

New trifluoromethyl derivatives of C₇₆ and C₈₂

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The present study concerns higher fullerenes of more than 70 carbon atoms. As is widely known, the number of possible isomers rapidly grows with the number of carbon atoms, the isomers that obey the Isolated Pentagon Rule (IPR) [1] being the most stable. Unambiguous structural determination of the fullerene molecules requires an X-ray study of pristine isomers or their derivatives. In this regard, the derivatized molecules frequently prove advantageous as the attached moieties suppress rotational disorder thereby enabling reliable determination of both cage connectivity and addition patterns. Here we report synthesis, separation, and structural characterization by means of single crystal X-ray diffraction of several new derivatives of C₇₆ and C₈₂.

A mixture of higher fullerenes was reacted with CF₃I in a sealed ampoule at 400°C. The C_m(CF₃)_n reaction products were dissolved in hexane and subjected to HPLC separation. Single crystals grown from three isolated fractions were studied by X-ray diffraction with the use of synchrotron radiation (BESSY, Free University, Berlin, Germany).

Two of the compounds obtained were found to contain the D₂-C₇₆ carbon cage. These molecules, C₇₆(CF₃)₁₆-II and C₇₆(CF₃)₁₆-III, appear to belong to one of the two previously known families of trifluoromethylated derivatives of C₇₆ [2]. The third compound, C₈₂(CF₃)₁₆, featured a certain disorder in the carbon cage (namely, alternating positions of two of the C-C bonds) caused by statistical distribution of enantiomeric molecules over the equivalent sites. The analysis of the disorder made it possible to attribute the carbon cage as the most stable isomer 3 of C₈₂. The reported isomer C₈₂(CF₃)₁₆ shows much similarity with the previously known C₈₂(CF₃)₁₈ [3], having 14 common CF₃ attachment sites.

We provide a general discussion of structural relationship, DFT calculated stability, and possible sequential addition pathways for the trifluoromethylated C₇₆ and C₈₂ known to date.

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