

Giant quantum anharmonic effects in Cyclo $[4n+ 2]$ carbon

Davide Romanin

Université Paris-Saclay, France

Cyclo $[4n+2]$ carbons are sp-bonded carbon rings in which Hückel rule predicts a fully symmetric structure that is, however, in competition with the second order Jahn–Teller (Peierls) distortion. This picture, however, neglects the crucial role played by nuclear quantum effects. In a recent work [Carbon Trends 9, 100207 (2022)] we investigated the magnitude of nuclear quantum effects on the stability, vibrational and optical properties of cyclo $[4n+2]$ carbons ($n=1,2,3,4$) in vacuum. We showed that quantum structural minimization reduces the energy separation between the different isomers and determines that the most stable one as the cumulenic phase, setting the transition from the polyenyic to the cumulenic form at $n=3$ (at odd with the classical structural optimization setting the transition at $n=2$). Moreover, the optical absorbance is completely reshaped by quantum anharmonic vibrations with redshifts ranging from 0.4 to 1.0 eV in the first excitonic absorption with respect to the static ionic picture. Our work outlines the crucial role of nuclear quantum effects in the understanding of carbon molecular systems.