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Dynamic Jahn-Teller effect in the expanded fullerides Cs3C60

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The mechanism of superconductivity in fulleride 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 fullerides where Mott localization happens because the distance between fulleride 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 fulleride 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

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