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1,7,16,30,36,47-Hexakis(perfluoroisopropyl)-1,7,16,30,36,47-hexahydro-(C_{60}–I_h)[5,6]fullerene

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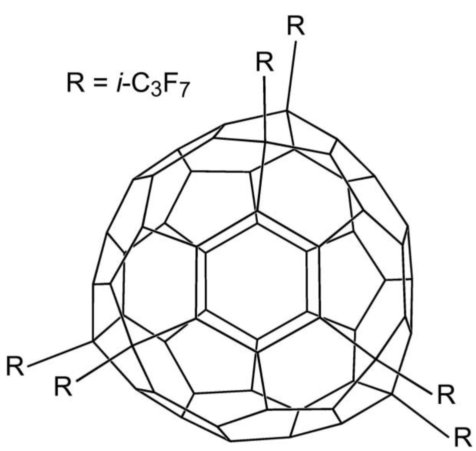
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.052; wR factor = 0.133; data-to-parameter ratio = 10.5.

The title compound, $C_{78}F_{42}$, is the first example of a perfluoroalkylfullerene with perfluoroisopropyl groups. The C_1 symmetry molecule has idealized C_3 symmetry with the six isopropyl groups arranged on three isolated *para*-C_6(*i*-C_3F_7)$_2$ hexagons. There are three intramolecular F$\cdots$F contacts between pairs of isopropyl groups that share the same hexagon; these contacts range from 2.616 (3) to 2.657 (3) Å.

Related literature

For related literature, see: Kareev, Kuvychko *et al.* (2006); Kareev, Shustova *et al.* (2006); Popov *et al.* (2007*a*,*b*); Tamm & Troyanov (2007).



Experimental

Crystal data

$C_{78}F_{42}$
M_r = 1734.78
Monoclinic, $P2_1/n$
a = 13.5877 (3) Å
b = 31.1809 (7) Å
c = 13.7240 (3) Å
β = 106.873 (1)°
V = 5564.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 (1) K
0.30 × 0.11 × 0.06 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 2003) T_{min} = 0.937, T_{max} = 0.988
75325 measured reflections
11386 independent reflections
6862 reflections with $I > 2\sigma(I)$
R_{int} = 0.083

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.133
S = 1.01
11386 reflections
1081 parameters
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2171).

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supplementary materials

Acta Cryst. (2007). E**63**, o4575 [**doi:10.1107/S1600536807053895**]

1,7,16,30,36,47-Hexakis(perfluoroisopropyl)-1,7,16,30,36,47-hexahydro(C_{60}-I_h)[5,6]fullerene

N. B. Shustova, I. V. Kuvychko, O. V. Boltalina and S. H. Strauss

Comment

Fullerenes with CF_3 or C_2F_5 groups generally have addition patterns that are ribbons of edge-sharing *meta*- and/or *para*-$C_6(R_f)_2$ hexagons (Popov *et al.*, 2007*a*; Popov *et al.*, 2007*b*; Tamm and Troyanov, 2007; Kareev, Kuvychko *et al.*, 2006). The i-C_3F_7 group was chosen to destabilize sterically such ribbons relative to addition patterns with multiple isolated *p*-$C_6(R_f)_2$ hexagons so that fullerene$(X)_n$ compounds with unprecedented addition patterns could be prepared and investigated.

The structure of the title compound, shown in Figure 1, consists of an icosahedral C_{60} cage and three isolated *p*-C_6(i-$C_3F_7)_2$ hexagons arranged so that the C_{60}(i-$C_3F_7)_6$ molecule has idealized C_3 symmetry (but the molecule has no crystallographically imposed symmetry). The conformations of the perfluoroalkyl groups result in the fluoromethine F atoms positioned over the shared hexagon, as shown in Figure 2. The three F···F distances range from 2.616 (3) to 2.657 (3) Å and the three F—C···C—F torsion angles range from 51.9 (3) to 56.4 (3) degrees. In contrast, the F···F distance and F—C···C—F torsion angle for the isolated *p*-$C_6(CF_3)_2$ hexagon in 1,6,11,18,24,27,52,55-$C_{60}(CF_3)_8$ are 2.695 (3) Å and 3.4 (2) degrees, respectively (Kareev, Shustova *et al.*, 2006). The differences are due in part to the different lengths of fluoromethine C—F bonds (these range from 1.372 (4) to 1.378 (4) in C_{60}(i-$C_3F_7)_6$) and trifluoromethyl C—F bonds (these range from 1.304 (3) to 1.347 (3) Å, and average 1.328 (1) Å, in 1,6,11,18,24,27,52,55-$C_{60}(CF_3)_8$) and range from 1.318 (4) to 1.353 (4) Å, and average 1.333 (1) Å, in C_{60}(i-$C_3F_7)_6$).

There are now more than 40 X-ray structures of fullerene$(CF_3)_n$ and fullerene$(C_2F_5)_n$ compounds (Popov *et al.*, 2007*a*; Popov *et al.*, 2007*b*; Tamm & Troyanov, 2007; Kareev, Newell *et al.*, 2006). The compound 1,7,16,36,46,49-$C_{60}(C_2F_5)_6$ is the only other fullerene$(R_f)_n$ with three or more isolated *p*-$C_6(R_f)_2$ hexagons (Kareev, Kuvychko *et al.*, 2006). The addition patterns of both compounds are very similar, as shown in the Schlegel diagrams in Figure 3. The continued study of fullerene(i-$C_3F_7)_n$ compounds will no doubt lead to other unprecedented addition patterns.

Experimental

The synthesis of the title compound was carried out by heating C_{60} and i-C_3F_7I in a sealed ampoule at 300–400 °C. Crystals of the HPLC-purified compound were grown by slow evaporation of a saturated toluene solution.

Refinement

The maximum (0.53 e/Å^3) and minimum (−0.32 e/Å^3) residual electron density peaks were located 1.16 Å from F833 and 0.55 Å from F823.

Figures

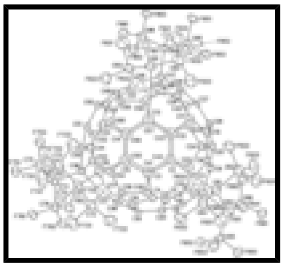

Fig. 1. The molecular structure of 1,7,16,30,36,47-C_{60}(i-C_3F_7)$_6$. Displacement ellipsoids are shown at the 50% probability level. The non-crystallographic C_3 axis is perpendicular to the plane of the page.

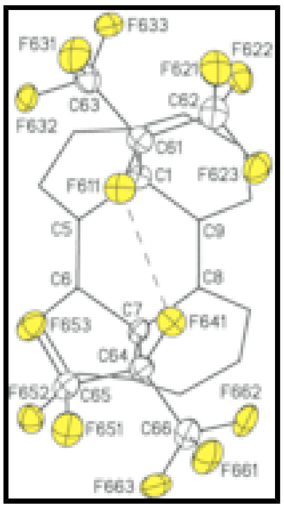

Fig. 2. A portion of the structure of 1,7,16,30,36,47-C_{60}(i-C_3F_7)$_6$ showing one of the three *para*-C_6(C_6(i-C_3F_7)$_2$ hexagons. The F611···F641 distance is 2.653 (3) Å and the F611—C61···C64—F641 torsion angle is 56.4 (3) degrees.

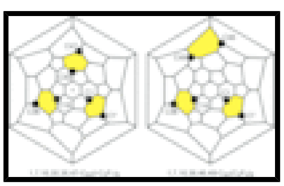

Fig. 3. (Left) Schlegel diagram of 1,7,16,30,36,47-C_{60}(i-C_3F_7)$_6$ showing the IUPAC lowest-locants for the cage carbon atoms to which the i-C_3F_7 groups are attached. The small triangle in the center denotes the molecular C_3 axis. (Right) Schlegel diagram of 1,7,16,36,46,49-C_{60}(C_2F_5)$_6$ showing the IUPAC lowest-locants for the cage carbon atoms to which the C_2F_5 groups are attached.

