Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4,10,19,25,41,55,60,67,69-Decakis(trifluoromethyl)-1,4,10,19,25,41,55,60,67,69-decahydro(C_{70}-D_{5h})[5,6]fullerene

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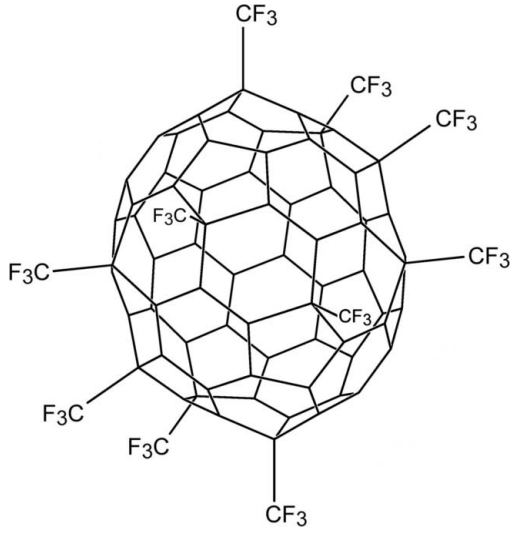
Received 28 August 2007; accepted 7 September 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.053; wR factor = 0.124; data-to-parameter ratio = 11.0.

The title compound, $C_{80}F_{30}$, is one of seven isomers of $C_{70}(CF_3)_{10}$ that have been isolated. The C_2-symmetry fullerene molecule has an idealized D_{5h} C_{70} core with the ten CF_3 groups arranged on a 'pole-to-pole' *para-meta-para-para-para-para-para-meta-para* (pmp^5mp) ribbon of edge-sharing $C_6(CF_3)_2$ hexagons. There are no cage Csp^3—Csp^3 bonds. There are intramolecular F···F contacts between pairs of CF_3 groups on the same hexagon that range from 2.560 (3) to 2.876 (3) Å. Two CF_3 groups are disordered with almost equal occupancies.

Related literature

For related literature, see: Avdoshenko *et al.* (2006); Goryunkov *et al.* (2006); Ignat'eva *et al.* (2006); Kareev *et al.* (2005, 2006*a*,*b*); Pham *et al.* (2007); Popov *et al.* (2007); Powell *et al.* (2002); Shustova *et al.* (2007).



Experimental

Crystal data

$C_{80}F_{30}$
M_r = 1530.80
Orthorhombic, *Pbcn*
a = 16.0658 (3) Å
b = 17.2662 (4) Å
c = 18.2153 (4) Å
V = 5052.84 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 100 (1) K
0.44 × 0.10 × 0.05 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.920, T_{max} = 0.990
53138 measured reflections
5853 independent reflections
3409 reflections with $I > 2\sigma(I)$
R_{int} = 0.098

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.124
S = 1.02
5853 reflections
534 parameters
25 restraints
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Data collection: *APEX2* (Bruker, 2000); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the US National Science Foundation for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2161).

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 doi:10.1107/S1600536807043991

supplementary materials

Acta Cryst. (2007). E**63**, o4073 [**doi:10.1107/S1600536807043991**]

1,4,10,19,25,41,55,60,67,69-Decakis(trifluoromethyl)-1,4,10,19,25,41,55,60,67,69-decahydro(C_{70}-D_{5h})[5,6]fullerene

N. B. Shustova, D. V. Peryshkov, O. V. Boltalina and S. H. Strauss

Comment

Recently reported high-temperature reactions of C_{70} with CF_3I have yielded more than two dozen $C_{70}(CF_3)_n$ derivatives (n = 2–18), most with relatively stable addition patterns that are chiral as well as unprecedented in fullerene$(X)_n$ chemistry (Kareev, Kuvychko, Lebedkin *et al.*, 2005; Kareev *et al.*, 2006*a*; Kareev *et al.*, 2006*b*; Avdoshenko *et al.*, 2006; Goryunkov *et al.*, 2006; Ignat'eva *et al.*, 2006; Popov, Kareev, Shustova *et al.*, 2007; Shustova, Peryshkov, Kareev, *et al.*, 2007). A member of the n = 10 set of seven isomers (Popov, Kareev, Shustova *et al.*, 2007), the title compound has been crystallized from toluene and we report its crystal structure here.

The structure of the title compound, as shown in Figs. 1 and 2, comprises an idealized $D_{5\,h}$ C_{70} core with ten sp^3 carbon atoms at positions 1, 4, 10, 19, 25, 41, 55, 60, 67, and 69 (Powell *et al.*, 2002), each of which is attached to a CF_3 group. The cage sp^3 carbon atoms are not adjacent to one another. The CF_3 groups are arranged on a *para-meta-para-para-para-para- meta-para* (pmp^{5}mp) ribbon of edge-sharing $C_6(CF_3)_2$ hexagons. The shared edges in each ribbon of hexagons are C(sp^3)-C(sp^2) bonds (*e.g.*, C1—C2, C4—C5, *etc*.), not C(sp^2)-C(sp^2) bonds. Thus, any pair of adjacent hexagons along the ribbon has a common CF_3 group.

