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1,6,11,16,18,24,27,36-Octakis(trifluoromethyl)-1,6,11,16,18,24,27,36-octahydro(C_{60}–I_h)[5,6]fullerene deuterochloroform solvate

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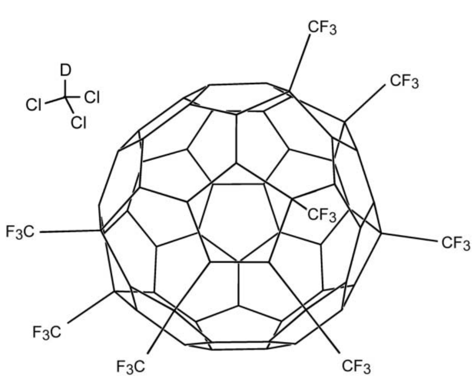
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.150; data-to-parameter ratio = 18.9.

The title compound, $C_{68}F_{24}{\cdot}CDCl_3$, is a solvate of one of five isomers of $C_{60}(CF_3)_8$ that have now been isolated. The fullerene molecule has an idealized I_h C_{60} core with the eight CF_3 groups arranged in an asymmetric fashion on a *para–para–para–meta–para–meta–para* 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, in the range 2.544 (2)–2.641 (2) Å.

Related literature

For related literature, see: Goryunkov *et al.* (2007); Kareev *et al.* (2005); Kareev, Lebedkin, Miller *et al.* (2006); Kareev, Lebedkin, Popov *et al.* (2006); Olmstead *et al.* (2003); Popov *et al.* (2007); Powell *et al.* (2002).



Experimental

Crystal data

$C_{68}F_{24}{\cdot}CDCl_3$
M_r = 1393.05
Monoclinic, $P2_1/c$
a = 14.5346 (6) Å
b = 15.5805 (7) Å
c = 20.1746 (9) Å
β = 99.821 (2)°
V = 4501.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 100 (2) K
0.34 × 0.20 × 0.05 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000) T_{min} = 0.888, T_{max} = 0.982
99651 measured reflections
16373 independent reflections
10149 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.150
S = 1.03
16373 reflections
865 parameters
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 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: TK2170).

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supplementary materials

Acta Cryst. (2007). E**63**, o3398 [doi:10.1107/S1600536807031704]

1,6,11,16,18,24,27,36-Octakis(trifluoromethyl)-1,6,11,16,18,24,27,36-octahydro(C_{60}-I_h)[5,6]fullerene deuterochloroform solvate

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Comment

Recently reported high-temperature reactions of C_{60} with CF_3I have yielded five $C_{60}(CF_3)_8$ derivatives, with thermodynamically stable addition patterns that are asymmetric as well as unprecedented in fullerene(X)$_n$ chemistry (Kareev *et al.*, 2005; Kareev, Lebedkin, Popov *et al.*, 2006; Kareev, Lebedkin, Miller *et al.*, 2006; Popov *et al.*, 2007). A member of this set of isomers, the title compound, (I), has been prepared and we report its crystal structure here. A lower-quality structure (C—C su's 0.004–0.005 Å) of the same molecule, as a toluene solvate, has recently been reported (Goryunkov *et al.*, 2007).

The structure of (I), Figs. 1 and 2, comprises an idealized I_h C_{60} core with eight sp^3 carbon atoms at positions 1, 6, 11, 16, 18, 24, 27, and 36 (Powell *et al.*, 2002), each of which is attached to a CF_3 group. The core sp^3 carbon atoms are not adjacent to one another. The CF_3 groups are arranged on a *para-para-para-meta-para-meta-para* ribbon of edge-sharing $C_6(CF_3)_2$ hexagons (*i.e.*, a p^3mpmp overall addition pattern; see Schlegel diagram in Fig. 3). Note that the shared edges in each ribbon of hexagons are C(sp^3)-C(sp^2) bonds (*e.g.*, C16—C17, C4—C18, *etc.*), not C(sp^2)-C(sp^2) bonds. Thus, any pair of adjacent hexagons along the ribbon have a common CF_3 group. As in all other published structures of fullerene(CF_3)$_n$ compounds, there are F···F intramolecular contacts between pairs of neighboring CF_3 groups that range from 2.544 (2) to 2.641 (2) Å.

Four of the shortest cage C—C bonds in (I) are C4—C5 1.344 (3) Å, C9—C10 1.368 (3) Å, C17—C37 1.355 (3) Å, and C25—C26 1.361 (3) Å. All four are significantly shorter than the shortest C—C bond in the most precise structure of empty C_{60} reported to date (C_{60}·Pt(octaethylporphyrin)), which is 1.379 (3) Å (Olmstead *et al.*, 2003). More importantly, these bonds are pentagon-hexagon junctions, and the shortest pent-hex junction in C_{60}·Pt(OEP) is 1.440 (3) Å (the longest pent-hex junction in C_{60}·Pt(OEP) is 1.461 (3) Å); OEP is octaethylporphyrin).

Experimental

The synthesis of (I) was carried out by heating C_{60} in a stream of CF_3I at 460 °C as previously described (Popov *et al.*, 2007). Crystals of the HPLC-purified compound were grown by slow evaporation of a saturated deuterochloroform solution.

Refinement

The maximum (0.81 e Å^{-3}) and minimum (−1.31 e Å^{-3}) residual electron density peaks were located 0.94 and 0.70 Å, respectively, from the Cl1 atom. The deuterium atom was geometrically placed (C—D = 1.00 Å) and refined as riding with U_{iso}(D) = 1.2U_{eq}(C).

Figures

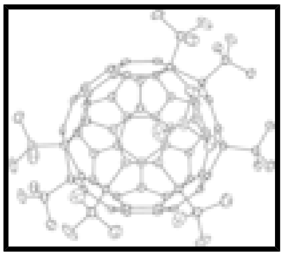

Fig. 1. The molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level.

