

## Electronic and geometric structure of a number of fullerene isomers $C_{90}$ and structure of their chlorine and perfluoroalkyl polyadducts

© Regina A. Tuktamysheva,<sup>1</sup> Ayrat R. Khamatgalimov,<sup>2</sup> and Valery I. Kovalenko<sup>1,2\*</sup>

<sup>1</sup>Department of Engineering Ecology. Kazan National Research Technological University. K. Marx St., 68. Kazan, 420015. Tatarstan Republic. Russia. Phone: +7 (843) 238-56-94. E-mail: koval@iopc.ru

<sup>2</sup>Physico-Chemical Research Division. A.E. Arbuzov Institute of Organic and Physical Chemistry.

Akad. Arbuzov St., 8. Kazan, 420088. Tatarstan Republic. Russia.

Phone: +7 (843) 273-93-65. E-mail: koval@iopc.ru

\*Supervising author; <sup>†</sup>Corresponding author

**Keywords:** fullerene  $C_{90}$ , IPR isomers, electronic structure, pyramidal, radical addition, chlorine and perfluoroalkyl derivatives, method of density functional theory.

### Abstract

For the first time we have shown the distribution of electron density and presented it as a traditional valence scheme, i.e. as simple, double and delocalized PI-bonds in molecules of IPR isomers of fullerene  $C_{90}$ :  $46(C_{2v})$ ,  $35(C_s)$ ,  $30(C_1)$ ,  $28(C_2)$ ,  $32(C_1)$ ,  $34(C_s)$ , which are the predecessors of polyadducts  $46(C_s)Cl_{32}$ ,  $35(C_s)Cl_{24}$ ,  $35(C_s)Cl_{28}$ ,  $30(C_1)Cl_{22}$ ,  $28(C_2)Cl_{26}$ ,  $32(C_1)Cl_{24}$ ,  $34(C_s)Cl_{32}$  and  $32(C_1)(CF_3)_{12}$ ,  $35(C_1)(CF_3)_{14}$ ,  $30(C_1)(CF_3)_{18}$ . The hexagons with delocalized  $\pi$ -bonds have been shown to be the most likely positions for addition of Cl and  $CF_3$  radicals that reflects the important role the fullerene molecular electronic structure plays in the radical addition reaction.