The two CF_3 groups in the middle of the ribbon are disordered and were refined as half atoms. Only one set of the two disordered pairs is shown in the figures. As in all other published structures of fullerene$(CF_3)_n$ compounds, there are F$\cdots$F intramolecular contacts between pairs of neighboring CF_3 groups. The range of F$\cdots$F distances that do not involve the disordered CF_3 groups is from 2.539 (3) to 2.756 (3) Å. The range of C$\cdots$F distances that do not involve the disordered CF_3 groups is from 1.323 (3) to 1.338 (3) Å.

The shortest cage C—C bond in the asymmetric unit is C8—C9, at 1.349 (4) Å. This is significantly shorter than the shortest C—C bond of this type in the most precise structure of empty C_{70} reported to date ($C_9H_3Cl_6N{\cdot}3(C_{70}){\cdot}3(C_6H_5Cl)$), which is 1.440 (4) Å (Pham *et al.*, 2007). More importantly, the C8—C9 bond is a pentagon-hexagon junction, and the shortest pent-hex junction in $C_9H_3Cl_6N{\cdot}3(C_{70}){\cdot}3(C_6H_5Cl)$) is also 1.440 (4) Å (the longest pent-hex junction in $C_9H_3Cl_6N{\cdot}3(C_{70}){\cdot}3(C_6H_5Cl)$) is 1.460 (4) Å.

Experimental

The synthesis of the title compound was carried out by heating C_{70} in a stream of CF_3I at 420 °C as previously described (Popov, Kareev, Shustova, *et al.* 2007). Crystals of the HPLC-purified compound were grown by slow evaporation of a saturated deuterochloroform solution.

Refinement

The maximum (0.47 e/Å^3) and minimum (−0.54 e/Å^3) residual electron density peaks were located 0.66 Å and 0.24 Å from F11.

Figures

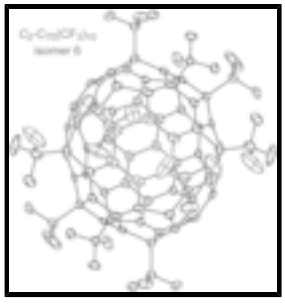


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are shown at the 50% probability level. The crystallographic C_2 axis is perpendicular to the plane of the page. Only one pair of the disordered CF_3 groups on the hexagon centered on the C_2 axis is shown.

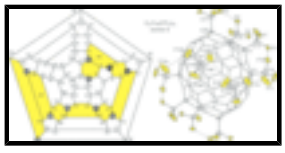


Fig. 2. (Left) Schlegel diagram showing the IUPAC lowest-locants for the cage carbon atoms. The C_2 axis passes through the center of the hexagon with C19 and C41 and bisects the C30—C50 bond. The CF_3 groups are attached to the cage carbon atoms depicted as black circles. Also shown is the ribbon of *meta*- and *para*-$C_6(CF_3)_2$ edge-sharing hexagons (the two *meta*-$C_6(CF_3)_2$ hexagons are indicated with the letter m). (Right) The structure showing the atom numbers for the CF_3 groups and the network of F···F contacts between CF_3 groups that share the same hexagon.

1,4,10,19,25,41,55,60,67,69-Decakis(trifluoromethyl)- 1,4,10,19,25,41,55,60,67,69-decahydro(C_{70}—D_{5h})[5,6]fullerene

Crystal data

$C_{80}F_{30}$	D_x = 2.012 Mg m^{-3}
M_r = 1530.80	Mo $K\alpha$ radiation λ = 0.71073 Å
Orthorhombic, *Pbcn*	Cell parameters from 999 reflections
a = 16.0658 (3) Å	θ = 1.7–27.9°
b = 17.2662 (4) Å	μ = 0.20 mm^{-1}
c = 18.2153 (4) Å	*T* = 100 (1) K
V = 5052.84 (19) Å^3	Plate, red
Z = 4	0.44 × 0.10 × 0.05 mm
F_{000} = 3000	

Data collection

Bruker Kappa APEXII diffractometer	5853 independent reflections
Radiation source: fine-focus sealed tube	3409 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.098

T = 100(1) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

T_{min} = 0.920, T_{max} = 0.990

53138 measured reflections

θ_{max} = 27.9º

θ_{min} = 1.7º

h = −19→21

k = −20→21

l = −23→19

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.053

$wR(F^2)$ = 0.124

S = 1.02

5853 reflections

534 parameters

25 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 4.0833P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.026

$\Delta\rho_{max}$ = 0.47 e Å^{-3}

$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.14807 (15)	0.84689 (16)	0.57610 (14)	0.0172 (6)	
C2	0.06726 (15)	0.89202 (16)	0.56364 (14)	0.0171 (6)	
C3	−0.00314 (15)	0.85035 (16)	0.54804 (14)	0.0179 (6)	
C4	−0.01274 (16)	0.76084 (17)	0.55711 (15)	0.0212 (7)	
C5	0.05113 (16)	0.73164 (16)	0.61305 (15)	0.0192 (6)	
C6	0.12706 (15)	0.76964 (16)	0.61409 (15)	0.0171 (6)	
C7	0.18225 (15)	0.76010 (16)	0.67239 (15)	0.0181 (6)	
C8	0.22979 (14)	0.83155 (16)	0.68340 (14)	0.0161 (6)	
C9	0.20545 (14)	0.88497 (16)	0.63383 (14)	0.0158 (6)	
C10	0.20897 (15)	0.97126 (16)	0.64795 (14)	0.0163 (6)	
C11	0.12152 (15)	1.00488 (16)	0.63621 (15)	0.0169 (6)	
C12	0.06016 (15)	0.97158 (16)	0.59058 (14)	0.0161 (6)	
C13	−0.02077 (15)	1.00408 (16)	0.59698 (15)	0.0181 (6)	

