# Synthesis and characterization of the novel isomer 1,4,10,19,25,41,60,69-$C_{70}(CF_3)_8$

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A large number of different individual structurally-characterized $C_{60}/_{70}(CF_3)_n$ compounds with $n$=2–18 is known. Under the typical conditions for trifluoromethylation, both with $CF_3I$ [1] and silver trifluoroacetate [2], the major product is $C_s$-symmetrical $C_{70}(CF_3)_8$. Additionally isolated and characterized were two more isomers of $C_{70}(CF_3)_8$ molecule with $C_2$-symmetry [1,3]. Here we report the synthesis and characterization of the novel asymmetrical 1,4,10,19,25,41,60,69-$C_{70}(CF_3)_8$ isomer.

For the preparation of $C_1$- $C_{70}(CF_3)_8$ the typical two-step method was used [1]. The reaction of $C_{70}$ and $CF_3I$ in a glass ampoule at 420 °C gave a mixture of $C_{70}(CF_3)_n$ compounds, $n$=10–18, as evidenced by MALDI mass spectra. Further reaction of this mixture with $C_{70}$ at 440 °C yielded lower trifluoromethylated fullerenes (n=2–10) *via* comproportionation. Isolation of novel isomer of $C_{70}(CF_3)_8$ was carried out by means of two-step HPLC separation.

On the basis of the $^{19}F$ NMR data and the quantum chemical calculations at the DFT level the addition pattern for the experimentally obtained new $C_1$-$C_{70}(CF_3)_8$ was suggested. 2D COSY $^{19}F$ NMR data reveal that the new isomer of $C_{70}(CF_3)_8$ represents trifluoromethylated fullerene molecule with the $C_1$-symmetry comprising a single continuous ribbon of edge-sharing *para*- and *meta*-$C_6(CF_3)_2$ hexagons.

[1] Mutig T., Kemnitz E., Troyanov S.I., *Mendeleev Commun*, **19**, 30 (2009).
[2] Dorozhkin E. I., Ignat'eva D. V., Tamm N. B., Goryunkov A. A., Khavrel P. A., Ioffe I. N., Popov A. A., Kuvychko I. V., Streletskiy A. V., Markov V. Y., Spandal J., Strauss S. H., Boltalina O. V., *Chem. Eur. J.* **12**, 3876 (2006).
[3] Mutig T., Ioffe I.N., Kemnitz E., Troyanov S.I., *Mendeleev Commun*. **18**, 73 (2008).