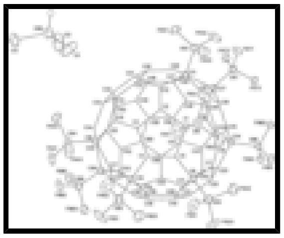

Fig. 2. The molecular structure of (I) showing the numbering scheme. Displacement ellipsoids are shown at the 50% probability level for selected atoms.

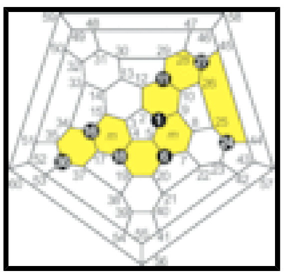

Fig. 3. Schlegel diagram of (I) showing the location of the CF_3 groups as black circles, the IUPAC lowest-locant numbers for the cage carbon atoms to which they are attached, and the ribbons or loops of *meta*- and *para*-$C_6(CF_3)_2$ edge-sharing hexagons (*meta*-$C_6(CF_3)_2$ hexagons are indicated by the letter m).

1,6,11,16,18,24,27,36-Octakis(trifluoromethyl)-1,6,11,16,18,24,27,36- octahydro(C_{60}—I_h)[5,6]fullerene deuterochloroform solvate

Crystal data

$C_{68}F_{24}$·$CDCl_3$	F_{000} = 2728
M_r = 1393.05	D_x = 2.055 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 999 reflections
a = 14.5346 (6) Å	θ = 1.7–32.6º
b = 15.5805 (7) Å	μ = 0.36 mm^{-1}
c = 20.1746 (9) Å	*T* = 100 (2) K
β = 99.821 (2)º	Plate, red
V = 4501.7 (3) Å^3	0.34 × 0.20 × 0.05 mm
Z = 4	

Data collection

Bruker Kappa APEXII diffractometer	16373 independent reflections
Radiation source: fine-focus sealed tube	10149 reflections with $I > 2\sigma(I)$

Monochromator: graphite	R_{int} = 0.058
T = 100(2) K	θ_{max} = 32.6°
φ and ω scans	θ_{min} = 1.7°
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -21 \rightarrow 20$
T_{min} = 0.888, T_{max} = 0.982	$k = -21 \rightarrow 23$
99651 measured reflections	$l = -30 \rightarrow 30$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 3.3603P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.150	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.03	$\Delta\rho_{max}$ = 0.81 e Å^{-3}
16373 reflections	$\Delta\rho_{min}$ = −1.31 e Å^{-3}
865 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 > 2sigma(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	0.22954 (14)	0.51270 (13)	0.71157 (10)	0.0119 (4)
C2	0.31195 (13)	0.47443 (13)	0.75999 (10)	0.0122 (4)
C3	0.37706 (14)	0.43914 (13)	0.72152 (10)	0.0120 (4)
C4	0.33256 (14)	0.44155 (13)	0.65064 (10)	0.0124 (4)
C5	0.24620 (14)	0.47497 (13)	0.64361 (10)	0.0122 (4)
C6	0.16767 (14)	0.45221 (13)	0.58603 (10)	0.0122 (4)
C7	0.08260 (13)	0.42002 (12)	0.61501 (10)	0.0116 (4)
C8	0.06967 (13)	0.43661 (12)	0.67850 (10)	0.0119 (4)
C9	0.14044 (13)	0.47654 (12)	0.72942 (10)	0.0118 (4)
C10	0.13275 (14)	0.44108 (13)	0.79026 (10)	0.0119 (4)
C11	0.21231 (14)	0.43500 (13)	0.84895 (10)	0.0126 (4)
C12	0.30475 (14)	0.44021 (13)	0.82144 (10)	0.0126 (4)
C13	0.36336 (14)	0.37005 (13)	0.84673 (10)	0.0131 (4)