1,7,16,30,36,47-Hexakis(perfluoroisopropyl)- 1,7,16,30,36,47-hexahydro(C_{60}–I_h)[5,6]fullerene

Crystal data

$C_{78}F_{42}$	F_{000} = 3384
M_r = 1734.78	D_x = 2.071 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation λ = 0.71073 Å
a = 13.5877 (3) Å	Cell parameters from 9868 reflections
b = 31.1809 (7) Å	θ = 2.3–26.4°
c = 13.7240 (3) Å	μ = 0.22 mm^{-1}
β = 106.8730 (10)°	*T* = 100 (1) K
V = 5564.2 (2) Å^3	Plate, red
Z = 4	0.30 × 0.11 × 0.06 mm

Data collection

Bruker Kappa APEX II diffractometer	11386 independent reflections
Radiation source: fine-focus sealed tube	6862 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.083$
$T = 100(1)$ K	$\theta_{max} = 26.4°$
φ and ω scans	$\theta_{min} = 1.7°$
Absorption correction: multi-scan SADABS (Sheldrick, 2003)	$h = -16 \rightarrow 16$
$T_{min} = 0.937$, $T_{max} = 0.988$	$k = -30 \rightarrow 38$
75325 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.052$	$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 5.908P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.53$ e Å^{-3}
11386 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
1081 parameters	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}
C1	0.6333 (3)	0.09622 (11)	0.3518 (3)	0.0163 (8)
C2	0.5209 (3)	0.08797 (11)	0.3546 (2)	0.0144 (7)
C3	0.4709 (3)	0.05947 (11)	0.2768 (3)	0.0160 (8)
C4	0.5354 (3)	0.05404 (11)	0.2077 (3)	0.0169 (8)
C5	0.6268 (2)	0.07914 (11)	0.2442 (3)	0.0150 (7)
C6	0.6666 (2)	0.10025 (11)	0.1759 (3)	0.0147 (7)
C7	0.7238 (2)	0.14363 (11)	0.1977 (3)	0.0150 (7)

C8	0.6891 (2)	0.16512 (11)	0.2821 (3)	0.0178 (8)
C9	0.6495 (2)	0.14421 (11)	0.3495 (2)	0.0158 (8)
C10	0.5857 (3)	0.17500 (11)	0.3876 (3)	0.0180 (8)
C11	0.4969 (3)	0.16276 (11)	0.4074 (2)	0.0175 (8)
C12	0.4641 (3)	0.11791 (11)	0.3891 (2)	0.0149 (7)
C13	0.3558 (3)	0.11734 (11)	0.3545 (2)	0.0163 (8)
C14	0.3077 (3)	0.08904 (11)	0.2773 (3)	0.0157 (8)
C15	0.3641 (3)	0.05823 (11)	0.2413 (2)	0.0159 (8)
C16	0.3059 (3)	0.04325 (11)	0.1323 (3)	0.0163 (8)
C17	0.3756 (3)	0.04820 (10)	0.0645 (3)	0.0145 (7)
C18	0.4894 (3)	0.04859 (11)	0.1061 (3)	0.0174 (8)
C19	0.5305 (3)	0.06950 (11)	0.0348 (3)	0.0151 (7)
C20	0.6163 (2)	0.09619 (11)	0.0695 (3)	0.0134 (7)
C21	0.6188 (2)	0.13636 (11)	0.0195 (3)	0.0154 (8)
C22	0.6725 (3)	0.16713 (12)	0.0947 (3)	0.0193 (8)
C23	0.6362 (3)	0.20845 (12)	0.0888 (3)	0.0199 (8)
C24	0.6283 (3)	0.23087 (11)	0.1806 (3)	0.0188 (8)
C25	0.6531 (2)	0.20971 (11)	0.2729 (3)	0.0168 (8)
C26	0.5899 (3)	0.21553 (11)	0.3394 (3)	0.0161 (7)
C27	0.5024 (3)	0.24146 (11)	0.3119 (3)	0.0163 (8)
C28	0.4110 (2)	0.22896 (11)	0.3369 (3)	0.0153 (7)
C29	0.4088 (3)	0.19032 (11)	0.3833 (2)	0.0163 (8)
C30	0.3112 (3)	0.16225 (11)	0.3666 (3)	0.0171 (8)
C31	0.2378 (2)	0.17523 (11)	0.2647 (2)	0.0138 (7)
C32	0.1883 (3)	0.14339 (11)	0.1858 (3)	0.0173 (8)
C33	0.2200 (2)	0.10183 (11)	0.1909 (3)	0.0161 (8)
C34	0.2238 (3)	0.07873 (11)	0.1017 (3)	0.0172 (8)
C35	0.1972 (2)	0.09910 (11)	0.0083 (3)	0.0167 (8)
C36	0.2458 (3)	0.08928 (11)	−0.0779 (2)	0.0156 (7)
C37	0.3495 (3)	0.06796 (11)	−0.0272 (3)	0.0150 (7)
C38	0.4439 (2)	0.08247 (11)	−0.0490 (2)	0.0147 (7)
C39	0.4465 (3)	0.12087 (11)	−0.0974 (2)	0.0156 (7)
C40	0.5349 (3)	0.14857 (12)	−0.0627 (3)	0.0195 (8)
C41	0.4995 (3)	0.19229 (12)	−0.0699 (3)	0.0187 (8)
C42	0.5499 (3)	0.22147 (11)	0.0046 (3)	0.0197 (8)
C43	0.4903 (3)	0.25257 (11)	0.0435 (3)	0.0207 (8)
C44	0.5381 (3)	0.25804 (11)	0.1508 (3)	0.0204 (8)
C45	0.4762 (3)	0.26333 (11)	0.2159 (3)	0.0184 (8)
C46	0.3656 (3)	0.26451 (11)	0.1767 (3)	0.0173 (8)
C47	0.3162 (3)	0.24977 (11)	0.2598 (3)	0.0155 (7)
C48	0.2406 (2)	0.21367 (11)	0.2182 (3)	0.0140 (7)
C49	0.1927 (2)	0.20879 (11)	0.1084 (3)	0.0146 (7)
C50	0.1596 (2)	0.16488 (11)	0.0896 (3)	0.0150 (7)
C51	0.1673 (2)	0.14345 (11)	0.0031 (3)	0.0157 (8)
C52	0.2074 (3)	0.16566 (12)	−0.0691 (3)	0.0184 (8)
C53	0.2647 (3)	0.13527 (11)	−0.1106 (2)	0.0185 (8)
C54	0.3546 (3)	0.14835 (12)	−0.1266 (2)	0.0189 (8)
C55	0.3890 (3)	0.19262 (11)	−0.1083 (2)	0.0170 (8)
C56	0.3325 (3)	0.22183 (11)	−0.0711 (3)	0.0179 (8)

