, UK

The mechanism of superconductivity in fullerene superconductors (A₃C₆₀, where A is an alkali metal) is being reconsidered from BCS towards another model, similar to cuprates: a phase diagram where an antiferromagnetic Mott insulator is changing into a strongly correlated superconductor. Typical model systems are the so-called expanded fullerenes where Mott localization happens because the distance between fullerene ions exceeds a critical value. Two cubic Cs₃C₆₀ polymorphs (A15 and fcc)¹ are the newest members of this class, with transition temperatures around 35 K at a few kilobars. The normal state of these compounds is low-spin ($S=1/2$) indicating a spin-pairing mechanism for which the Jahn-Teller-effect was proposed. We will present evidence by infrared spectroscopy for a dynamic Jahn-Teller effect in the insulating state of the expanded fullerene Cs₃C₆₀ in the temperature range 28-480 K at ambient pressure. Jahn-Teller distortions of the size ~ 0.04 Angstroms can be easily detected by vibrational spectroscopy, due to the symmetry lowering of the fullerene balls. The temperature dependence of the spectra can be explained by a molecular effect, the gradual transformation of two temperature-dependent solid-state conformers to a single one, typical and unique for Jahn-Teller systems in solids.² These results unequivocally establish the relevance of the dynamic Jahn-Teller effect overcoming Hund's rule local exchange interactions, leading to a magnetic Mott-Jahn-Teller insulator.³

¹ Y. Takabayashi, A.Y. Ganin, P. Jeglic, D. Arcon, T. Takano, Y. Iwasa, Y. Ohishi, M. Takata, N. Takeshita, K. Prassides, M.J. Rosseinsky: *Science* 323, 1585 (2009)

² I.B. Bersuker: "The Jahn-Teller Effect", Cambridge University Press, 2006

³ M. Capone, M. Fabrizio, C. Castellani, E. Tosatti: *Rev. Mod. Phys.* 81, 943 (2009)

Primary author: KAMARAS, Katalin (Wigner Research Centre for Physics, Hungarian Academy of Sciences)

Presenter: KAMARAS, Katalin (Wigner Research Centre for Physics, Hungarian Academy of Sciences)

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