C14	−0.09317 (15)	0.96120 (17)	0.57594 (14)	0.0187 (6)	
C15	−0.08409 (15)	0.88541 (18)	0.55430 (14)	0.0208 (7)	
C16	−0.14344 (15)	0.82795 (17)	0.57804 (15)	0.0203 (7)	
C17	−0.10068 (15)	0.75657 (17)	0.58928 (15)	0.0216 (7)	
C18	−0.12203 (16)	0.71052 (17)	0.64672 (16)	0.0224 (7)	
C19	−0.06088 (16)	0.65728 (16)	0.68667 (16)	0.0227 (7)	
C20	0.02896 (16)	0.68342 (16)	0.67393 (16)	0.0213 (7)	
C21	0.08471 (16)	0.67492 (16)	0.73207 (16)	0.0219 (7)	
C22	0.16204 (15)	0.71231 (16)	0.73075 (15)	0.0201 (6)	
C23	0.18732 (15)	0.73373 (17)	0.80518 (15)	0.0208 (7)	
C24	0.23331 (15)	0.79965 (17)	0.81776 (15)	0.0191 (6)	
C25	0.27335 (15)	0.84797 (16)	0.75587 (15)	0.0196 (6)	
C26	0.24996 (15)	0.93044 (17)	0.77931 (15)	0.0188 (6)	
C27	0.21993 (15)	0.98455 (16)	0.73100 (14)	0.0179 (6)	
C28	0.15831 (16)	1.03892 (16)	0.75525 (15)	0.0193 (6)	
C29	0.09863 (16)	1.05095 (16)	0.69643 (15)	0.0187 (6)	
C30	0.01394 (16)	1.07106 (15)	0.71141 (15)	0.0174 (6)	
C31	−0.04340 (15)	1.05362 (16)	0.65680 (15)	0.0173 (6)	
C32	−0.13118 (15)	1.04049 (16)	0.67284 (15)	0.0185 (6)	
C33	−0.16206 (15)	0.98408 (17)	0.62258 (15)	0.0203 (6)	
C45	0.20949 (15)	0.84927 (17)	0.87587 (15)	0.0209 (7)	
C46	0.21946 (15)	0.92902 (17)	0.85350 (15)	0.0203 (7)	
C71	0.36707 (16)	0.83212 (18)	0.75032 (16)	0.0232 (7)	
C72	0.27308 (16)	1.01737 (17)	0.60260 (15)	0.0208 (6)	
C73	0.19695 (16)	0.83397 (17)	0.50429 (15)	0.0218 (7)	
C74	−0.00903 (18)	0.7147 (2)	0.48471 (18)	0.0334 (8)	
F1	0.40336 (9)	0.87577 (10)	0.69942 (9)	0.0298 (4)	
F2	0.40463 (9)	0.84669 (11)	0.81408 (9)	0.0356 (5)	
F3	0.38117 (10)	0.75794 (10)	0.73328 (10)	0.0354 (5)	
F4	0.34564 (9)	0.98094 (10)	0.59759 (9)	0.0324 (4)	
F5	0.24686 (9)	1.03264 (10)	0.53477 (8)	0.0281 (4)	
F6	0.28737 (11)	1.08613 (10)	0.63398 (9)	0.0373 (5)	
F7	0.24219 (11)	0.89500 (11)	0.48588 (10)	0.0401 (5)	
F8	0.24879 (11)	0.77447 (11)	0.51097 (9)	0.0424 (5)	
F9	0.14794 (10)	0.81972 (11)	0.44729 (9)	0.0376 (5)	
F10	0.06645 (10)	0.69174 (11)	0.46686 (9)	0.0389 (5)	
F11	−0.05481 (16)	0.65144 (16)	0.48843 (15)	0.1015 (12)	
F12	−0.03764 (16)	0.75595 (16)	0.42896 (11)	0.0793 (9)	
F13	−0.0496 (3)	0.5632 (3)	0.5902 (3)	0.053 (2)	0.511 (8)
F14	−0.0479 (5)	0.5247 (3)	0.7019 (4)	0.060 (3)	0.511 (8)
F15	−0.1603 (3)	0.5624 (4)	0.6519 (4)	0.0402 (15)	0.511 (8)
C75	−0.0798 (8)	0.5751 (6)	0.6567 (7)	0.021 (3)	0.511 (8)
F13A	−0.1288 (5)	0.5590 (4)	0.6213 (4)	0.0464 (19)	0.489 (8)
F14A	−0.0029 (3)	0.5355 (2)	0.6456 (4)	0.052 (2)	0.489 (8)
F15A	−0.0943 (4)	0.5270 (3)	0.7297 (3)	0.0397 (14)	0.489 (8)
C75A	−0.0701 (9)	0.5695 (6)	0.6721 (7)	0.026 (4)	0.489 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0157 (12)	0.0214 (16)	0.0144 (15)	−0.0016 (11)	0.0022 (11)	−0.0013 (13)
C2	0.0184 (13)	0.0260 (17)	0.0068 (13)	0.0017 (11)	0.0034 (10)	0.0004 (13)
C3	0.0195 (13)	0.0248 (17)	0.0094 (14)	−0.0003 (11)	0.0003 (11)	−0.0056 (13)
C4	0.0186 (14)	0.0266 (18)	0.0184 (16)	−0.0040 (12)	0.0028 (11)	−0.0114 (13)
C5	0.0203 (13)	0.0177 (16)	0.0196 (15)	0.0012 (11)	0.0043 (11)	−0.0097 (13)
C6	0.0166 (13)	0.0166 (16)	0.0182 (15)	0.0006 (11)	0.0056 (11)	−0.0055 (13)
C7	0.0127 (12)	0.0184 (16)	0.0231 (16)	0.0043 (11)	0.0049 (11)	−0.0021 (13)
C8	0.0114 (12)	0.0199 (16)	0.0170 (15)	0.0009 (10)	0.0036 (10)	−0.0018 (13)
C9	0.0137 (12)	0.0206 (16)	0.0130 (14)	−0.0009 (11)	0.0056 (10)	−0.0028 (13)
C10	0.0164 (12)	0.0186 (16)	0.0139 (14)	−0.0031 (11)	0.0000 (11)	−0.0009 (12)
C11	0.0210 (13)	0.0145 (15)	0.0153 (15)	−0.0021 (11)	0.0045 (11)	0.0035 (12)
C12	0.0204 (13)	0.0206 (17)	0.0073 (14)	0.0002 (11)	0.0020 (11)	0.0038 (12)
C13	0.0224 (14)	0.0208 (17)	0.0109 (15)	0.0017 (11)	0.0016 (11)	0.0052 (13)
C14	0.0187 (13)	0.0283 (18)	0.0092 (14)	0.0046 (12)	−0.0030 (10)	0.0050 (13)
C15	0.0176 (13)	0.037 (2)	0.0075 (14)	0.0006 (12)	−0.0022 (11)	−0.0045 (13)
C16	0.0169 (13)	0.0309 (18)	0.0133 (15)	−0.0002 (12)	−0.0059 (11)	−0.0079 (13)
C17	0.0154 (13)	0.0305 (18)	0.0188 (16)	−0.0068 (12)	0.0001 (11)	−0.0135 (14)
C18	0.0193 (13)	0.0237 (17)	0.0242 (17)	−0.0070 (12)	0.0012 (12)	−0.0120 (14)
C19	0.0218 (14)	0.0168 (17)	0.0294 (17)	−0.0046 (11)	0.0076 (12)	−0.0073 (14)
C20	0.0199 (13)	0.0136 (16)	0.0305 (18)	−0.0005 (11)	0.0073 (12)	−0.0088 (14)
C21	0.0215 (14)	0.0111 (15)	0.0332 (18)	0.0027 (11)	0.0083 (12)	0.0012 (13)
C22	0.0161 (13)	0.0172 (16)	0.0272 (17)	0.0059 (11)	0.0044 (12)	0.0020 (14)
C23	0.0159 (13)	0.0227 (17)	0.0237 (16)	0.0071 (11)	0.0014 (12)	0.0080 (14)
C24	0.0115 (12)	0.0268 (18)	0.0190 (15)	0.0054 (11)	−0.0003 (11)	0.0086 (13)
C25	0.0138 (12)	0.0265 (17)	0.0185 (15)	0.0000 (11)	−0.0001 (11)	0.0031 (14)
C26	0.0107 (12)	0.0283 (17)	0.0174 (15)	−0.0040 (11)	0.0003 (11)	−0.0010 (14)
C27	0.0162 (12)	0.0206 (16)	0.0168 (15)	−0.0077 (11)	0.0008 (11)	−0.0025 (13)
C28	0.0199 (13)	0.0170 (16)	0.0209 (16)	−0.0075 (11)	0.0027 (11)	−0.0023 (13)
C29	0.0238 (14)	0.0133 (16)	0.0191 (16)	−0.0032 (11)	0.0032 (12)	0.0064 (13)
C30	0.0263 (14)	0.0072 (14)	0.0187 (15)	0.0004 (11)	0.0029 (12)	0.0011 (12)
C31	0.0214 (13)	0.0157 (16)	0.0150 (15)	0.0039 (11)	0.0027 (11)	0.0070 (12)
C32	0.0205 (13)	0.0201 (16)	0.0147 (15)	0.0085 (11)	−0.0006 (11)	0.0050 (13)
C33	0.0180 (13)	0.0288 (18)	0.0140 (15)	0.0082 (12)	−0.0034 (11)	0.0061 (13)
C45	0.0126 (12)	0.0342 (19)	0.0161 (15)	0.0017 (12)	−0.0060 (11)	0.0053 (14)
C46	0.0123 (12)	0.0337 (19)	0.0148 (15)	−0.0040 (12)	−0.0046 (11)	0.0005 (14)
C71	0.0151 (13)	0.033 (2)	0.0218 (16)	0.0016 (12)	−0.0007 (12)	0.0051 (15)
C72	0.0211 (14)	0.0236 (18)	0.0177 (16)	−0.0044 (12)	−0.0005 (11)	−0.0014 (14)
C73	0.0168 (13)	0.0291 (18)	0.0194 (16)	−0.0016 (12)	0.0018 (12)	−0.0023 (14)
C74	0.0258 (16)	0.043 (2)	0.0315 (19)	−0.0086 (15)	0.0094 (14)	−0.0174 (17)
F1	0.0171 (8)	0.0452 (12)	0.0270 (10)	−0.0027 (7)	0.0034 (7)	0.0059 (9)
F2	0.0168 (8)	0.0643 (13)	0.0256 (10)	−0.0002 (8)	−0.0042 (7)	0.0052 (9)
F3	0.0215 (8)	0.0346 (12)	0.0501 (12)	0.0089 (7)	0.0046 (8)	0.0034 (9)
F4	0.0177 (8)	0.0434 (11)	0.0361 (11)	−0.0030 (7)	0.0064 (7)	0.0092 (9)
F5	0.0277 (8)	0.0388 (11)	0.0177 (9)	−0.0057 (7)	0.0022 (7)	0.0079 (8)

