

Trifluoromethyl derivatives of fullerene C₇₆, C₇₆(CF₃)₁₄₋₁₈

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Data collection for single crystals of C₇₆(CF₃)_n was carried out with a MAR225 CCD detector at 100 K using synchrotron radiation at the BESSY storage ring, BL 14.2 ($\lambda = 0.9050 \text{ \AA}$, PSF of the Free University of Berlin, Germany). The structures were solved using direct methods (SHELXS97) or with the shake-and-bake program SHELXD and anisotropically refined with SHELXL97. Crystallographic data and some details of data collection and structure refinement are found in Table 1S. Two crystal structures contain solvated molecules (hexane or toluene). Hydrogen atoms of non-disordered solvent molecules were included in calculated positions. In the crystal structures, one, two, or three CF₃ groups are orientationally disordered between two positions each. Solvated hexane molecule in the structure of C₇₆(CF₃)₁₈·0.5C₆H₁₄ is strongly disordered between two positions around an inversion centre.

Table 1S. Crystallographic data and some details of data collection and refinement for four C₇₆(CF₃)_n structures.

Isomer	C ₇₆ (CF ₃) ₁₄ -I	C ₇₆ (CF ₃) ₁₆ -I	C ₇₆ (CF ₃) ₁₈ -I	C ₇₆ (CF ₃) ₁₈ -II
Solvent	C ₆ H ₅ (CH ₃)	-	0.5 C ₆ H ₁₄	-
<i>M</i>	1971.03	2016.92	2198.03	2154.94
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group; <i>Z</i>	<i>P</i> 2 ₁ / <i>n</i> ; 4	<i>P</i> $\bar{1}$; 2	<i>P</i> $\bar{1}$; 2	<i>P</i> $\bar{1}$; 2
<i>a</i> / \AA	13.946(1)	12.782(1)	14.6663(3)	11.566(1)
<i>b</i> / \AA	28.493(2)	14.503(1)	14.8569(3)	14.073(1)
<i>c</i> / \AA	17.758(1)	18.416(1)	17.6749(3)	22.098(2)
α / °	90	82.430(3)	84.4847(6)	91.762(3)
β / °	107.955(2)	82.059(1)	75.6282(6)	98.562(4)
γ / °	90	71.100(1)	79.5249(6)	109.635(3)
Volume / \AA^3	6712.7(8)	3236.0(4)	3663.3(1)	3337.3(5)
<i>D_c</i> / g cm ⁻³ ; μ / mm ⁻¹	1.950; 0.196	2.070; 0.218	1.993; 0.213	2.144; 0.231
Temperature / K	100(2)	100(2)	100(2)	100(2)
Refls collected / <i>R</i> _{int}	77894 / 0.094	42939 / 0.040	45032 / 0.048	45258 / 0.061
Data / parameters	14089 / 1309	11702 / 1289	12364 / 1455	12261 / 1388
<i>R</i> ₁ [<i>I</i> ≥ 2σ(<i>I</i>)]/w <i>R</i> ₂ (all)	0.065 / 0.173	0.068 / 0.156	0.056 / 0.135	0.083 / 0.235
Δρ (max / min)/e \AA^{-3}	0.57 / -0.58	0.77 / -0.66	0.70 / -0.70	0.75 / -0.61

CCDC 743440 – 743443 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. For details, see ‘Notice to Authors’, *Mendeleev Commun.*, Issue 1, 2010.