

Structure of Halofullerenes Using Experimental and Theoretical Approaches

Sergey Troyanov^a, Natalia Shustova^a, Alex Popov^a, Ilya Ioffe^a, Erhard Kemnitz^b, ^a*Department of Chemistry, Moscow State University, Russia.* ^b*Institute of Chemistry, Humboldt University Berlin, Germany.*
E-mail: troyanov@thermo.chem.msu.ru

Halogenated fullerenes are compounds of profound fundamental and practical importance. Investigation of these fullerene derivatives is complicated by the formation of compound and/or isomer mixtures. Theoretical calculations at the DFT level of theory allow a reliable prediction of relative energy, geometry, and spectroscopic properties of halofullerene molecules containing more than 100 atoms.

In the absence of experimental crystallographic data, a comparison of experimental and calculated IR spectra was indicative for a choice of molecular structures for C₇₀Br₁₀ or C₆₀Cl₂₄, which have been later confirmed by X-ray crystallography (partially with the use of synchrotron radiation). For the mixture of two compounds with known X-ray structures, C₆₀Cl₂₈ and C₆₀Cl₃₀, the experimental IR spectra were interpreted by comparison with the calculated ones using subtle differences for compounds possessing very similar structures. For the mixture of isomeric molecules in the same crystal (examples: C₇₀Cl₂₈ [1], C₆₀F₄₈, and C₇₈Br₁₈ [2]), theoretically predicted structures were helpful in the search for suitable disordering model in LS refinements.

Thus, simultaneous use of X-ray crystallography, IR spectroscopy, and theoretical calculations resulted in obtaining highly valuable structural information for many halogenated fullerenes.

[1] Troyanov S.I., Shustova N.B., Ioffe I.N., Turnbull A.P., Kemnitz E., *Chem. Commun.*, 2005, 72. [2] Troyanov S., Kemnitz E., *Eur. J. Org. Chem.* 2003, 3916.

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