Abstract Submitted
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Theory of Jahn Teller signatures in the infrared absorption of C_{60}^{3-} [1] S. SHAHAB NAGHAVI, SISSA, Trieste, Italy, MICHELE FABRIZIO, ERIO TOSATTI, SISSA, CNR-IOM Democritos and ICTP, Trieste, Italy, CONDENSED MATTER PHYSICS TEAM — Among the molecular superconductors, trivalent fullerides such as Cs_3C_{60}, with three folded degenerate HOMO and a fully ordered pressure induced superconductor-insulator are still intriguing. The orbital degeneracy of the fulleride ion C_{60}^{-3} implies that besides a Jahn-Teller distorted state with S=1/2 and high-lying spin (S=3/2) excitation known from NMR, another undetected orbital excitation with S=1/2 should exist. Building upon accurate density hybrid functional theory calculations where properties such as the infrared (IR) spectrum and its Jahn-Teller features are well described, we extracted the AB-INITIO orbital and spin spectrum of a C_{60}^{-3} ion in different spin and orbital states including a new low lying L=2 S=1/2 excitation. Despite a Jahn-Teller distortion so small to be observable in its IR spectrum, this state is found to gain a large zero-point energy, placing it just above the L=1, S=1/2 ion ground state, and way below the L=0, S=3/2 high lying excitation. We can now elegantly explain the surprising early thermal disappearance of the low-temperature Jahn-Teller IR spectral features and splitting without a concurrent rise of spin susceptibility that would instead be required by population of the high spin S=3/2 excitation.

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