C57	0.3840 (3)	0.25256 (11)	0.0060 (3)	0.0207 (8)
C58	0.3209 (3)	0.25820 (11)	0.0750 (3)	0.0211 (8)
C59	0.2307 (2)	0.23014 (11)	0.0393 (3)	0.0163 (8)
C60	0.2390 (3)	0.20813 (12)	−0.0511 (3)	0.0191 (8)
C61	0.7163 (3)	0.07237 (12)	0.4393 (3)	0.0211 (8)
C62	0.7457 (3)	0.09788 (13)	0.5399 (3)	0.0258 (9)
C63	0.6866 (3)	0.02601 (13)	0.4587 (3)	0.0259 (9)
C64	0.8445 (3)	0.14036 (12)	0.2256 (3)	0.0198 (8)
C65	0.8817 (3)	0.10239 (12)	0.1730 (3)	0.0231 (9)
C66	0.8961 (3)	0.18259 (13)	0.2059 (3)	0.0254 (9)
C71	0.2632 (3)	−0.00448 (12)	0.1279 (3)	0.0217 (8)
C72	0.3421 (3)	−0.03605 (11)	0.1916 (3)	0.0226 (8)
C73	0.1612 (3)	−0.00728 (13)	0.1544 (3)	0.0285 (9)
C74	0.1741 (3)	0.06129 (12)	−0.1656 (3)	0.0195 (8)
C75	0.0790 (3)	0.08585 (13)	−0.2320 (3)	0.0247 (9)
C76	0.2324 (3)	0.04054 (13)	−0.2341 (3)	0.0248 (9)
C81	0.2564 (3)	0.16416 (12)	0.4551 (3)	0.0216 (8)
C82	0.1908 (3)	0.12459 (12)	0.4584 (3)	0.0225 (9)
C83	0.3326 (3)	0.17322 (13)	0.5605 (3)	0.0294 (10)
C84	0.2669 (3)	0.28753 (11)	0.3065 (3)	0.0181 (8)
C85	0.3356 (3)	0.32729 (11)	0.3346 (3)	0.0212 (8)
C86	0.1592 (3)	0.29994 (11)	0.2378 (3)	0.0209 (8)
F611	0.80470 (15)	0.06890 (7)	0.41034 (16)	0.0287 (5)
F621	0.80504 (17)	0.07521 (7)	0.61711 (16)	0.0321 (5)
F622	0.66226 (16)	0.10955 (7)	0.56547 (15)	0.0297 (5)
F623	0.79801 (17)	0.13319 (7)	0.53091 (16)	0.0346 (6)
F631	0.76810 (18)	0.00455 (7)	0.51475 (17)	0.0362 (6)
F632	0.64986 (17)	0.00433 (7)	0.37240 (16)	0.0279 (5)
F633	0.61469 (17)	0.02545 (7)	0.50738 (16)	0.0311 (5)
F641	0.88280 (14)	0.13275 (7)	0.32809 (15)	0.0260 (5)
F651	0.98236 (15)	0.10383 (7)	0.18588 (17)	0.0319 (5)
F652	0.83554 (15)	0.10227 (7)	0.07281 (16)	0.0285 (5)
F653	0.86110 (15)	0.06529 (7)	0.21100 (17)	0.0292 (5)
F661	0.99620 (15)	0.18263 (7)	0.25622 (18)	0.0338 (6)
F662	0.85483 (16)	0.21631 (7)	0.23915 (18)	0.0337 (6)
F663	0.88577 (16)	0.18792 (7)	0.10707 (17)	0.0329 (6)
F711	0.24276 (17)	−0.01883 (7)	0.02927 (15)	0.0283 (5)
F721	0.31623 (18)	−0.07650 (7)	0.16486 (18)	0.0360 (6)
F722	0.34970 (18)	−0.03225 (7)	0.29069 (16)	0.0329 (6)
F723	0.43549 (16)	−0.02996 (7)	0.18104 (17)	0.0293 (5)
F731	0.13276 (18)	−0.04834 (7)	0.15836 (18)	0.0378 (6)
F732	0.08582 (16)	0.01214 (8)	0.08282 (19)	0.0375 (6)
F733	0.16705 (17)	0.01098 (7)	0.24359 (18)	0.0346 (6)
F741	0.13473 (16)	0.02827 (6)	−0.12255 (15)	0.0256 (5)
F751	0.01111 (16)	0.05892 (8)	−0.29029 (17)	0.0379 (6)
F752	0.10518 (17)	0.11463 (8)	−0.29092 (17)	0.0387 (6)
F753	0.03068 (15)	0.10617 (7)	−0.17345 (16)	0.0321 (6)
F761	0.16948 (16)	0.02142 (8)	−0.31524 (16)	0.0341 (6)
F762	0.29605 (17)	0.01033 (7)	−0.18262 (17)	0.0339 (6)

F763	0.28763 (17)	0.06945 (7)	−0.26690 (16)	0.0328 (6)
F811	0.18824 (16)	0.19794 (7)	0.43554 (16)	0.0280 (5)
F821	0.12408 (18)	0.13216 (8)	0.51088 (18)	0.0393 (6)
F822	0.25071 (18)	0.09149 (7)	0.50469 (17)	0.0365 (6)
F823	0.13816 (16)	0.11148 (7)	0.36677 (16)	0.0303 (5)
F831	0.28580 (18)	0.17033 (8)	0.63388 (16)	0.0405 (6)
F832	0.36870 (18)	0.21329 (8)	0.56370 (17)	0.0373 (6)
F833	0.41085 (17)	0.14643 (8)	0.58299 (16)	0.0351 (6)
F841	0.25277 (15)	0.27327 (6)	0.39657 (15)	0.0236 (5)
F851	0.30260 (16)	0.35327 (7)	0.39559 (16)	0.0300 (5)
F852	0.33652 (16)	0.34939 (6)	0.25144 (16)	0.0283 (5)
F853	0.43237 (15)	0.31704 (6)	0.38514 (16)	0.0261 (5)
F861	0.09038 (15)	0.26999 (7)	0.24179 (17)	0.0275 (5)
F862	0.15848 (16)	0.30427 (7)	0.14115 (15)	0.0259 (5)
F863	0.12588 (16)	0.33685 (6)	0.26575 (16)	0.0269 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0123 (17)	0.0181 (19)	0.0184 (19)	0.0023 (15)	0.0042 (15)	0.0041 (15)
C2	0.0154 (18)	0.0159 (19)	0.0111 (17)	0.0027 (15)	0.0024 (15)	0.0079 (14)
C3	0.0239 (19)	0.0095 (18)	0.0160 (18)	0.0009 (15)	0.0081 (16)	0.0061 (14)
C4	0.0181 (19)	0.0107 (18)	0.0206 (19)	0.0038 (15)	0.0036 (16)	0.0026 (15)
C5	0.0118 (17)	0.0135 (18)	0.0178 (18)	0.0064 (14)	0.0013 (15)	−0.0005 (15)
C6	0.0079 (16)	0.0154 (19)	0.0203 (19)	0.0053 (14)	0.0034 (15)	−0.0027 (15)
C7	0.0106 (17)	0.0156 (19)	0.0193 (18)	−0.0003 (14)	0.0050 (15)	0.0003 (15)
C8	0.0086 (17)	0.022 (2)	0.0202 (19)	−0.0038 (15)	−0.0005 (15)	−0.0040 (16)
C9	0.0100 (17)	0.023 (2)	0.0100 (17)	0.0020 (15)	−0.0034 (14)	−0.0027 (15)
C10	0.0158 (18)	0.022 (2)	0.0115 (17)	−0.0016 (15)	−0.0034 (15)	−0.0048 (15)
C11	0.023 (2)	0.019 (2)	0.0083 (17)	−0.0006 (16)	0.0013 (15)	−0.0017 (14)
C12	0.0195 (18)	0.0172 (19)	0.0066 (16)	−0.0018 (15)	0.0014 (14)	0.0013 (14)
C13	0.0220 (19)	0.0176 (19)	0.0129 (17)	0.0055 (15)	0.0107 (16)	0.0062 (15)
C14	0.0124 (17)	0.0183 (19)	0.0172 (18)	−0.0022 (15)	0.0056 (15)	0.0041 (15)
C15	0.023 (2)	0.0115 (18)	0.0119 (17)	−0.0058 (15)	0.0041 (15)	0.0024 (14)
C16	0.0168 (18)	0.0145 (19)	0.0167 (18)	−0.0056 (15)	0.0036 (15)	−0.0005 (15)
C17	0.0170 (18)	0.0079 (18)	0.0155 (18)	−0.0011 (14)	−0.0001 (15)	−0.0046 (14)
C18	0.0208 (19)	0.0123 (18)	0.0205 (19)	0.0053 (15)	0.0081 (16)	−0.0024 (15)
C19	0.0173 (18)	0.0153 (19)	0.0157 (18)	0.0026 (15)	0.0093 (15)	−0.0031 (15)
C20	0.0090 (16)	0.0149 (19)	0.0189 (18)	0.0030 (14)	0.0081 (15)	−0.0034 (15)
C21	0.0127 (17)	0.0175 (19)	0.0189 (19)	0.0000 (14)	0.0093 (16)	−0.0021 (15)
C22	0.0129 (18)	0.024 (2)	0.025 (2)	−0.0013 (16)	0.0110 (16)	0.0054 (16)
C23	0.0145 (18)	0.020 (2)	0.029 (2)	−0.0098 (16)	0.0122 (17)	0.0005 (16)
C24	0.0181 (19)	0.020 (2)	0.0216 (19)	−0.0114 (16)	0.0101 (16)	−0.0083 (16)
C25	0.0086 (17)	0.0142 (19)	0.026 (2)	−0.0047 (14)	0.0033 (15)	−0.0061 (16)
C26	0.0147 (18)	0.0172 (19)	0.0146 (18)	−0.0059 (15)	0.0013 (15)	−0.0045 (15)
C27	0.0188 (19)	0.0124 (18)	0.0172 (18)	−0.0014 (15)	0.0043 (15)	−0.0075 (15)
C28	0.0143 (18)	0.0137 (18)	0.0178 (18)	−0.0010 (14)	0.0045 (15)	−0.0076 (15)
C29	0.0211 (19)	0.0179 (19)	0.0094 (17)	0.0023 (15)	0.0038 (15)	−0.0048 (14)