C14	0.43056 (14)	0.33913 (13)	0.81079 (10)	0.0131 (4)
C15	0.43964 (13)	0.37626 (13)	0.74774 (10)	0.0125 (4)
C16	0.48223 (14)	0.31089 (13)	0.70478 (10)	0.0138 (4)
C17	0.42311 (14)	0.30696 (13)	0.63493 (10)	0.0132 (4)
C18	0.36765 (13)	0.38418 (13)	0.59986 (10)	0.0125 (4)
C19	0.28377 (14)	0.33905 (13)	0.55855 (10)	0.0131 (4)
C20	0.19455 (14)	0.36916 (13)	0.55264 (10)	0.0129 (4)
C21	0.11890 (14)	0.30888 (13)	0.54595 (10)	0.0130 (4)
C22	0.04858 (14)	0.33898 (13)	0.58249 (10)	0.0127 (4)
C23	−0.00237 (13)	0.28128 (13)	0.61350 (10)	0.0132 (4)
C24	−0.03997 (13)	0.30422 (13)	0.67805 (10)	0.0120 (4)
C25	0.01605 (13)	0.37749 (13)	0.71364 (10)	0.0119 (4)
C26	0.05413 (14)	0.37925 (13)	0.78009 (10)	0.0121 (4)
C27	0.04584 (14)	0.30608 (13)	0.82818 (10)	0.0132 (4)
C28	0.14437 (14)	0.28551 (13)	0.86735 (10)	0.0133 (4)
C29	0.21721 (14)	0.34206 (13)	0.87615 (10)	0.0137 (4)
C30	0.31094 (14)	0.31034 (14)	0.88086 (10)	0.0138 (4)
C31	0.32936 (14)	0.22274 (14)	0.87955 (10)	0.0149 (4)
C32	0.39982 (14)	0.19058 (14)	0.84261 (10)	0.0149 (4)
C33	0.44895 (14)	0.24785 (13)	0.80846 (10)	0.0142 (4)
C34	0.46981 (13)	0.22705 (13)	0.74309 (10)	0.0136 (4)
C35	0.43829 (14)	0.15167 (13)	0.71288 (11)	0.0148 (4)
C36	0.40829 (14)	0.14344 (13)	0.63628 (11)	0.0152 (4)
C37	0.38769 (14)	0.23243 (13)	0.60682 (10)	0.0135 (4)
C38	0.30168 (14)	0.24885 (13)	0.55832 (10)	0.0137 (4)
C39	0.23019 (15)	0.19004 (13)	0.54784 (10)	0.0143 (4)
C40	0.13594 (14)	0.22051 (13)	0.54197 (10)	0.0136 (4)
C41	0.08435 (14)	0.16073 (13)	0.57607 (10)	0.0139 (4)
C42	0.01719 (14)	0.19157 (13)	0.61230 (10)	0.0137 (4)
C43	0.00952 (14)	0.15484 (13)	0.67717 (10)	0.0131 (4)
C44	−0.01543 (13)	0.22188 (13)	0.71973 (10)	0.0128 (4)
C45	0.02385 (14)	0.22293 (13)	0.78671 (10)	0.0132 (4)
C46	0.08854 (14)	0.15709 (13)	0.81393 (10)	0.0141 (4)
C47	0.16171 (14)	0.19491 (13)	0.86302 (10)	0.0143 (4)
C48	0.25307 (15)	0.16337 (14)	0.87047 (10)	0.0155 (4)
C49	0.27510 (15)	0.09381 (13)	0.82797 (11)	0.0159 (4)
C50	0.36617 (14)	0.11167 (13)	0.81069 (11)	0.0153 (4)
C52	0.31046 (15)	0.05660 (13)	0.69644 (11)	0.0160 (4)
C51	0.38363 (14)	0.09373 (13)	0.74610 (11)	0.0159 (4)
C53	0.31764 (15)	0.09096 (13)	0.63196 (11)	0.0162 (4)
C54	0.23746 (15)	0.10979 (13)	0.58680 (10)	0.0153 (4)
C55	0.14711 (15)	0.09228 (13)	0.60372 (11)	0.0154 (4)
C56	0.13946 (15)	0.05629 (13)	0.66603 (11)	0.0156 (4)
C57	0.06917 (14)	0.08813 (13)	0.70320 (10)	0.0141 (4)
C58	0.10952 (15)	0.08903 (13)	0.77358 (11)	0.0151 (4)
C59	0.20490 (15)	0.05780 (13)	0.78024 (11)	0.0156 (4)
C60	0.22246 (15)	0.03785 (13)	0.71339 (11)	0.0158 (4)
C61	0.23418 (15)	0.61124 (13)	0.70994 (11)	0.0160 (4)
C62	0.13984 (15)	0.52462 (14)	0.53379 (11)	0.0169 (4)

C63	0.20979 (15)	0.50065 (14)	0.90533 (11)	0.0169 (4)
C64	0.58647 (14)	0.33052 (14)	0.70584 (11)	0.0166 (4)
C65	0.42188 (15)	0.43631 (14)	0.55408 (11)	0.0177 (4)
C66	−0.14472 (14)	0.32420 (13)	0.66104 (10)	0.0135 (4)
C67	−0.02525 (15)	0.32071 (14)	0.87504 (10)	0.0155 (4)
C68	0.47841 (15)	0.09581 (14)	0.60102 (12)	0.0188 (4)
C69	0.68341 (18)	0.30051 (17)	0.98786 (14)	0.0290 (5)
D691	0.6858	0.3219	1.0349	0.035*
Cl1	0.62123 (6)	0.37552 (5)	0.93253 (4)	0.0537 (2)
Cl2	0.62609 (6)	0.20279 (5)	0.98064 (6)	0.0564 (2)
Cl3	0.79819 (5)	0.29047 (5)	0.97296 (4)	0.04089 (18)
F611	0.31448 (10)	0.63788 (8)	0.69331 (8)	0.0255 (3)
F612	0.22776 (10)	0.64561 (8)	0.76941 (7)	0.0252 (3)
F613	0.16494 (10)	0.64384 (9)	0.66515 (7)	0.0264 (3)
F621	0.21276 (10)	0.57120 (9)	0.52435 (7)	0.0278 (3)
F622	0.07730 (10)	0.57817 (9)	0.55216 (7)	0.0279 (3)
F623	0.10111 (11)	0.49154 (9)	0.47448 (7)	0.0278 (3)
F631	0.28373 (10)	0.49032 (9)	0.95411 (7)	0.0271 (3)
F632	0.13408 (11)	0.49217 (11)	0.93358 (8)	0.0332 (4)
F633	0.21160 (11)	0.58085 (9)	0.88351 (7)	0.0271 (3)
F641	0.62551 (9)	0.27344 (9)	0.67054 (8)	0.0265 (3)
F642	0.63347 (9)	0.32981 (10)	0.76843 (7)	0.0282 (3)
F643	0.59864 (9)	0.40800 (9)	0.68020 (8)	0.0267 (3)
F651	0.46681 (12)	0.38468 (10)	0.51812 (8)	0.0378 (4)
F652	0.48295 (10)	0.48998 (10)	0.58856 (8)	0.0323 (4)
F653	0.36383 (10)	0.48368 (10)	0.51031 (7)	0.0279 (3)
F661	−0.15923 (9)	0.39304 (8)	0.62046 (7)	0.0201 (3)
F662	−0.18186 (8)	0.34158 (9)	0.71544 (6)	0.0182 (3)
F663	−0.19178 (8)	0.25846 (8)	0.62891 (6)	0.0186 (3)
F671	−0.00442 (10)	0.38995 (9)	0.91402 (7)	0.0227 (3)
F672	−0.02650 (9)	0.25319 (9)	0.91616 (6)	0.0193 (3)
F673	−0.11104 (9)	0.33158 (9)	0.84072 (6)	0.0213 (3)
F681	0.49604 (9)	0.01739 (9)	0.62755 (7)	0.0248 (3)
F682	0.56018 (9)	0.13640 (9)	0.60644 (8)	0.0271 (3)
F683	0.44498 (10)	0.08603 (9)	0.53539 (7)	0.0259 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0119 (9)	0.0102 (8)	0.0136 (9)	−0.0004 (7)	0.0017 (7)	0.0007 (7)
C2	0.0099 (8)	0.0116 (9)	0.0146 (9)	−0.0026 (7)	0.0002 (7)	−0.0015 (7)
C3	0.0111 (9)	0.0114 (9)	0.0133 (9)	−0.0035 (7)	0.0016 (7)	0.0012 (7)
C4	0.0127 (9)	0.0109 (9)	0.0136 (9)	−0.0034 (7)	0.0023 (7)	0.0011 (7)
C5	0.0120 (9)	0.0114 (9)	0.0136 (9)	−0.0012 (7)	0.0032 (7)	0.0030 (7)
C6	0.0124 (9)	0.0127 (9)	0.0116 (9)	−0.0013 (7)	0.0018 (7)	0.0028 (7)
C7	0.0093 (8)	0.0113 (9)	0.0135 (9)	0.0008 (7)	−0.0004 (7)	0.0038 (7)
C8	0.0095 (8)	0.0107 (9)	0.0149 (9)	0.0014 (7)	0.0002 (7)	0.0015 (7)
C9	0.0099 (8)	0.0104 (9)	0.0149 (9)	0.0005 (7)	0.0012 (7)	−0.0002 (7)

