Physico-Chemical nanomaterials science

Peculiarities of the antioxidant action of exomodified fullerenes C_{60} at the oxidation of organic compounds

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During for the last 10 years, we have studied the antioxidant properties of a large group of modified fullerenes based on C_{60} [1, 2]. Directed synthesis of potential antioxidants (AO) carried out at the Institute of Chemical Physics (c. Chernogolovka). This paper presents the study results of antioxidant properties of fullerenes exomodified depending on the degree of functionalization, location and nature of functional groups in the carbon skeleton (Table.): $C_{60}Cl_6$, $C_{60}Cl_{28}$, $C_{60}Fl_{48}$,

Full 4. Full 5. Full 6.
$$F_{-20} = \frac{F_{-20}}{C_{60}} + \frac{F_{-20}}{NH - CH_3} + \frac{F_{-20}}{C_{60}} + \frac{F_{-20}}{NH - CH_3} + \frac{F_{-20}}{C_{-16}} + \frac{F_{-20}}{NH - CH_3} + \frac{F_{-20}}{NH$$

Testing antioxidant polysubstituted derivatives of fullerene C_{60} model was conducted in conditions of initiated oxidation of benzyl alcohol at 50 °C and 1 atm. The initiator of free radicals is 2,2'-azo-bis-izobutyronitryl.

Table The rate constants of the chain termination of oxidation benzyl alcohol by fullerenes (50 °C)

Formula	C ₆₀	$C_{60}Cl_6$	$C_{60}Cl_{28}$	$C_{60}F_{48}$	Full 1	Full 2	Full 3	Full 4	Full 5	Full 6	Full 7
k_{ROO} , 10^3 , $1/(\text{mol} \cdot \text{s})$	0,143	0,446	0,547	0,13	21,5	11,7	15,6	0,61	2,78	1,0	6,35
$k_{\rm R}$, 10^7 , $1/(\text{mol} \cdot \text{s})$	1,3	1,5	2,37	8,9	-	1,5	8,24	0,114	-	-	-
f	2	2	2	2	2	2	2	> <u>25</u>	<u>> 16</u>	<u>> 21</u>	2

Conclusions

- 1. Exohalogenation of C_{60} fullerene surface leads to a selective oxidation of the cliff by alkyl radicals ($C_{60} \rightarrow C_{60}Cl_{28} \rightarrow C_{60}Cl_{28} \rightarrow C_{60}F_{48}$).
 - 2. Fluoridation frame C_{60} retains its active interaction with alkyl radicals ($C_{60}F_{48} \leftrightarrow \text{Full 2}$).
- 3. Modification nitrogen-containing heterocyclic substituents groups leads to repeated breakage radicals on substituents (gross stoichiometric *f*> 16 at 4 Full, Full 5, Full 6).
- 4. By increasing the branching of substituents (more than 5) exomodified fullerenes interact only with peroxy radicals (Full 1, Full 5, Full 6, Full 7).
- 5. When modifying fullerenes polyfluorinated substituents are growing activity of its interaction with peroxy radicals (Full 2).

We first determined that oxidation chains fullerenes held simultaneously with both peroxides and alkyl radicals. For the first time were estimated rate constants of oxidation chains breaking of organic compounds exomodified fullerenes. The realization of catalytic oxidation chains of benzyl alcohol exomodified nitrogen-containing fullerenes.

The authors express gratitude P.A. Troshin for the sample exomodified fullerene C₆₀.

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