F6	0.0518 (11)	0.0297 (11)	0.0302 (10)	−0.0222 (8)	0.0131 (8)	−0.0067 (9)
F7	0.0467 (11)	0.0412 (12)	0.0325 (11)	−0.0192 (9)	0.0217 (9)	−0.0082 (9)
F8	0.0464 (11)	0.0493 (13)	0.0315 (11)	0.0266 (9)	0.0178 (9)	0.0039 (10)
F9	0.0282 (9)	0.0677 (14)	0.0168 (9)	−0.0052 (9)	0.0048 (7)	−0.0127 (9)
F10	0.0309 (10)	0.0548 (13)	0.0310 (11)	0.0059 (9)	0.0081 (8)	−0.0190 (9)
F11	0.0947 (18)	0.101 (2)	0.109 (2)	−0.0763 (16)	0.0727 (17)	−0.0905 (18)
F12	0.0927 (18)	0.112 (2)	0.0335 (13)	0.0535 (15)	−0.0346 (12)	−0.0437 (14)
F13	0.071 (4)	0.036 (3)	0.054 (3)	−0.021 (2)	0.030 (3)	−0.026 (2)
F14	0.088 (6)	0.021 (3)	0.072 (5)	−0.001 (3)	−0.054 (5)	0.001 (3)
F15	0.025 (2)	0.031 (3)	0.064 (4)	−0.008 (2)	−0.003 (2)	−0.016 (3)
C75	0.018 (5)	0.016 (6)	0.028 (6)	−0.002 (4)	−0.001 (4)	−0.005 (4)
F13A	0.066 (5)	0.024 (3)	0.049 (4)	−0.004 (3)	−0.029 (4)	−0.007 (3)
F14A	0.039 (3)	0.021 (3)	0.096 (6)	−0.0068 (18)	0.038 (3)	−0.022 (3)
F15A	0.064 (4)	0.020 (2)	0.036 (3)	−0.011 (2)	0.006 (2)	0.001 (2)
C75A	0.019 (5)	0.040 (9)	0.019 (6)	−0.004 (5)	0.002 (4)	−0.003 (5)