C30	0.0214 (19)	0.0173 (19)	0.0137 (18)	0.0006 (15)	0.0068 (16)	0.0003 (15)
C31	0.0101 (17)	0.0191 (19)	0.0156 (17)	0.0009 (14)	0.0091 (15)	−0.0009 (15)
C32	0.0123 (18)	0.019 (2)	0.025 (2)	−0.0022 (15)	0.0118 (16)	−0.0007 (16)
C33	0.0118 (17)	0.020 (2)	0.0177 (18)	−0.0048 (15)	0.0062 (15)	0.0000 (15)
C34	0.0111 (17)	0.022 (2)	0.0186 (19)	−0.0094 (15)	0.0046 (15)	−0.0057 (15)
C35	0.0053 (16)	0.025 (2)	0.0175 (18)	−0.0021 (15)	−0.0004 (14)	−0.0049 (16)
C36	0.0158 (18)	0.0184 (19)	0.0103 (17)	0.0018 (15)	0.0001 (15)	−0.0031 (14)
C37	0.0146 (17)	0.0142 (18)	0.0150 (18)	−0.0017 (15)	0.0022 (15)	−0.0069 (15)
C38	0.0154 (18)	0.0157 (19)	0.0137 (17)	0.0006 (15)	0.0051 (15)	−0.0082 (14)
C39	0.0198 (19)	0.021 (2)	0.0064 (16)	0.0041 (16)	0.0044 (15)	0.0016 (14)
C40	0.024 (2)	0.024 (2)	0.0154 (18)	0.0025 (17)	0.0135 (16)	0.0016 (16)
C41	0.021 (2)	0.022 (2)	0.0162 (19)	0.0017 (16)	0.0115 (16)	0.0084 (16)
C42	0.0202 (19)	0.021 (2)	0.022 (2)	−0.0029 (16)	0.0120 (17)	0.0074 (16)
C43	0.031 (2)	0.0118 (19)	0.0204 (19)	−0.0043 (16)	0.0095 (17)	0.0041 (15)
C44	0.026 (2)	0.0093 (19)	0.025 (2)	−0.0050 (16)	0.0061 (17)	0.0026 (15)
C45	0.0211 (19)	0.0087 (18)	0.023 (2)	−0.0020 (15)	0.0029 (16)	−0.0043 (15)
C46	0.024 (2)	0.0072 (18)	0.023 (2)	0.0025 (15)	0.0107 (17)	−0.0003 (15)
C47	0.0211 (19)	0.0120 (18)	0.0151 (18)	0.0007 (15)	0.0077 (16)	−0.0013 (14)
C48	0.0126 (17)	0.0131 (18)	0.0178 (18)	0.0022 (14)	0.0070 (15)	−0.0034 (15)
C49	0.0097 (17)	0.0147 (19)	0.0193 (18)	0.0053 (14)	0.0038 (15)	0.0000 (15)
C50	0.0074 (16)	0.021 (2)	0.0165 (18)	0.0023 (15)	0.0032 (14)	−0.0002 (15)
C51	0.0054 (16)	0.022 (2)	0.0154 (18)	0.0025 (14)	−0.0030 (14)	−0.0027 (15)
C52	0.0147 (18)	0.024 (2)	0.0130 (18)	0.0082 (16)	−0.0016 (15)	0.0008 (15)
C53	0.023 (2)	0.023 (2)	0.0067 (17)	0.0010 (16)	−0.0007 (15)	−0.0005 (15)
C54	0.026 (2)	0.026 (2)	0.0050 (16)	0.0059 (17)	0.0046 (15)	0.0024 (15)
C55	0.023 (2)	0.018 (2)	0.0106 (17)	0.0008 (15)	0.0066 (16)	0.0055 (15)
C56	0.0178 (18)	0.022 (2)	0.0140 (18)	0.0077 (16)	0.0048 (15)	0.0105 (15)
C57	0.030 (2)	0.0150 (19)	0.0194 (19)	0.0047 (16)	0.0108 (17)	0.0090 (16)
C58	0.025 (2)	0.0132 (19)	0.026 (2)	0.0069 (16)	0.0097 (18)	0.0087 (16)
C59	0.0111 (17)	0.0121 (18)	0.0239 (19)	0.0076 (14)	0.0021 (15)	0.0063 (15)
C60	0.0173 (18)	0.024 (2)	0.0144 (18)	0.0109 (16)	0.0025 (15)	0.0097 (16)
C61	0.0183 (19)	0.024 (2)	0.021 (2)	0.0029 (16)	0.0063 (16)	0.0005 (16)
C62	0.026 (2)	0.027 (2)	0.020 (2)	0.0042 (18)	−0.0018 (18)	0.0036 (17)
C63	0.029 (2)	0.029 (2)	0.017 (2)	0.0105 (18)	0.0011 (18)	0.0007 (17)
C64	0.0115 (18)	0.025 (2)	0.022 (2)	−0.0018 (16)	0.0027 (16)	0.0006 (16)
C65	0.0127 (19)	0.025 (2)	0.031 (2)	−0.0003 (16)	0.0068 (17)	0.0008 (18)
C66	0.0089 (19)	0.027 (2)	0.039 (2)	−0.0003 (16)	0.0058 (18)	−0.0075 (19)
C71	0.025 (2)	0.020 (2)	0.0181 (19)	−0.0074 (16)	0.0038 (17)	−0.0041 (16)
C72	0.029 (2)	0.0117 (19)	0.028 (2)	−0.0050 (16)	0.0106 (18)	−0.0009 (16)
C73	0.030 (2)	0.021 (2)	0.033 (2)	−0.0079 (18)	0.007 (2)	−0.0022 (18)
C74	0.0164 (18)	0.024 (2)	0.0154 (18)	−0.0002 (16)	−0.0002 (16)	−0.0021 (16)
C75	0.020 (2)	0.033 (2)	0.0170 (19)	0.0010 (18)	−0.0022 (17)	−0.0077 (18)
C76	0.019 (2)	0.034 (2)	0.018 (2)	−0.0015 (18)	−0.0007 (17)	−0.0109 (18)
C81	0.025 (2)	0.021 (2)	0.021 (2)	0.0051 (17)	0.0096 (17)	0.0022 (16)
C82	0.025 (2)	0.028 (2)	0.019 (2)	−0.0026 (18)	0.0130 (18)	−0.0038 (17)
C83	0.036 (2)	0.032 (3)	0.022 (2)	−0.004 (2)	0.0126 (19)	0.0003 (18)
C84	0.0216 (19)	0.018 (2)	0.0172 (18)	0.0021 (15)	0.0092 (16)	0.0009 (15)
C85	0.023 (2)	0.016 (2)	0.024 (2)	0.0028 (16)	0.0066 (17)	−0.0043 (16)
C86	0.024 (2)	0.016 (2)	0.025 (2)	−0.0002 (16)	0.0099 (17)	−0.0039 (16)