C10	0.0114 (9)	0.0118 (9)	0.0123 (9)	−0.0001 (7)	0.0016 (7)	−0.0021 (7)
C11	0.0125 (9)	0.0138 (9)	0.0113 (8)	−0.0018 (7)	0.0012 (7)	−0.0017 (7)
C12	0.0117 (9)	0.0116 (9)	0.0140 (9)	−0.0037 (7)	0.0006 (7)	−0.0038 (7)
C13	0.0127 (9)	0.0141 (9)	0.0115 (9)	−0.0028 (7)	−0.0008 (7)	−0.0005 (7)
C14	0.0097 (9)	0.0138 (9)	0.0144 (9)	−0.0015 (7)	−0.0016 (7)	0.0001 (7)
C15	0.0080 (8)	0.0138 (9)	0.0154 (9)	−0.0027 (7)	0.0011 (7)	−0.0005 (7)
C16	0.0103 (9)	0.0138 (9)	0.0169 (9)	−0.0014 (7)	0.0010 (7)	0.0004 (7)
C17	0.0103 (9)	0.0152 (9)	0.0149 (9)	−0.0006 (7)	0.0039 (7)	0.0006 (7)
C18	0.0105 (9)	0.0149 (9)	0.0127 (9)	−0.0006 (7)	0.0038 (7)	0.0018 (7)
C19	0.0143 (9)	0.0169 (10)	0.0090 (8)	−0.0017 (7)	0.0041 (7)	0.0006 (7)
C20	0.0154 (9)	0.0142 (9)	0.0089 (8)	−0.0008 (7)	0.0019 (7)	0.0014 (7)
C21	0.0120 (9)	0.0185 (10)	0.0083 (8)	−0.0011 (7)	0.0007 (7)	−0.0002 (7)
C22	0.0107 (9)	0.0169 (10)	0.0096 (8)	0.0002 (7)	−0.0010 (7)	0.0007 (7)
C23	0.0090 (8)	0.0169 (10)	0.0124 (9)	−0.0008 (7)	−0.0015 (7)	0.0003 (7)
C24	0.0085 (8)	0.0126 (9)	0.0148 (9)	−0.0016 (7)	0.0016 (7)	0.0011 (7)
C25	0.0096 (8)	0.0125 (9)	0.0138 (9)	−0.0005 (7)	0.0030 (7)	0.0004 (7)
C26	0.0108 (8)	0.0137 (9)	0.0127 (9)	0.0008 (7)	0.0041 (7)	−0.0009 (7)
C27	0.0115 (9)	0.0166 (9)	0.0116 (9)	−0.0011 (7)	0.0027 (7)	0.0014 (7)
C28	0.0146 (9)	0.0171 (10)	0.0085 (8)	−0.0012 (7)	0.0029 (7)	0.0014 (7)
C29	0.0157 (9)	0.0164 (10)	0.0086 (8)	−0.0010 (8)	0.0011 (7)	−0.0005 (7)
C30	0.0134 (9)	0.0180 (10)	0.0087 (8)	−0.0018 (7)	−0.0014 (7)	0.0002 (7)
C31	0.0141 (9)	0.0180 (10)	0.0111 (9)	−0.0003 (8)	−0.0017 (7)	0.0031 (7)
C32	0.0124 (9)	0.0158 (10)	0.0149 (9)	0.0025 (7)	−0.0021 (7)	0.0038 (7)
C33	0.0098 (9)	0.0157 (9)	0.0153 (9)	0.0005 (7)	−0.0030 (7)	0.0023 (7)
C34	0.0073 (8)	0.0148 (9)	0.0181 (9)	0.0021 (7)	0.0002 (7)	0.0031 (8)
C35	0.0116 (9)	0.0143 (9)	0.0181 (10)	0.0033 (7)	0.0010 (7)	0.0010 (8)
C36	0.0131 (9)	0.0130 (9)	0.0194 (10)	0.0011 (7)	0.0027 (8)	−0.0015 (8)
C37	0.0108 (9)	0.0160 (9)	0.0145 (9)	0.0003 (7)	0.0043 (7)	−0.0005 (7)
C38	0.0136 (9)	0.0169 (9)	0.0110 (8)	0.0004 (7)	0.0037 (7)	−0.0013 (7)
C39	0.0156 (9)	0.0158 (10)	0.0121 (9)	−0.0002 (7)	0.0037 (7)	−0.0045 (7)
C40	0.0138 (9)	0.0170 (10)	0.0097 (8)	−0.0017 (7)	0.0013 (7)	−0.0020 (7)
C41	0.0117 (9)	0.0159 (9)	0.0132 (9)	−0.0036 (7)	−0.0006 (7)	−0.0031 (7)
C42	0.0099 (9)	0.0156 (9)	0.0147 (9)	−0.0034 (7)	−0.0003 (7)	−0.0033 (7)
C43	0.0101 (9)	0.0129 (9)	0.0159 (9)	−0.0040 (7)	0.0006 (7)	−0.0002 (7)
C44	0.0092 (8)	0.0136 (9)	0.0161 (9)	−0.0024 (7)	0.0034 (7)	0.0002 (7)
C45	0.0111 (9)	0.0131 (9)	0.0158 (9)	−0.0033 (7)	0.0038 (7)	0.0009 (7)
C46	0.0133 (9)	0.0142 (9)	0.0149 (9)	−0.0033 (7)	0.0031 (7)	0.0031 (7)
C47	0.0152 (9)	0.0163 (10)	0.0118 (9)	−0.0023 (8)	0.0034 (7)	0.0045 (7)
C48	0.0166 (10)	0.0171 (10)	0.0118 (9)	0.0006 (8)	0.0000 (7)	0.0067 (7)
C49	0.0171 (10)	0.0128 (9)	0.0168 (10)	0.0003 (7)	−0.0001 (8)	0.0057 (8)
C50	0.0139 (9)	0.0122 (9)	0.0184 (10)	0.0022 (7)	−0.0013 (8)	0.0057 (8)
C52	0.0159 (10)	0.0101 (9)	0.0214 (10)	0.0014 (7)	0.0015 (8)	−0.0014 (8)
C51	0.0136 (9)	0.0111 (9)	0.0220 (10)	0.0030 (7)	0.0004 (8)	0.0022 (8)
C53	0.0157 (10)	0.0109 (9)	0.0224 (10)	0.0006 (7)	0.0040 (8)	−0.0039 (8)
C54	0.0160 (10)	0.0137 (9)	0.0166 (9)	−0.0002 (7)	0.0039 (8)	−0.0049 (7)
C55	0.0152 (9)	0.0115 (9)	0.0184 (10)	−0.0021 (7)	−0.0005 (8)	−0.0043 (7)
C56	0.0162 (10)	0.0095 (9)	0.0207 (10)	−0.0030 (7)	0.0020 (8)	−0.0025 (8)
C57	0.0131 (9)	0.0106 (9)	0.0182 (10)	−0.0041 (7)	0.0017 (7)	−0.0005 (7)
C58	0.0160 (10)	0.0111 (9)	0.0181 (10)	−0.0025 (7)	0.0029 (8)	0.0040 (7)