Geometric parameters (Å, °)

C1—C2	1.531 (4)	C21—C19^{i}	1.559 (4)
C1—C6	1.540 (4)	C22—C23	1.463 (4)
C1—C73	1.542 (4)	C23—C24	1.376 (4)
C1—C9	1.545 (4)	C23—C18^{i}	1.424 (4)
C2—C3	1.370 (4)	C24—C45	1.415 (4)
C2—C12	1.463 (4)	C24—C25	1.543 (4)
C3—C15	1.439 (4)	C25—C26	1.533 (4)
C3—C4	1.562 (4)	C25—C71	1.534 (4)
C4—C17	1.531 (4)	C26—C27	1.371 (4)
C4—C5	1.531 (4)	C26—C46	1.438 (4)
C4—C74	1.542 (4)	C27—C28	1.434 (4)
C5—C6	1.385 (4)	C28—C32^{i}	1.381 (4)
C5—C20	1.432 (4)	C28—C29	1.453 (4)
C6—C7	1.393 (4)	C29—C30	1.430 (4)
C7—C22	1.384 (4)	C30—C31	1.389 (4)
C7—C8	1.465 (4)	C30—C30^{i}	1.475 (5)
C8—C9	1.349 (4)	C31—C32	1.458 (4)
C8—C25	1.521 (4)	C32—C28^{i}	1.381 (4)
C9—C10	1.513 (4)	C32—C33	1.426 (4)
C10—C11	1.535 (3)	C33—C46^{i}	1.394 (4)
C10—C27	1.540 (4)	C45—C16^{i}	1.402 (4)
C10—C72	1.542 (4)	C45—C46	1.445 (4)
C11—C29	1.404 (4)	C46—C33^{i}	1.394 (4)
C11—C12	1.412 (4)	C71—F1	1.330 (3)
C12—C13	1.421 (4)	C71—F2	1.333 (3)
C13—C14	1.431 (4)	C71—F3	1.337 (3)
C13—C31	1.432 (4)	C72—F4	1.328 (3)
C14—C15	1.374 (4)	C72—F5	1.332 (3)
C14—C33	1.450 (4)	C72—F6	1.338 (3)

