The functionalization of C_2-p^7-$C_{70}(CF_3)_8$ by the Bingel reaction

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An extensive development of synthetic methods for the trifluoromethylation of C_{60} and C_{70} resulted in a large number of different individual structurally-characterized $C_{60/70}(CF_3)_n$ with n=2–18. The methods of their following derivatization are under active studying [1].

Here we report the functionalization of a trifluoromethylated fullerene C_2-1,4,11,19,31,41,51,60-$C_{70}(CF_3)_8$, *via* the Bingel reaction for the first time. In C_2-p^7-$C_{70}(CF_3)_8$ all CF_3 groups arrange in the continuous ribbon of edge-sharing *para*-$C_6(CF_3)_2$ hexagons in the equatorial region of the molecule, remaining free both poles for further functionalization.

For the preparation of C_2-p^7-$C_{70}(CF_3)_8$ the typical two-step method [2] was used. The room temperature Bingel reaction of the HPLC-purified C_2-p^7-$C_{70}(CF_3)_8$ yielded the mixture of single isomer of $C_{70}(CF_3)_8[C(CO_2Et)_2]$ monoadduct and two isomers of $C_{70}(CF_3)_8[C(CO_2Et)_2]_2$ bisadduct.

The structures of isolated derivatives of C_2-p^7-$C_{70}(CF_3)_8$ were determined by means of ^{1}H and ^{19}F NMR spectroscopy and quantum chemical calculations at the DFT level. The structure of one isomer of bisadduct, $C_{70}(CF_3)_8[C(CO_2Et)_2]_2$-I, was revealed by X-ray single crystal analysis.

[1] Ovchinnikova N.S., Goryunkov A.A., Khavrel P.A., Belov N.M., Apenova M.G., Ioffe I.N., Yurovskaya M.A., Troyanov S.I., Sidorov L.N., Kemnitz E. *Dalton Trans*., **40**, 959 (2011); Takano Y., Herranz M.A., Kareev I.E., Strauss S.H., Boltalina O.V., Akasaka T., Martin N., *J. Org. Chem*. **74**, 6902 (2009); Ovchinnikova N.S., Ignateva D.V., Tamm N.B., Avdoshenko S.M., Goryunkov A.A., Ioffe I.N., Markov V.Y., Troyanov S.I., Sidorov L.N., Yurovskaya M.A., Kemnitz E., *New J. Chem*. **32**, 89 (2008).

[2] Mutig T., Kemnitz E., Troyanov S.I., *Mendeleev Commun*. **19**, 30 (2009).