C59	0.0153 (10)	0.0109 (9)	0.0202 (10)	−0.0007 (7)	0.0019 (8)	0.0047 (8)
C60	0.0178 (10)	0.0081 (9)	0.0211 (10)	−0.0008 (7)	0.0021 (8)	0.0000 (7)
C61	0.0149 (9)	0.0125 (9)	0.0214 (10)	−0.0003 (7)	0.0051 (8)	0.0010 (8)
C62	0.0153 (10)	0.0186 (10)	0.0162 (10)	−0.0014 (8)	0.0008 (8)	0.0056 (8)
C63	0.0169 (10)	0.0181 (10)	0.0158 (9)	−0.0022 (8)	0.0028 (8)	−0.0030 (8)
C64	0.0117 (9)	0.0157 (10)	0.0228 (10)	−0.0001 (7)	0.0040 (8)	−0.0005 (8)
C65	0.0155 (10)	0.0189 (10)	0.0196 (10)	−0.0013 (8)	0.0060 (8)	0.0025 (8)
C66	0.0101 (9)	0.0152 (9)	0.0147 (9)	−0.0012 (7)	0.0012 (7)	0.0000 (7)
C67	0.0159 (10)	0.0178 (10)	0.0131 (9)	−0.0021 (8)	0.0031 (7)	0.0013 (8)
C68	0.0162 (10)	0.0161 (10)	0.0247 (11)	0.0013 (8)	0.0049 (8)	−0.0029 (8)
C69	0.0256 (12)	0.0289 (13)	0.0322 (13)	0.0020 (10)	0.0040 (10)	0.0001 (11)
Cl1	0.0641 (5)	0.0305 (4)	0.0525 (5)	0.0121 (3)	−0.0302 (4)	−0.0050 (3)
Cl2	0.0327 (4)	0.0348 (4)	0.1032 (8)	−0.0068 (3)	0.0158 (4)	0.0022 (4)
Cl3	0.0261 (3)	0.0569 (5)	0.0438 (4)	−0.0025 (3)	0.0176 (3)	0.0046 (3)
F611	0.0221 (7)	0.0147 (6)	0.0430 (8)	−0.0057 (5)	0.0150 (6)	0.0004 (6)
F612	0.0369 (8)	0.0144 (6)	0.0260 (7)	−0.0014 (6)	0.0104 (6)	−0.0060 (5)
F613	0.0263 (7)	0.0165 (6)	0.0343 (8)	0.0046 (5)	−0.0013 (6)	0.0071 (6)
F621	0.0191 (7)	0.0282 (8)	0.0344 (8)	−0.0077 (6)	−0.0001 (6)	0.0177 (6)
F622	0.0296 (8)	0.0238 (7)	0.0313 (8)	0.0124 (6)	0.0080 (6)	0.0124 (6)
F623	0.0379 (8)	0.0251 (7)	0.0164 (6)	−0.0038 (6)	−0.0074 (6)	0.0063 (5)
F631	0.0291 (8)	0.0303 (8)	0.0177 (6)	0.0015 (6)	−0.0075 (6)	−0.0080 (6)
F632	0.0291 (8)	0.0420 (9)	0.0328 (8)	−0.0133 (7)	0.0182 (7)	−0.0217 (7)
F633	0.0440 (9)	0.0151 (6)	0.0218 (7)	0.0016 (6)	0.0045 (6)	−0.0037 (5)
F641	0.0128 (6)	0.0263 (7)	0.0421 (8)	−0.0010 (5)	0.0091 (6)	−0.0121 (6)
F642	0.0140 (6)	0.0456 (9)	0.0231 (7)	−0.0055 (6)	−0.0023 (5)	0.0012 (6)
F643	0.0161 (6)	0.0197 (7)	0.0451 (9)	−0.0042 (5)	0.0071 (6)	0.0073 (6)
F651	0.0480 (10)	0.0303 (8)	0.0457 (10)	0.0067 (7)	0.0385 (8)	0.0066 (7)
F652	0.0276 (8)	0.0387 (9)	0.0296 (8)	−0.0201 (7)	0.0017 (6)	0.0085 (7)
F653	0.0258 (7)	0.0323 (8)	0.0256 (7)	−0.0016 (6)	0.0042 (6)	0.0164 (6)
F661	0.0151 (6)	0.0218 (7)	0.0227 (7)	0.0026 (5)	0.0008 (5)	0.0084 (5)
F662	0.0120 (6)	0.0260 (7)	0.0169 (6)	0.0010 (5)	0.0039 (5)	−0.0018 (5)
F663	0.0114 (6)	0.0203 (6)	0.0226 (6)	−0.0046 (5)	−0.0008 (5)	−0.0043 (5)
F671	0.0252 (7)	0.0234 (7)	0.0219 (7)	−0.0044 (6)	0.0109 (5)	−0.0073 (5)
F672	0.0182 (6)	0.0238 (7)	0.0171 (6)	−0.0014 (5)	0.0069 (5)	0.0055 (5)
F673	0.0125 (6)	0.0342 (8)	0.0173 (6)	0.0025 (5)	0.0028 (5)	0.0042 (5)
F681	0.0211 (7)	0.0169 (6)	0.0360 (8)	0.0066 (5)	0.0036 (6)	−0.0026 (6)
F682	0.0149 (6)	0.0264 (7)	0.0425 (9)	−0.0024 (5)	0.0120 (6)	−0.0114 (6)
F683	0.0256 (7)	0.0288 (8)	0.0237 (7)	0.0048 (6)	0.0053 (6)	−0.0076 (6)