C15—C16	1.442 (4)	C73—F7	1.323 (3)
C16—C45^{i}	1.402 (4)	C73—F9	1.326 (3)
C16—C17	1.426 (4)	C73—F8	1.328 (3)
C17—C18	1.358 (4)	C74—F10	1.316 (3)
C18—C23^{i}	1.424 (4)	C74—F11	1.319 (4)
C18—C19	1.530 (4)	C74—F12	1.323 (4)
C19—C20	1.530 (4)	F13—C75	1.322 (12)
C19—C75	1.551 (10)	F14—C75	1.303 (12)
C19—C75A	1.546 (11)	F15—C75	1.315 (12)
C19—C21^{i}	1.559 (4)	F13A—C75A	1.332 (13)
C20—C21	1.395 (4)	F14A—C75A	1.321 (13)
C21—C22	1.400 (4)	F15A—C75A	1.339 (13)
C2—C1—C6	108.8 (2)	C7—C22—C23	119.7 (2)
C2—C1—C73	112.3 (2)	C21—C22—C23	110.3 (2)
C6—C1—C73	111.6 (2)	C24—C23—C18^{i}	121.7 (3)
C2—C1—C9	113.0 (2)	C24—C23—C22	120.8 (3)
C6—C1—C9	101.2 (2)	C18^{i}—C23—C22	107.1 (2)
C73—C1—C9	109.6 (2)	C23—C24—C45	118.7 (2)
C3—C2—C12	119.9 (2)	C23—C24—C25	123.3 (3)
C3—C2—C1	117.6 (2)	C45—C24—C25	109.4 (2)
C12—C2—C1	119.6 (2)	C8—C25—C26	107.6 (2)
C2—C3—C15	120.6 (3)	C8—C25—C71	111.2 (2)
C2—C3—C4	125.4 (2)	C26—C25—C71	115.1 (2)
C15—C3—C4	108.6 (2)	C8—C25—C24	110.0 (2)
C17—C4—C5	110.4 (2)	C26—C25—C24	101.3 (2)
C17—C4—C74	109.8 (2)	C71—C25—C24	111.2 (2)
C5—C4—C74	111.9 (2)	C27—C26—C46	119.7 (2)
C17—C4—C3	100.3 (2)	C27—C26—C25	122.7 (2)
C5—C4—C3	109.3 (2)	C46—C26—C25	109.2 (2)
C74—C4—C3	114.6 (2)	C26—C27—C28	119.4 (2)
C6—C5—C20	118.9 (2)	C26—C27—C10	124.7 (2)
C6—C5—C4	116.3 (2)	C28—C27—C10	108.7 (2)
C20—C5—C4	122.7 (2)	C32^{i}—C28—C27	121.5 (3)
C5—C6—C7	121.0 (3)	C32^{i}—C28—C29	119.2 (2)
C5—C6—C1	126.7 (2)	C27—C28—C29	108.8 (2)
C7—C6—C1	107.8 (2)	C11—C29—C30	122.4 (2)
C22—C7—C6	120.4 (2)	C11—C29—C28	108.8 (2)
C22—C7—C8	121.3 (2)	C30—C29—C28	121.5 (2)
C6—C7—C8	109.7 (2)	C31—C30—C29	116.2 (2)
C9—C8—C7	109.5 (2)	C31—C30—C30^{i}	118.8 (3)
C9—C8—C25	126.0 (2)	C29—C30—C30^{i}	118.1 (3)
C7—C8—C25	121.0 (2)	C30—C31—C13	120.4 (2)
C8—C9—C10	123.3 (2)	C30—C31—C32	122.1 (2)
C8—C9—C1	109.7 (2)	C13—C31—C32	107.8 (2)
C10—C9—C1	123.9 (2)	C28^{i}—C32—C33	119.1 (3)
C9—C10—C11	108.3 (2)	C28^{i}—C32—C31	119.9 (2)