F611	0.0200 (11)	0.0358 (13)	0.0301 (12)	0.0073 (10)	0.0070 (10)	0.0060 (10)
F621	0.0306 (12)	0.0367 (14)	0.0209 (12)	0.0071 (11)	−0.0052 (10)	0.0043 (10)
F622	0.0281 (12)	0.0372 (14)	0.0202 (11)	0.0071 (10)	0.0015 (10)	−0.0026 (10)
F623	0.0331 (13)	0.0341 (14)	0.0276 (13)	−0.0109 (11)	−0.0053 (11)	−0.0001 (11)
F631	0.0420 (14)	0.0280 (13)	0.0315 (13)	0.0137 (11)	−0.0007 (12)	0.0081 (11)
F632	0.0371 (13)	0.0205 (12)	0.0243 (12)	0.0041 (10)	0.0058 (11)	0.0012 (10)
F633	0.0400 (13)	0.0303 (13)	0.0266 (12)	0.0004 (11)	0.0154 (11)	0.0053 (10)
F641	0.0146 (11)	0.0383 (14)	0.0222 (12)	0.0002 (9)	0.0008 (9)	−0.0003 (10)
F651	0.0132 (11)	0.0373 (14)	0.0467 (14)	−0.0006 (10)	0.0109 (10)	−0.0078 (11)
F652	0.0221 (11)	0.0363 (14)	0.0283 (13)	0.0009 (10)	0.0092 (10)	−0.0067 (10)
F653	0.0250 (12)	0.0197 (12)	0.0454 (14)	0.0039 (9)	0.0143 (11)	0.0034 (10)
F661	0.0159 (12)	0.0328 (14)	0.0525 (15)	−0.0077 (10)	0.0094 (11)	−0.0083 (11)
F662	0.0245 (12)	0.0230 (12)	0.0571 (16)	−0.0053 (10)	0.0173 (12)	−0.0102 (11)
F663	0.0309 (13)	0.0344 (14)	0.0383 (14)	−0.0074 (10)	0.0175 (11)	0.0049 (11)
F711	0.0371 (13)	0.0231 (12)	0.0223 (12)	−0.0101 (10)	0.0048 (10)	−0.0059 (9)
F721	0.0432 (14)	0.0156 (12)	0.0469 (15)	−0.0046 (10)	0.0093 (12)	0.0005 (11)
F722	0.0432 (14)	0.0337 (14)	0.0220 (12)	−0.0040 (11)	0.0099 (11)	0.0048 (10)
F723	0.0272 (12)	0.0241 (13)	0.0391 (14)	0.0030 (10)	0.0134 (11)	0.0051 (10)
F731	0.0400 (14)	0.0268 (14)	0.0492 (15)	−0.0157 (11)	0.0171 (12)	−0.0023 (11)
F732	0.0197 (12)	0.0390 (15)	0.0492 (15)	−0.0056 (11)	0.0027 (12)	0.0031 (12)
F733	0.0382 (14)	0.0336 (14)	0.0397 (14)	−0.0110 (11)	0.0236 (12)	−0.0079 (11)
F741	0.0287 (12)	0.0251 (12)	0.0215 (11)	−0.0066 (10)	0.0049 (10)	−0.0028 (9)
F751	0.0223 (12)	0.0489 (16)	0.0317 (13)	0.0044 (11)	−0.0090 (11)	−0.0186 (12)
F752	0.0363 (14)	0.0479 (16)	0.0265 (13)	0.0073 (12)	0.0005 (11)	0.0132 (12)
F753	0.0176 (11)	0.0456 (15)	0.0285 (13)	0.0083 (10)	−0.0006 (10)	−0.0128 (11)
F761	0.0277 (12)	0.0466 (15)	0.0239 (12)	−0.0016 (11)	0.0011 (10)	−0.0193 (11)
F762	0.0309 (13)	0.0338 (14)	0.0301 (13)	0.0139 (11)	−0.0021 (11)	−0.0123 (11)
F763	0.0332 (13)	0.0409 (14)	0.0286 (13)	−0.0032 (11)	0.0157 (11)	−0.0089 (11)
F811	0.0349 (13)	0.0272 (13)	0.0270 (12)	0.0076 (10)	0.0170 (11)	0.0010 (10)
F821	0.0420 (14)	0.0488 (16)	0.0375 (14)	−0.0124 (12)	0.0278 (12)	−0.0071 (12)
F822	0.0494 (15)	0.0276 (13)	0.0347 (13)	−0.0008 (12)	0.0158 (12)	0.0092 (11)
F823	0.0294 (12)	0.0375 (14)	0.0265 (13)	−0.0118 (11)	0.0121 (10)	−0.0056 (10)
F831	0.0485 (15)	0.0584 (17)	0.0203 (12)	−0.0078 (13)	0.0192 (12)	−0.0047 (11)
F832	0.0469 (15)	0.0375 (15)	0.0315 (13)	−0.0169 (12)	0.0178 (12)	−0.0144 (11)
F833	0.0357 (14)	0.0480 (15)	0.0183 (12)	0.0052 (12)	0.0028 (11)	0.0016 (11)
F841	0.0324 (12)	0.0235 (12)	0.0191 (11)	0.0045 (10)	0.0139 (10)	0.0000 (9)
F851	0.0353 (13)	0.0197 (12)	0.0338 (13)	0.0046 (10)	0.0082 (11)	−0.0101 (10)
F852	0.0355 (13)	0.0193 (12)	0.0283 (12)	−0.0048 (10)	0.0066 (11)	0.0032 (10)
F853	0.0234 (12)	0.0198 (12)	0.0306 (12)	0.0013 (9)	0.0006 (10)	−0.0078 (10)
F861	0.0224 (11)	0.0235 (12)	0.0391 (13)	−0.0005 (9)	0.0128 (10)	−0.0019 (10)
F862	0.0289 (12)	0.0277 (13)	0.0211 (12)	0.0069 (10)	0.0073 (10)	−0.0001 (9)
F863	0.0280 (12)	0.0212 (12)	0.0322 (12)	0.0078 (10)	0.0100 (10)	−0.0058 (10)

Geometric parameters (Å, °)

C1—C9	1.514 (5)	C44—C45	1.404 (5)
C1—C5	1.548 (5)	C45—C46	1.442 (5)
C1—C2	1.559 (4)	C46—C58	1.365 (5)
C1—C61	1.575 (5)	C46—C47	1.552 (5)

