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Polymeric forms of radical-fullerenes C_{74} (D_{3h}) and C_{76} (T_d)

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Abstract

Theoretical rationalization of the experimentally observed of polymer forms formation of C_{74} (D_{3h}) and C_{76} (T_d) fullerenes was performed. It is decisively showed that radical nature of these fullerenes is the driving force for the formation of linear and cyclic oligomers of biradical C_{74} (D_{3h}) and tetradadical C_{76} (T_d) during the electroarc synthesis of fullerenes. A regularity in the distribution of the spin densities in linear oligomeric forms of the C_{74} (D_{3h}) fullerene is revealed: radical substructures on the chain ends remain radical, while the central parts have closed electron shells. Open-shell triplet configurations of dimer molecules remains more favorable including trimers, tetramers and pentamers of C_{74} (D_{3h}) having a chain structure. When transitioning from dimers of fullerene C_{74} (D_{3h}) to trimers, and further to tetramers and pentamers having a chain structure, a significant increases in energy gain is observed. The analysis of the published experimental data demonstrates the reconcilable picture of this IPR C_{74} (D_{3h}) radical fullerene "life". It is noted that interfullerene carbon bonds in oligomers are rather weak. This makes it easy to switch from polymer forms to individual molecules of radical C_{74} (D_{3h}) and C_{76} (T_d).

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