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## «SCALY» MAGNETISM OF CARPET-LIKE POLYMERS OF C<sub>60</sub>

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Since its discovery, high-temperature magnetism of carbon crystals, formed by polymerized layers of covalently bound C<sub>60</sub> molecules, still has been an intriguing phenomenon of obscure origin. The paper is devoted to disclosing the problem by quantum-chemical calculations of large clusters of both hexagonally and tetragonally packed carpet-like C<sub>60</sub> layers. The calculations have been performed in the broken symmetry SSP HF approximation [1] by using AM1 semi empirical technique of the NANOPACK parallel codes [2]. Exchange integrals J are considered as the main characteristics of magnetic phenomena. They are determined as

$$J = \frac{E_{S=0}^{UHF} - E_{S_{\max}}^{UHF}}{S_{\max}^2}, \quad \text{where } E_{S=0}^{UHF} \quad \text{and} \quad E_{S_{\max}}^{UHF}$$

are the cluster energies in the broken symmetry singlet state as well as in the state with the highest multiplicity  $2S_{\max}+1$  related to spin  $S_{\max}=n/2$ . The number of non-paired odd electrons n for a cluster with k polymerized C<sub>60</sub> molecules fills in the region of  $60k \div 52k$  and  $60k \div 48k$  for tetragonal and hexagonal structures, respectively.

Clusters considered in the paper cover k varying from 2 to 10. As shown, exchange integrals J<sub>mol</sub> related to one C<sub>60</sub> molecule slightly decreases with respect to a free molecule while k is growing but still remains negative and too large by value to provide magnetic behavior. Therefore, the molecules themselves can not provide magnetism of ideal crystals consisted of polymerized molecules. However, the exchange integral of a cluster of k C<sub>60</sub> molecules as a whole is determined as  $|J_{cl}| \sim J_{mol}/k$  [1] so that at big k it may approach value to be enough for magnetic behavior observation. This conclusion is well consistent with a recent experimental finding of a direct connection between magnetic behavior of polymerized carbon crystals and well observed domain structure of the latter [3].

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### Литература

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