C2—C12	1.380 (5)	C47—C48	1.519 (5)
C2—C3	1.404 (5)	C47—C84	1.579 (5)
C3—C15	1.391 (5)	C48—C49	1.465 (5)
C3—C4	1.476 (5)	C49—C59	1.376 (5)
C4—C18	1.364 (5)	C49—C50	1.441 (5)
C4—C5	1.430 (5)	C50—C51	1.392 (5)
C5—C6	1.378 (5)	C51—C52	1.439 (5)
C6—C20	1.426 (5)	C52—C60	1.392 (5)
C6—C7	1.545 (5)	C52—C53	1.445 (5)
C7—C8	1.526 (5)	C53—C54	1.365 (5)
C7—C22	1.565 (5)	C54—C55	1.456 (5)
C7—C64	1.577 (5)	C55—C56	1.380 (5)
C8—C9	1.363 (5)	C56—C60	1.440 (5)
C8—C25	1.467 (5)	C56—C57	1.449 (5)
C9—C10	1.486 (5)	C57—C58	1.461 (5)
C10—C11	1.367 (5)	C58—C59	1.468 (5)
C10—C26	1.435 (5)	C59—C60	1.451 (5)
C11—C29	1.432 (5)	C61—F611	1.374 (4)
C11—C12	1.467 (5)	C61—C62	1.542 (5)
C12—C13	1.408 (5)	C61—C63	1.545 (5)
C13—C14	1.388 (5)	C62—F622	1.332 (4)
C13—C30	1.554 (5)	C62—F621	1.333 (4)
C14—C15	1.406 (5)	C62—F623	1.335 (4)
C14—C33	1.472 (5)	C63—F632	1.329 (4)
C15—C16	1.547 (5)	C63—F631	1.331 (4)
C16—C17	1.516 (5)	C63—F633	1.334 (4)
C16—C34	1.541 (5)	C64—F641	1.372 (4)
C16—C71	1.592 (5)	C64—C65	1.545 (5)
C17—C37	1.353 (5)	C64—C66	1.551 (5)
C17—C18	1.484 (5)	C65—F651	1.329 (4)
C18—C19	1.418 (5)	C65—F653	1.331 (4)
C19—C20	1.398 (5)	C65—F652	1.335 (4)
C19—C38	1.444 (5)	C66—F663	1.332 (4)
C20—C21	1.433 (5)	C66—F662	1.333 (4)
C21—C40	1.405 (5)	C66—F661	1.335 (4)
C21—C22	1.443 (5)	C71—F711	1.375 (4)
C22—C23	1.374 (5)	C71—C72	1.529 (5)
C23—C42	1.445 (5)	C71—C73	1.535 (5)
C23—C24	1.473 (5)	C72—F721	1.332 (4)
C24—C25	1.380 (5)	C72—F723	1.332 (4)
C24—C44	1.448 (5)	C72—F722	1.338 (4)
C25—C26	1.435 (4)	C73—F733	1.332 (4)
C26—C27	1.396 (5)	C73—F732	1.340 (5)
C27—C45	1.433 (5)	C73—F731	1.343 (4)
C27—C28	1.435 (5)	C74—F741	1.371 (4)
C28—C29	1.367 (5)	C74—C76	1.537 (5)
C28—C47	1.552 (5)	C74—C75	1.550 (5)
C29—C30	1.550 (5)	C75—F752	1.324 (4)
C30—C31	1.517 (5)	C75—F751	1.330 (4)

C30—C81	1.599 (5)	C75—F753	1.336 (4)
C31—C48	1.364 (5)	C76—F763	1.332 (4)
C31—C32	1.479 (5)	C76—F761	1.332 (4)
C32—C33	1.361 (5)	C76—F762	1.334 (4)
C32—C50	1.430 (5)	C81—F811	1.376 (4)
C33—C34	1.435 (5)	C81—C82	1.530 (5)
C34—C35	1.381 (5)	C81—C83	1.541 (5)
C35—C51	1.437 (5)	C82—F823	1.318 (4)
C35—C36	1.543 (4)	C82—F821	1.333 (4)
C36—C37	1.531 (5)	C82—F822	1.353 (4)
C36—C53	1.546 (5)	C83—F833	1.316 (5)
C36—C74	1.574 (5)	C83—F832	1.338 (5)
C37—C38	1.469 (4)	C83—F831	1.341 (4)
C38—C39	1.375 (5)	C84—F841	1.378 (4)
C39—C40	1.444 (5)	C84—C85	1.532 (5)
C39—C54	1.471 (5)	C84—C86	1.543 (5)
C40—C41	1.439 (5)	C85—F851	1.332 (4)
C41—C42	1.391 (5)	C85—F853	1.335 (4)
C41—C55	1.440 (5)	C85—F852	1.336 (4)
C42—C43	1.461 (5)	C86—F862	1.330 (4)
C43—C57	1.385 (5)	C86—F863	1.333 (4)
C43—C44	1.436 (5)	C86—F861	1.334 (4)

C9—C1—C5	106.8 (3)	C48—C47—C28	106.4 (3)
C9—C1—C2	108.2 (3)	C48—C47—C46	109.4 (3)
C5—C1—C2	100.5 (3)	C28—C47—C46	100.0 (3)
C9—C1—C61	114.0 (3)	C48—C47—C84	112.7 (3)
C5—C1—C61	113.2 (3)	C28—C47—C84	113.6 (3)
C2—C1—C61	113.1 (3)	C46—C47—C84	113.7 (3)
C12—C2—C3	119.6 (3)	C31—C48—C49	109.0 (3)
C12—C2—C1	123.1 (3)	C31—C48—C47	125.7 (3)
C3—C2—C1	110.3 (3)	C49—C48—C47	120.9 (3)
C15—C3—C2	120.7 (3)	C59—C49—C50	119.8 (3)
C15—C3—C4	121.7 (3)	C59—C49—C48	121.0 (3)
C2—C3—C4	108.3 (3)	C50—C49—C48	107.8 (3)
C18—C4—C5	121.3 (3)	C51—C50—C32	119.6 (3)
C18—C4—C3	119.3 (3)	C51—C50—C49	120.8 (3)
C5—C4—C3	109.3 (3)	C32—C50—C49	107.0 (3)
C6—C5—C4	119.7 (3)	C50—C51—C35	120.7 (3)
C6—C5—C1	124.1 (3)	C50—C51—C52	119.6 (3)
C4—C5—C1	109.0 (3)	C35—C51—C52	109.8 (3)
C5—C6—C20	119.2 (3)	C60—C52—C51	119.7 (3)
C5—C6—C7	124.1 (3)	C60—C52—C53	121.3 (3)
C20—C6—C7	109.9 (3)	C51—C52—C53	108.1 (3)
C8—C7—C6	106.5 (3)	C54—C53—C52	118.5 (3)
C8—C7—C22	109.0 (3)	C54—C53—C36	123.8 (3)
C6—C7—C22	99.7 (3)	C52—C53—C36	109.9 (3)
C8—C7—C64	111.9 (3)	C53—C54—C55	120.8 (3)
C6—C7—C64	114.8 (3)	C53—C54—C39	120.7 (3)
C22—C7—C64	114.1 (3)	C55—C54—C39	107.5 (3)

C9—C8—C25	108.9 (3)	C56—C55—C41	120.1 (3)
C9—C8—C7	125.1 (3)	C56—C55—C54	120.3 (3)
C25—C8—C7	121.3 (3)	C41—C55—C54	107.8 (3)
C8—C9—C10	108.3 (3)	C55—C56—C60	119.3 (3)
C8—C9—C1	125.1 (3)	C55—C56—C57	120.3 (3)
C10—C9—C1	121.9 (3)	C60—C56—C57	108.8 (3)
C11—C10—C26	119.5 (3)	C43—C57—C56	120.1 (3)
C11—C10—C9	121.9 (3)	C43—C57—C58	120.3 (3)
C26—C10—C9	107.6 (3)	C56—C57—C58	107.6 (3)
C10—C11—C29	120.9 (3)	C46—C58—C57	120.6 (3)
C10—C11—C12	118.3 (3)	C46—C58—C59	120.5 (3)
C29—C11—C12	109.9 (3)	C57—C58—C59	107.6 (3)
C2—C12—C13	120.7 (3)	C49—C59—C60	119.9 (3)
C2—C12—C11	122.1 (3)	C49—C59—C58	120.1 (3)
C13—C12—C11	107.8 (3)	C60—C59—C58	107.6 (3)
C14—C13—C12	118.7 (3)	C52—C60—C56	119.5 (3)
C14—C13—C30	122.8 (3)	C52—C60—C59	120.3 (3)
C12—C13—C30	110.8 (3)	C56—C60—C59	108.3 (3)
C13—C14—C15	121.2 (3)	F611—C61—C62	106.1 (3)
C13—C14—C33	122.4 (3)	F611—C61—C63	105.7 (3)
C15—C14—C33	107.4 (3)	C62—C61—C63	109.9 (3)
C3—C15—C14	118.5 (3)	F611—C61—C1	108.0 (3)
C3—C15—C16	122.4 (3)	C62—C61—C1	112.4 (3)
C14—C15—C16	111.6 (3)	C63—C61—C1	114.1 (3)
C17—C16—C34	107.0 (3)	F622—C62—F621	107.5 (3)
C17—C16—C15	109.1 (3)	F622—C62—F623	108.4 (3)
C34—C16—C15	100.0 (3)	F621—C62—F623	107.2 (3)
C17—C16—C71	111.0 (3)	F622—C62—C61	111.0 (3)
C34—C16—C71	115.7 (3)	F621—C62—C61	112.2 (3)
C15—C16—C71	113.4 (3)	F623—C62—C61	110.4 (3)
C37—C17—C18	108.4 (3)	F632—C63—F631	107.1 (3)
C37—C17—C16	125.1 (3)	F632—C63—F633	107.4 (3)
C18—C17—C16	122.1 (3)	F631—C63—F633	108.2 (3)
C4—C18—C19	119.5 (3)	F632—C63—C61	111.8 (3)
C4—C18—C17	120.8 (3)	F631—C63—C61	110.8 (3)
C19—C18—C17	108.3 (3)	F633—C63—C61	111.4 (3)
C20—C19—C18	119.7 (3)	F641—C64—C65	105.6 (3)
C20—C19—C38	120.7 (3)	F641—C64—C66	105.6 (3)
C18—C19—C38	106.5 (3)	C65—C64—C66	110.1 (3)
C19—C20—C6	120.4 (3)	F641—C64—C7	108.5 (3)
C19—C20—C21	119.4 (3)	C65—C64—C7	113.2 (3)
C6—C20—C21	109.9 (3)	C66—C64—C7	113.2 (3)
C40—C21—C20	119.6 (3)	F651—C65—F653	107.6 (3)
C40—C21—C22	121.2 (3)	F651—C65—F652	107.1 (3)
C20—C21—C22	108.4 (3)	F653—C65—F652	108.2 (3)
C23—C22—C21	118.9 (3)	F651—C65—C64	112.0 (3)
C23—C22—C7	123.5 (3)	F653—C65—C64	110.4 (3)
C21—C22—C7	109.6 (3)	F652—C65—C64	111.3 (3)
C22—C23—C42	120.4 (3)	F663—C66—F662	108.7 (3)

