On the electronic and vibrational contributions to the static electric properties of molecular complexes under spatial confinement

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The studies of spatially confined atomic and molecular systems have become a topic of great significance during the past few decades and nowadays increasingly attract attention of researchers from various fields of science. Among many physical and chemical properties, strongly affected by the confining environments, the linear and nonlinear electric properties are of pivotal importance due to the rapid development of molecular nonlinear optics [1-4]. In particular, it has been shown that the spatial confinement diminishes the electronic and vibrational contributions to the hyper(polarizabilities) of model linear molecules (HCN, HCCH, CO_2) [5]. However, the electronic contributions are affected to the larger extent than their vibrational counterparts. Moreover, it has been found that the spatial restriction more significantly influences the harmonic vibrational terms than the anharmonic ones. To further examine this issue we analyze, for the first time, the influence of spatial confinement on the electronic and vibrational contributions to the hyper(polarizabilities) of hydrogen-bonded molecular complexes (HCN···HCN and HCN···HNC), which exhibit moderate anharmonic contributions to vibrational electric properties. The external spatial confinement is assumed in the form of cylindrically symmetric harmonic oscillator potential, which mimics a nanotube-like confining environment.

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