Trifluoromethylated [60]Fullerenes. Synthesis, Spectroscopic Characterization and Properties.

Alexey A. Goryunkov, Vitaliy Yu. Markov, Alexei V. Streletskii, Lev N. Sidorov, Olga V. Boltalina

Department of Chemistry, Moscow State University, Leninskie Gory 1-3, 119992 Moscow, Russia

Donald Dick and Steven H. Strauss

Chemistry Department, Colorado State University, 80523 Fort Collins, CO, USA

Trifluoromethylated derivatives of fullerenes have not been studied as intensely as their fluorine counterparts.¹⁻³ Only two CF₃ derivatives were structurally characterized - $C_{60}F_{17}CF_3^4$ and $C_{60}(CF_3)_2^5$. However. trifluoromethylated fullerenes showed considerable stability towards hydrolysis and relatively high thermal stability, which makes them even more attractive than fluorofullerenes from the practical standpoint.

This work presents our recent developments in synthesis, the spectroscopic characterization and some properties of trifluoromethylated [60]fullerenes. Reaction between AgCF₃COO (AgTFA) and [60]fullerene performed under dynamic vacuum conditions and in the closed system was applied for preparation of the samples with varying number of CF₃ groups. The effect of the reagent ratio, reaction temperature and systematically was investigated, time revealing that distribution of $C_{60}(CF_3)_n$ products is mainly regulated by the ratio between C₆₀ and AgTFA. The highest addition level was reached - up to 24 CF_3 groups were detected by mass spectrometry in some samples. Methods of purification and isolation of the specific compounds will be discussed.

Three mass spectrometric techniques were applied - EI, ESI and MALDI - all showing different degree of fragmentation, with prevailing CF_3 loss. Prominent differences in the relative distribution of odd- and even-numbered ions were noted for different ionization methods and discussed. The molecular origin of the even-numbered peaks in the EI MS was proven with the use of ionization efficiency curves, differences in appearance energy between molecular and fragment ions comprised 3-4 eV.

References

- Wasserman, E.; Fagan, P.J.; Krisic, P.J.; Mcwen, C.N.; Lazar, J.; Parker, D.H.; Herron, N. *Science* 262, 404-407. 1993.
- 2. Fritz, H.P.; Hiemeyer, R. *Carbon* **33**, 1601-1609. 1995.
- Uzkikh, I.S.; Dorozhkin, E.I.; Boltalina, O.V.; Boltalin, A.I. *Doklady Chemistry* 379, 204-207. 2001.
- Boltalina, O.V.; Hitchcock, P.B.; Troshin, P.A.; Street, J.M.; Taylor, R. J. Chem. Soc., Perkin Trans. 2, 2410-2414. 2000.
- Avent, A.G.; Boltalina, O.V.; Goryunkov, A.; Darwish, A.D.; Markov, V.Yu.; Taylor, R. *Fullerenes*, *Nanotubes and Carbon Nanostructures* 10, 235–241. 2002.