Geometric parameters (Å, °)

C1—C9	1.511 (3)	C35—C51	1.441 (3)
C1—C2	1.532 (3)	C35—C36	1.538 (3)
C1—C61	1.537 (3)	C36—C37	1.518 (3)
C1—C5	1.548 (3)	C36—C68	1.531 (3)
C2—C12	1.370 (3)	C36—C53	1.540 (3)
C2—C3	1.432 (3)	C37—C38	1.473 (3)
C3—C15	1.379 (3)	C38—C39	1.374 (3)
C3—C4	1.466 (3)	C39—C40	1.436 (3)

C4—C5	1.344 (3)	C39—C54	1.471 (3)
C4—C18	1.512 (3)	C40—C41	1.442 (3)
C5—C6	1.525 (3)	C41—C42	1.400 (3)
C6—C7	1.539 (3)	C41—C55	1.452 (3)
C6—C20	1.540 (3)	C42—C43	1.450 (3)
C6—C62	1.550 (3)	C43—C57	1.397 (3)
C7—C8	1.351 (3)	C43—C44	1.437 (3)
C7—C22	1.469 (3)	C44—C45	1.375 (3)
C8—C9	1.463 (3)	C45—C46	1.436 (3)
C8—C25	1.465 (3)	C46—C58	1.402 (3)
C9—C10	1.368 (3)	C46—C47	1.449 (3)
C10—C26	1.482 (3)	C47—C48	1.400 (3)
C10—C11	1.510 (3)	C48—C49	1.451 (3)
C11—C63	1.535 (3)	C49—C59	1.396 (3)
C11—C12	1.541 (3)	C49—C50	1.452 (3)
C11—C29	1.546 (3)	C50—C51	1.398 (3)
C12—C13	1.426 (3)	C52—C60	1.410 (3)
C13—C14	1.398 (3)	C52—C53	1.427 (3)
C13—C30	1.449 (3)	C52—C51	1.451 (3)
C14—C15	1.424 (3)	C53—C54	1.383 (3)
C14—C33	1.449 (3)	C54—C55	1.438 (3)
C15—C16	1.535 (3)	C55—C56	1.398 (3)
C16—C17	1.521 (3)	C56—C60	1.434 (3)
C16—C64	1.542 (3)	C56—C57	1.454 (3)
C16—C34	1.544 (3)	C57—C58	1.441 (3)
C17—C37	1.355 (3)	C58—C59	1.454 (3)
C17—C18	1.550 (3)	C59—C60	1.448 (3)
C18—C19	1.526 (3)	C61—F612	1.332 (2)
C18—C65	1.544 (3)	C61—F613	1.333 (2)
C19—C20	1.365 (3)	C61—F611	1.334 (2)
C19—C38	1.429 (3)	C62—F621	1.325 (2)
C20—C21	1.435 (3)	C62—F622	1.332 (3)
C21—C40	1.404 (3)	C62—F623	1.336 (3)
C21—C22	1.437 (3)	C63—F633	1.327 (3)
C22—C23	1.381 (3)	C63—F632	1.329 (3)
C23—C42	1.427 (3)	C63—F631	1.337 (3)
C23—C24	1.538 (3)	C64—F641	1.326 (2)
C24—C25	1.511 (3)	C64—F642	1.329 (3)
C24—C66	1.534 (3)	C64—F643	1.337 (3)
C24—C44	1.542 (3)	C65—F652	1.327 (3)
C25—C26	1.361 (3)	C65—F651	1.327 (3)
C26—C27	1.515 (3)	C65—F653	1.335 (3)
C27—C67	1.532 (3)	C66—F662	1.331 (2)
C27—C45	1.546 (3)	C66—F663	1.336 (2)
C27—C28	1.547 (3)	C66—F661	1.344 (2)
C28—C29	1.366 (3)	C67—F673	1.330 (2)
C28—C47	1.439 (3)	C67—F671	1.339 (2)
C29—C30	1.437 (3)	C67—F672	1.342 (2)
C30—C31	1.392 (3)	C68—F682	1.334 (3)

