

Jahn-Teller distortions and excitation energies in C_{60} ions

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Abstract

Based on previously computed parameters for the electron-phonon couplings and the Coulomb exchange, we compute and classify the static Jahn-Teller distortions, i.e. the minima of the lowest adiabatic potential energy surface, of C_{60} ions for all charge and spin states. We compute the intra-band electronic excitation energies in the different optimal geometries in the sudden approximation, and find a spread of the electronic states of roughly 1 eV. We also obtain the leading vibronic quantum corrections to the ground-state energy, equal to zero-point energy lowering due to the softening of the phonons at the adiabatic Jahn-Teller minima: these non-adiabatic corrections are so large that for some cases states of different spin symmetry turn lower than the high-spin adiabatic ground state.