First principles study of the vibronic coupling in positively charged C_{60}^{+}

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Abstract

Orbital vibronic coupling parameters for C_{60}^{+} were derived by using frozen-phonon approach via density functional theory calculations with hybrid B3LYP and CAM-B3LYP functional. Based on these derived vibronic coupling parameters, the static Jahn-Teller effect of C_{60}^{+} were analyzed. At the global minima of adiabatic potential energy surface (APES), the Jahn-Teller deformation shows a D_{5d} structure with stabilization energies of 110 and 129 meV with B3LYP and CAM-B3LYP respectively. These stabilization energies are two times larger than that in C_{60}^{-}, suggesting the crucial role of the dynamical Jahn-Teller effect in C_{60}^{+}. Present coupling parameters enable us to assess the actual situation of dynamical Jahn-Teller effect in C_{60}^{+} and also that of excited C_{60} in combination with the established coupling parameters for C_{60}^{-}.

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