C31—C48	1.432 (3)	C68—F683	1.339 (3)
C31—C32	1.455 (3)	C68—F681	1.341 (3)
C32—C33	1.396 (3)	C69—Cl2	1.730 (3)
C32—C50	1.435 (3)	C69—Cl3	1.752 (3)
C33—C34	1.440 (3)	C69—Cl1	1.756 (3)
C34—C35	1.366 (3)		

C9—C1—C2	108.16 (16)	C68—C36—C35	114.22 (17)
C9—C1—C61	114.83 (16)	C37—C36—C53	110.66 (17)
C2—C1—C61	111.72 (16)	C68—C36—C53	110.32 (17)
C9—C1—C5	109.83 (16)	C35—C36—C53	101.20 (17)
C2—C1—C5	101.17 (15)	C17—C37—C38	110.38 (18)
C61—C1—C5	110.26 (16)	C17—C37—C36	125.69 (18)
C12—C2—C3	120.04 (18)	C38—C37—C36	120.48 (18)
C12—C2—C1	123.83 (18)	C39—C38—C19	121.51 (19)
C3—C2—C1	108.72 (17)	C39—C38—C37	121.35 (19)
C15—C3—C2	121.22 (18)	C19—C38—C37	107.64 (17)
C15—C3—C4	122.99 (18)	C38—C39—C40	118.56 (19)
C2—C3—C4	107.25 (17)	C38—C39—C54	120.06 (19)
C5—C4—C3	111.20 (18)	C40—C39—C54	107.80 (18)
C5—C4—C18	125.05 (18)	C21—C40—C39	119.66 (18)
C3—C4—C18	120.14 (17)	C21—C40—C41	119.67 (18)
C4—C5—C6	123.67 (18)	C39—C40—C41	108.28 (18)
C4—C5—C1	109.75 (17)	C42—C41—C40	119.53 (19)
C6—C5—C1	123.58 (17)	C42—C41—C55	119.99 (19)
C5—C6—C7	109.37 (16)	C40—C41—C55	108.30 (18)
C5—C6—C20	108.41 (16)	C41—C42—C23	120.23 (19)
C7—C6—C20	99.94 (15)	C41—C42—C43	120.22 (19)
C5—C6—C62	115.05 (17)	C23—C42—C43	108.96 (17)
C7—C6—C62	111.23 (16)	C57—C43—C44	121.31 (18)
C20—C6—C62	111.75 (16)	C57—C43—C42	119.63 (18)
C8—C7—C22	119.81 (18)	C44—C43—C42	108.57 (17)
C8—C7—C6	123.27 (18)	C45—C44—C43	119.42 (19)
C22—C7—C6	109.96 (16)	C45—C44—C24	123.01 (18)
C7—C8—C9	123.53 (18)	C43—C44—C24	109.71 (17)
C7—C8—C25	120.66 (18)	C44—C45—C46	120.17 (19)
C9—C8—C25	107.21 (17)	C44—C45—C27	123.71 (18)
C10—C9—C8	107.64 (17)	C46—C45—C27	109.29 (17)
C10—C9—C1	124.68 (18)	C58—C46—C45	120.77 (19)
C8—C9—C1	121.32 (17)	C58—C46—C47	119.84 (19)
C9—C10—C26	108.51 (17)	C45—C46—C47	109.10 (18)
C9—C10—C11	124.05 (18)	C48—C47—C28	120.70 (19)
C26—C10—C11	122.48 (17)	C48—C47—C46	120.18 (19)
C10—C11—C63	115.30 (17)	C28—C47—C46	108.95 (18)
C10—C11—C12	108.21 (16)	C47—C48—C31	119.13 (19)
C63—C11—C12	111.37 (16)	C47—C48—C49	119.98 (19)
C10—C11—C29	108.65 (16)	C31—C48—C49	108.30 (18)
C63—C11—C29	111.50 (16)	C59—C49—C48	119.92 (19)
C12—C11—C29	100.78 (16)	C59—C49—C50	120.0 (2)
C2—C12—C13	119.29 (18)	C48—C49—C50	107.51 (18)