C9—C10—C27	108.5 (2)	C33—C32—C31	108.3 (2)
C11—C10—C27	100.7 (2)	C46^{i}—C33—C32	119.7 (2)
C9—C10—C72	116.3 (2)	C46^{i}—C33—C14	120.1 (3)
C11—C10—C72	110.0 (2)	C32—C33—C14	107.3 (2)
C27—C10—C72	111.9 (2)	C16^{i}—C45—C24	119.6 (3)
C29—C11—C12	120.5 (2)	C16^{i}—C45—C46	120.2 (3)
C29—C11—C10	110.2 (2)	C24—C45—C46	109.6 (2)
C12—C11—C10	124.5 (2)	C33^{i}—C46—C26	120.5 (3)
C11—C12—C13	115.5 (2)	C33^{i}—C46—C45	119.2 (2)
C11—C12—C2	121.7 (2)	C26—C46—C45	108.6 (2)
C13—C12—C2	118.0 (2)	F1—C71—F2	107.6 (2)
C12—C13—C14	121.2 (2)	F1—C71—F3	107.9 (2)
C12—C13—C31	122.0 (2)	F2—C71—F3	107.8 (2)
C14—C13—C31	107.8 (2)	F1—C71—C25	112.0 (2)
C15—C14—C13	118.9 (2)	F2—C71—C25	110.7 (2)
C15—C14—C33	120.6 (3)	F3—C71—C25	110.6 (2)
C13—C14—C33	108.8 (2)	F4—C72—F5	107.9 (2)
C14—C15—C3	121.3 (2)	F4—C72—F6	107.4 (2)
C14—C15—C16	119.9 (2)	F5—C72—F6	106.0 (2)
C3—C15—C16	109.4 (3)	F4—C72—C10	112.3 (2)
C45^{i}—C16—C17	120.4 (3)	F5—C72—C10	112.8 (2)
C45^{i}—C16—C15	119.9 (3)	F6—C72—C10	110.1 (2)
C17—C16—C15	108.6 (2)	F7—C73—F9	106.0 (2)
C18—C17—C16	119.7 (2)	F7—C73—F8	107.2 (2)
C18—C17—C4	123.8 (3)	F9—C73—F8	107.5 (2)
C16—C17—C4	110.4 (2)	F7—C73—C1	112.3 (2)
C17—C18—C23^{i}	119.7 (3)	F9—C73—C1	112.9 (2)
C17—C18—C19	123.8 (2)	F8—C73—C1	110.7 (2)
C23^{i}—C18—C19	110.5 (2)	F10—C74—F11	106.1 (3)
C18—C19—C20	110.9 (2)	F10—C74—F12	107.0 (3)
C18—C19—C75	104.9 (5)	F11—C74—F12	107.0 (3)
C20—C19—C75	113.7 (5)	F10—C74—C4	113.7 (2)
C18—C19—C75A	116.5 (6)	F11—C74—C4	111.3 (3)
C20—C19—C75A	110.7 (5)	F12—C74—C4	111.4 (3)
C75—C19—C75A	12.4 (8)	F14—C75—F13	109.3 (10)
C18—C19—C21^{i}	100.2 (2)	F14—C75—F15	108.6 (9)
C20—C19—C21^{i}	108.6 (2)	F13—C75—F15	105.9 (10)
C75—C19—C21^{i}	117.7 (5)	F14—C75—C19	108.2 (8)
C75A—C19—C21^{i}	109.4 (5)	F13—C75—C19	113.1 (8)
C21—C20—C5	119.3 (2)	F15—C75—C19	111.6 (8)
C21—C20—C19	117.4 (3)	F13A—C75A—F14A	105.4 (10)
C5—C20—C19	121.6 (2)	F13A—C75A—F15A	105.3 (9)
C20—C21—C22	120.5 (3)	F14A—C75A—F15A	106.2 (10)
C20—C21—C19^{i}	125.7 (2)	F13A—C75A—C19	108.7 (9)
C22—C21—C19^{i}	108.9 (2)	F14A—C75A—C19	114.8 (9)
C7—C22—C21	119.7 (3)	F15A—C75A—C19	115.5 (9)

Symmetry codes: (i) −*x*, *y*, −*z*+3/2.

Correspondence of IUPAC lowest locants with crystallographic atom numbers for C_2-1,4,10,19,25,41,55,60,67,69-$C_{70}(CF_3)_{10}$

C1	C1
C2	C2
C3	C3
C4	C4
C5	C5
C6	C6
C7	C7
C8	C8
C9	C9
C10	C10
C11	C11
C12	C12
C13	C13
C14	C14
C15	C15
C16	C16
C17	C17
C18	C18
C19	C19
C20	C20
C21	C21
C22	C22
C23	C23
C24	C24
C25	C25
C26	C26
C27	C27
C28	C28
C29	C29
C30	C30
C31	C31
C32	C32
C33	C33
C34	C46*a*
C35	C45*a*
C36	C24*a*
C37	C23*a*
C38	C22*a*
C39	C21*a*
C40	C20*a*
C41	C19*a*
C42	C18*a*
C43	C17*a*

C44	C16*a*
C45	C45
C46	C46
C47	C33*a*
C48	C32*a*
C49	C31*a*
C50	C30*a*
C51	C29*a*
C52	C28*a*
C53	C27*a*
C54	C26*a*
C55	C25*a*
C56	C8a
C57	C7a
C58	C6a
C59	C5a
C60	C4a
C61	C3a
C62	C15*a*
C63	C14*a*
C64	C13*a*
C65	C12*a*
C66	C11*a*
C67	C10*a*
C68	C9a
C69	C1a
C70	C2a

