PARTITIONING OF INTERACTION-INDUCED NONLINEAR

OPTICAL PROPERTIES OF MOLECULAR COMPLEXES

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Elucidation of the effects of different fundamental intermolecular interactions on the nonlinear optical properties is pivotal for proposing efficient strategies to obtain new materials with tailored properties in complex environments. The aim of the talk is to present the scheme of the decomposition of the electronic and nuclear-relaxation interaction-induced (excess) hyperpolarizabilities of molecular complexes. The excess property is defined as the difference between a property of the complex and the net properties of the noninteracting subsystems. The decomposition scheme was applied to ten hydrogen-bonded molecular complexes and their electronic and vibrational excess (hyper)polarizabilities were partitioned into different interaction energy contributions (electrostatic, exchange, induction and dispersion). It will be demonstrated that the physical origin of the electronic and vibrational excess properties is completely different. In the case of vibrational contributions, the decomposition pattern is very similar for the polarizability and first and second hyperpolarizabilities. The exchange contributions to excess vibrational properties are the largest and they have different sign than the electrostatic, induction and dispersion terms. On the other hand, no general patterns can be established for the electronic excess properties.

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