SEMINAIRE ISMO

Denis Sabirov

Laboratory of Mathematical Chemistry, Institute of Petrochemistry and Catalysis of Russian Academy of Sciences, Ufa, Russia

Dipole polarizability of fullerene derivatives and its use in physical chemistry and materials science

Fullerenes is the only molecular form of carbon, therefore, their chemical and physical behavior are deducible from molecular properties. The studies of our group is focused on the DFT calculations of the dipole polarizability of fullerene compounds and elucidating their relations with chemical structure and physicochemical processes.

This report (a) generalizes known experimental and theoretical data on α values of fullerenes and their derivatives and (b) shows their usability for chemical and materials science issues.

According to different theoretical methodologies (semiempirical methods, DFT, perturbation theory, coupled clusters theory etc.) and experimental techniques (ellipsometry, electron energy-loss spectroscopy, molecular beam deflection, and near-field interferometry), polarizabilities of fullerenes and their derivatives are very high (e.g., ~80 and ~100 $Å^3$ for C_{60} and C_{70}). The measured α values increase from isolated molecules to fullerene clusters and solid state (fullerite) in contrast to typical organic molecules. We discuss the dipole polarizabilities of the main classes of fullerene compounds (fullerenes and their ions, exohedral one-cage and multi-cage derivatives, endohedral complexes); the size-dependences of fullerene static and dynamic polarizabilities; effects of mechanical deformations and charging of the fullerene core.

The numerical estimates of α has descriptive and predictive potential for fullerene chemistry and materials science. We discuss the works on fullerenes whereby the role of dipole polarizability is crucial for :

(a) fullerene reactivity (including theoretical astrochemistry of C_{60});

(b) anion–π catalysis with fullerenes;

(c) organic photovoltaics (fullerene-adduct molecular switches and fullerene-adduct-based organic solar cells);

(d) dielectric screening the molecules inside the fullerene cages;

(e) chromatographic behavior of fullerene compounds;

(f) ordering of the $C_{60/70}$ nanostructures.

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Université Paris-Sud - 91405 ORSAY Cedex