C22—C23—C24	120.5 (3)	F663—C66—F661	108.5 (3)
C42—C23—C24	107.9 (3)	F662—C66—F661	106.8 (3)
C25—C24—C44	120.0 (3)	F663—C66—C64	111.3 (3)
C25—C24—C23	120.0 (3)	F662—C66—C64	110.7 (3)
C44—C24—C23	107.6 (3)	F661—C66—C64	110.7 (3)
C24—C25—C26	119.4 (3)	F711—C71—C72	105.2 (3)
C24—C25—C8	121.2 (3)	F711—C71—C73	106.0 (3)
C26—C25—C8	108.1 (3)	C72—C71—C73	111.1 (3)
C27—C26—C10	119.4 (3)	F711—C71—C16	108.0 (3)
C27—C26—C25	121.4 (3)	C72—C71—C16	113.2 (3)
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C26—C27—C45	119.4 (3)	F721—C72—F723	106.7 (3)
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C28—C29—C30	124.2 (3)	F733—C73—F731	108.1 (3)
C11—C29—C30	108.5 (3)	F732—C73—F731	107.0 (3)
C31—C30—C29	106.9 (3)	F733—C73—C71	112.1 (3)
C31—C30—C13	108.4 (3)	F732—C73—C71	110.6 (3)
C29—C30—C13	100.4 (3)	F731—C73—C71	110.7 (3)
C31—C30—C81	111.3 (3)	F741—C74—C76	106.4 (3)
C29—C30—C81	115.7 (3)	F741—C74—C75	105.1 (3)
C13—C30—C81	113.4 (3)	C76—C74—C75	109.8 (3)
C48—C31—C32	108.4 (3)	F741—C74—C36	108.6 (3)
C48—C31—C30	124.4 (3)	C76—C74—C36	112.8 (3)
C32—C31—C30	122.2 (3)	C75—C74—C36	113.6 (3)
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C50—C32—C31	107.8 (3)	F751—C75—F753	106.5 (3)
C32—C33—C34	121.6 (3)	F752—C75—C74	111.6 (3)
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C34—C33—C14	109.3 (3)	F753—C75—C74	110.7 (3)
C35—C34—C33	119.8 (3)	F763—C76—F761	108.0 (3)
C35—C34—C16	123.8 (3)	F763—C76—F762	108.4 (3)
C33—C34—C16	109.3 (3)	F761—C76—F762	106.7 (3)
C34—C35—C51	118.8 (3)	F763—C76—C74	111.2 (3)
C34—C35—C36	124.4 (3)	F761—C76—C74	112.3 (3)
C51—C35—C36	109.3 (3)	F762—C76—C74	110.1 (3)
C37—C36—C35	106.2 (3)	F811—C81—C82	105.0 (3)
C37—C36—C53	109.0 (3)	F811—C81—C83	105.9 (3)
C35—C36—C53	100.5 (3)	C82—C81—C83	111.0 (3)
C37—C36—C74	113.0 (3)	F811—C81—C30	108.4 (3)
C35—C36—C74	112.9 (3)	C82—C81—C30	113.3 (3)
C53—C36—C74	114.2 (3)	C83—C81—C30	112.7 (3)
C17—C37—C38	108.7 (3)	F823—C82—F821	107.7 (3)
C17—C37—C36	125.3 (3)	F823—C82—F822	107.3 (3)

C38—C37—C36	121.1 (3)	F821—C82—F822	107.0 (3)
C39—C38—C19	120.0 (3)	F823—C82—C81	112.4 (3)
C39—C38—C37	120.8 (3)	F821—C82—C81	111.5 (3)
C19—C38—C37	108.0 (3)	F822—C82—C81	110.7 (3)
C38—C39—C40	119.8 (3)	F833—C83—F832	108.8 (3)
C38—C39—C54	120.0 (3)	F833—C83—F831	107.9 (3)
C40—C39—C54	107.5 (3)	F832—C83—F831	106.7 (3)
C21—C40—C41	119.3 (3)	F833—C83—C81	112.4 (3)
C21—C40—C39	120.5 (3)	F832—C83—C81	110.0 (3)
C41—C40—C39	108.3 (3)	F831—C83—C81	110.9 (3)
C42—C41—C40	119.1 (3)	F841—C84—C85	105.6 (3)
C42—C41—C55	120.2 (3)	F841—C84—C86	105.9 (3)
C40—C41—C55	108.9 (3)	C85—C84—C86	110.6 (3)
C41—C42—C23	121.1 (3)	F841—C84—C47	108.0 (3)
C41—C42—C43	119.7 (3)	C85—C84—C47	114.0 (3)
C23—C42—C43	107.6 (3)	C86—C84—C47	112.2 (3)
C57—C43—C44	119.6 (3)	F851—C85—F853	106.2 (3)
C57—C43—C42	119.5 (3)	F851—C85—F852	108.1 (3)
C44—C43—C42	108.6 (3)	F853—C85—F852	108.4 (3)
C45—C44—C43	119.4 (3)	F851—C85—C84	111.0 (3)
C45—C44—C24	120.2 (3)	F853—C85—C84	111.9 (3)
C43—C44—C24	108.3 (3)	F852—C85—C84	111.0 (3)
C44—C45—C27	119.6 (3)	F862—C86—F863	107.1 (3)
C44—C45—C46	121.1 (3)	F862—C86—F861	108.0 (3)
C27—C45—C46	108.1 (3)	F863—C86—F861	106.9 (3)
C58—C46—C45	119.0 (3)	F862—C86—C84	111.5 (3)
C58—C46—C47	123.3 (3)	F863—C86—C84	112.4 (3)
C45—C46—C47	110.1 (3)	F861—C86—C84	110.6 (3)