Fig. 1

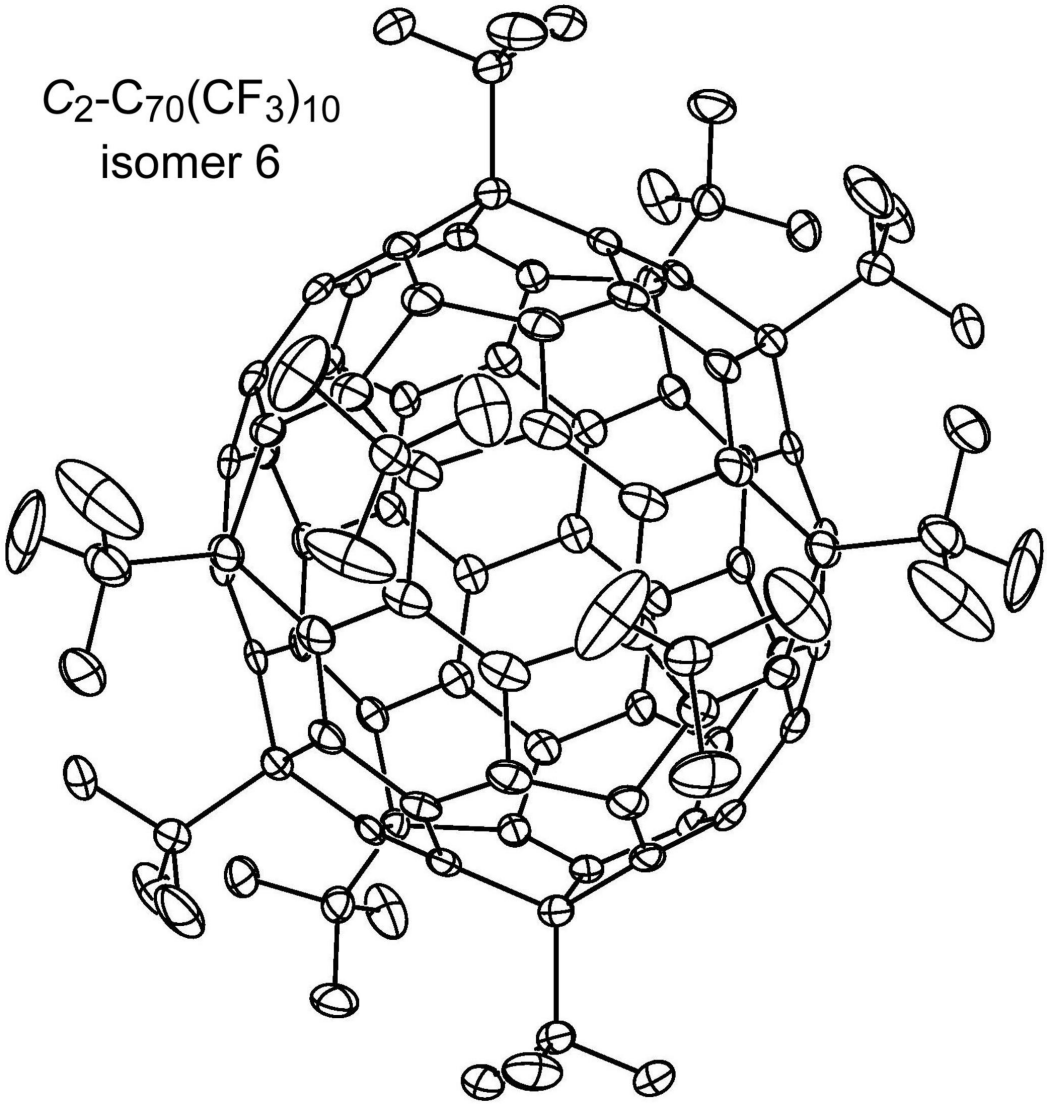
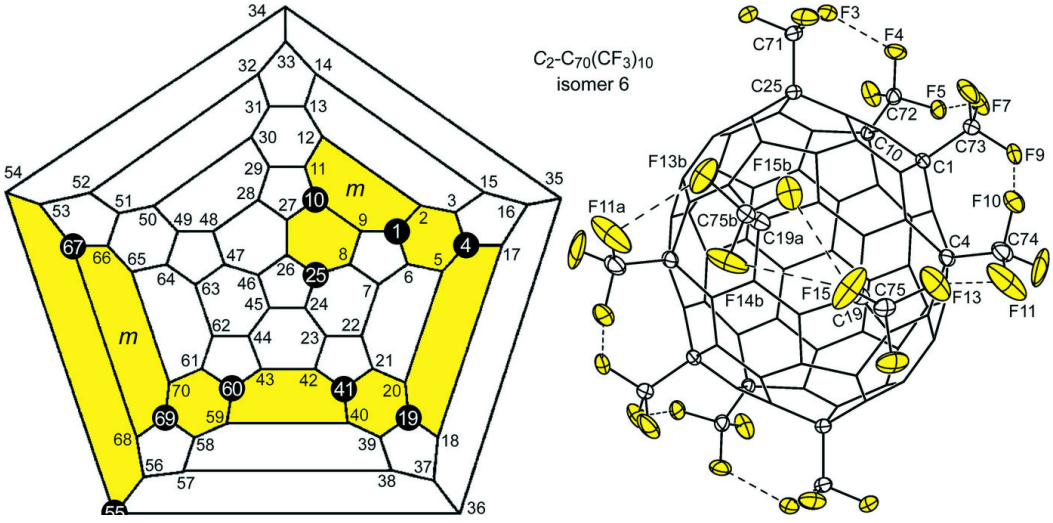


Fig. 2


C_2-$C_{70}(CF_3)_{10}$
isomer 6
m
m
F3
F4
C71
C25
F5
C72
F7
C10
C73
F9
C1
F13b
F15b
F10
F11a
C75b
C19a
C4
C74
F14b
F15
C75
F13
C19
F11