Bromination of [70]fullerene

N.I. Denisenko, A.A. Popov, I.V. Kouvitchko, O.V. Boltalina
Chemistry Department, Moscow State University, 119899 Moscow, Russia

Bromofullerenes $C_{60}Br_6$ and $C_{60}Br_8$ have been synthesized by bromination of the C_{60} solution in carbon tetrachloride and carbon disulfide, respectively [1]. Direct bromination of [60]fullerene yields $C_{60}Br_{24}$ [2,3]. X-ray single crystal structures of the bromofullerenes were determined [2]. Birkett et al. noted that bromination degree of [70]fullerene is close to $C_{60}Br_{24}$ [1].

Previously, we found that $C_{60}Br_8*2Br_2$ was formed at the first stage of the direct bromination of C_{60} Precipitation of the poorly soluble in Br_2 $C_{60}Br_8*Br_2$ hampered further bromination [4]. In order to obtain bromo[70]fullerenes direct bromination at RT as a function of time of the reaction was investigated. We varied reaction time from 5 minutes to 1 month. Compositions of the obtained samples were determined with the use of thermal gravimetry (TG) and differential scanning calorimetry (DSC). Decomposition of all samples occurred in two stages (detected by both TG and DSC). For example, two endothermic effects were observed at 75^0C and 133^0C for the sample obtained by direct bromination during 5 minutes (x(Br)=13 according to TG data); whereas the sample synthesized after 1 month, contained up to 17 Br atoms per fullerene molecule. The IR spectra of the samples (with different time of bromination) were identical.

Direct bromination under UV-irradiation yielded the products with composition about 10 bromine atoms per [70]fullerene molecule, and the IR spectra were similar to the ones mentioned above.

Bromination of the saturated solutions of [70]fullerene in 1,2-dichlorobenzene led to the formation of the dark orange precipitates. Decomposition of all the samples occurred in one stage (as detected by TG), and their composition was determined as $C_{70}Br_{10}$. The IR spectra of the samples (obtained by using different bromine concentrations) were identical to those synthesized in the direct bromination. The conjectured molecular structures of the synthesized bromo[70]fullerenes are proposed on the basis of the experimental results and with the support of the theoretical calculations.

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