Real Space partitioning of the first hyperpolarizability through Atoms in Molecules

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The first static hyperpolarizability is partitioned within the framework of the Quantum Theory of Atoms in Molecules (QTAIM) through two partitioning schemes. The first one uses a two-state model, while the second one is based on finite differences approach. We have fragmented the principal hyperpolarizability component into contributions, arising from atoms polarizations and charge transfer. The purposed schemes were used to decompose the hyperpolarizability of 14 Donnor–π–Acceptor (D-π–A) systems. The results show the dominant role of the charge transfer component. Besides, a relevant correlation is observed between the donor-acceptor strength and the activation of the π-moiety, which increases the principal hyperpolarizability component contribution. In addition, acceptor moieties of different compounds exhibit substantial transferable hyperpolarizability values. These observations shed insight on the complex relationship between functional group features and the molecular nonlinear optical properties, a relevant information for the design of molecules for optical applications.

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Since 2023 is the Head of the Chemistry Department at the Universidad de Guanajuato. Scientific contributions: Chemical Bond models thorough Quantum Chemical Topology; Computer Aid Material Designing for environmental remediation, for example in the study of CO_2 adsorption and catalytic reduction; Drug designing assisted by computer, using grammar evolutive algorithms for the designing drugs against SARS-CoV-2 and cancer; García-Revilla also worked in the characterization of linear and no-linear optical properties of organic molecules. Author of more than 40 JCR published articles, 800 citations. Awards: National Researcher SNII-II.