Fig. 1

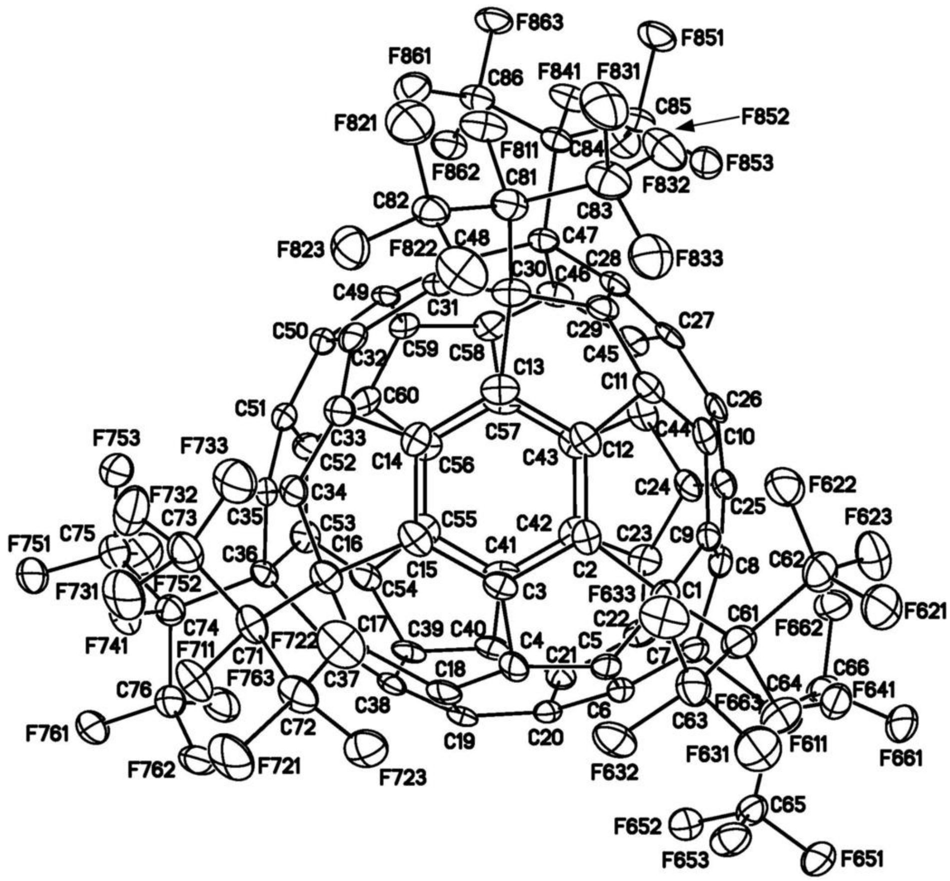
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Fig. 2

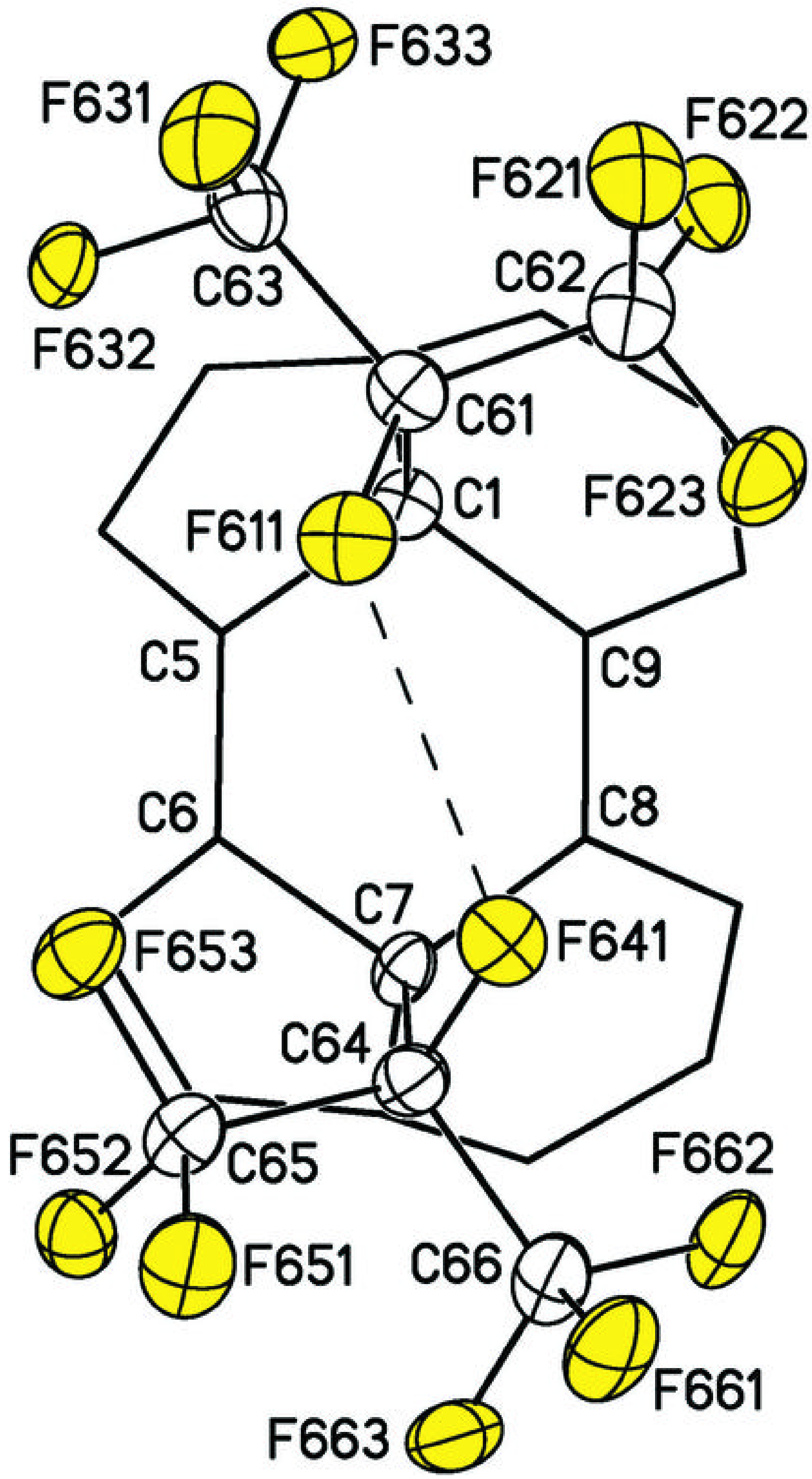
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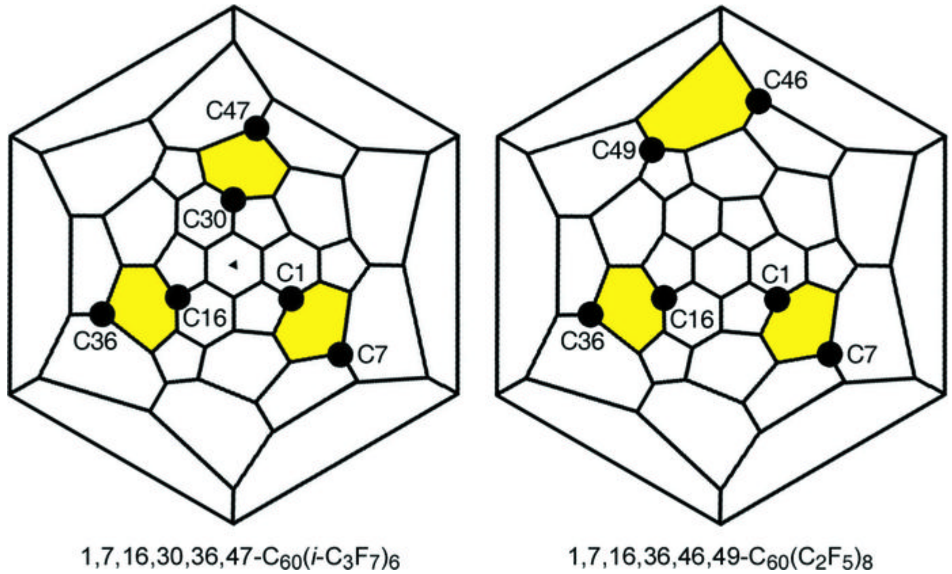
Fig. 3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