C2—C12—C11	123.53 (18)	C51—C50—C32	119.18 (19)
C13—C12—C11	109.58 (17)	C51—C50—C49	120.23 (19)
C14—C13—C12	120.41 (18)	C32—C50—C49	108.15 (18)
C14—C13—C30	119.73 (19)	C60—C52—C53	120.63 (19)
C12—C13—C30	109.39 (18)	C60—C52—C51	120.24 (19)
C13—C14—C15	120.20 (18)	C53—C52—C51	108.71 (18)
C13—C14—C33	120.27 (18)	C50—C51—C35	120.70 (19)
C15—C14—C33	108.90 (18)	C50—C51—C52	119.68 (19)
C3—C15—C14	118.40 (18)	C35—C51—C52	109.03 (18)
C3—C15—C16	123.91 (18)	C54—C53—C52	119.7 (2)
C14—C15—C16	110.05 (17)	C54—C53—C36	122.77 (19)
C17—C16—C15	109.35 (16)	C52—C53—C36	110.03 (18)
C17—C16—C64	114.79 (17)	C53—C54—C55	120.30 (19)
C15—C16—C64	110.52 (16)	C53—C54—C39	120.53 (19)
C17—C16—C34	109.50 (16)	C55—C54—C39	107.62 (18)
C15—C16—C34	100.71 (16)	C56—C55—C54	120.36 (19)
C64—C16—C34	111.06 (16)	C56—C55—C41	119.94 (19)
C37—C17—C16	122.44 (18)	C54—C55—C41	107.99 (18)
C37—C17—C18	110.07 (17)	C55—C56—C60	119.50 (19)
C16—C17—C18	124.00 (17)	C55—C56—C57	119.84 (19)
C4—C18—C19	108.18 (16)	C60—C56—C57	108.06 (18)
C4—C18—C65	111.10 (17)	C43—C57—C58	119.03 (19)
C19—C18—C65	110.96 (16)	C43—C57—C56	120.37 (19)
C4—C18—C17	111.02 (16)	C58—C57—C56	107.93 (18)
C19—C18—C17	101.33 (16)	C46—C58—C57	119.17 (19)
C65—C18—C17	113.74 (16)	C46—C58—C59	119.87 (19)
C20—C19—C38	120.56 (19)	C57—C58—C59	108.02 (18)
C20—C19—C18	123.22 (18)	C49—C59—C60	120.29 (19)
C38—C19—C18	109.02 (17)	C49—C59—C58	120.18 (19)
C19—C20—C21	118.99 (19)	C60—C59—C58	107.61 (18)
C19—C20—C6	123.97 (18)	C52—C60—C56	119.45 (19)
C21—C20—C6	110.10 (17)	C52—C60—C59	119.52 (19)
C40—C21—C20	120.50 (18)	C56—C60—C59	108.39 (18)
C40—C21—C22	119.83 (18)	F612—C61—F613	107.26 (17)
C20—C21—C22	109.81 (18)	F612—C61—F611	107.46 (17)
C23—C22—C21	120.22 (19)	F613—C61—F611	107.62 (17)
C23—C22—C7	121.54 (18)	F612—C61—C1	111.86 (17)
C21—C22—C7	107.15 (17)	F613—C61—C1	111.36 (17)
C22—C23—C42	120.41 (19)	F611—C61—C1	111.06 (17)
C22—C23—C24	121.86 (18)	F621—C62—F622	107.31 (18)
C42—C23—C24	110.04 (17)	F621—C62—F623	107.92 (17)
C25—C24—C66	112.75 (16)	F622—C62—F623	106.71 (17)
C25—C24—C23	109.74 (16)	F621—C62—C6	111.97 (17)
C66—C24—C23	109.89 (16)	F622—C62—C6	112.22 (17)
C25—C24—C44	108.28 (16)	F623—C62—C6	110.46 (17)
C66—C24—C44	114.77 (16)	F633—C63—F632	107.49 (18)
C23—C24—C44	100.71 (16)	F633—C63—F631	107.37 (17)
C26—C25—C8	107.67 (17)	F632—C63—F631	107.01 (18)
C26—C25—C24	125.40 (18)	F633—C63—C11	112.18 (17)

C8—C25—C24	122.21 (17)	F632—C63—C11	112.20 (17)
C25—C26—C10	108.90 (17)	F631—C63—C11	110.33 (17)
C25—C26—C27	123.53 (18)	F641—C64—F642	107.87 (17)
C10—C26—C27	122.97 (17)	F641—C64—F643	107.51 (18)
C26—C27—C67	114.77 (17)	F642—C64—F643	107.14 (18)
C26—C27—C45	108.41 (16)	F641—C64—C16	111.64 (17)
C67—C27—C45	111.08 (16)	F642—C64—C16	110.86 (17)
C26—C27—C28	108.38 (16)	F643—C64—C16	111.61 (17)
C67—C27—C28	112.26 (16)	F652—C65—F651	108.73 (18)
C45—C27—C28	101.00 (16)	F652—C65—F653	106.81 (18)
C29—C28—C47	120.06 (19)	F651—C65—F653	106.74 (18)
C29—C28—C27	124.23 (18)	F652—C65—C18	112.46 (18)
C47—C28—C27	109.19 (17)	F651—C65—C18	110.93 (18)
C28—C29—C30	119.46 (19)	F653—C65—C18	110.92 (17)
C28—C29—C11	124.79 (18)	F662—C66—F663	108.05 (16)
C30—C29—C11	109.35 (17)	F662—C66—F661	107.23 (16)
C31—C30—C29	121.28 (19)	F663—C66—F661	107.58 (16)
C31—C30—C13	120.15 (19)	F662—C66—C24	112.55 (16)
C29—C30—C13	108.49 (18)	F663—C66—C24	111.05 (16)
C30—C31—C48	119.26 (19)	F661—C66—C24	110.17 (16)
C30—C31—C32	120.13 (19)	F673—C67—F671	107.52 (18)
C48—C31—C32	108.03 (18)	F673—C67—F672	108.14 (17)
C33—C32—C50	119.37 (19)	F671—C67—F672	107.09 (16)
C33—C32—C31	119.78 (19)	F673—C67—C27	111.66 (16)
C50—C32—C31	108.01 (18)	F671—C67—C27	111.94 (17)
C32—C33—C34	120.90 (19)	F672—C67—C27	110.29 (17)
C32—C33—C14	119.91 (19)	F682—C68—F683	107.64 (18)
C34—C33—C14	108.63 (18)	F682—C68—F681	107.00 (18)
C35—C34—C33	119.69 (19)	F683—C68—F681	107.66 (18)
C35—C34—C16	124.27 (19)	F682—C68—C36	112.74 (18)
C33—C34—C16	109.21 (17)	F683—C68—C36	110.89 (18)
C34—C35—C51	120.05 (19)	F681—C68—C36	110.69 (18)
C34—C35—C36	122.42 (19)	Cl2—C69—Cl3	111.47 (15)
C51—C35—C36	109.31 (18)	Cl2—C69—Cl1	110.11 (15)
C37—C36—C68	111.31 (17)	Cl3—C69—Cl1	110.62 (15)
C37—C36—C35	108.69 (17)		

Fig. 1

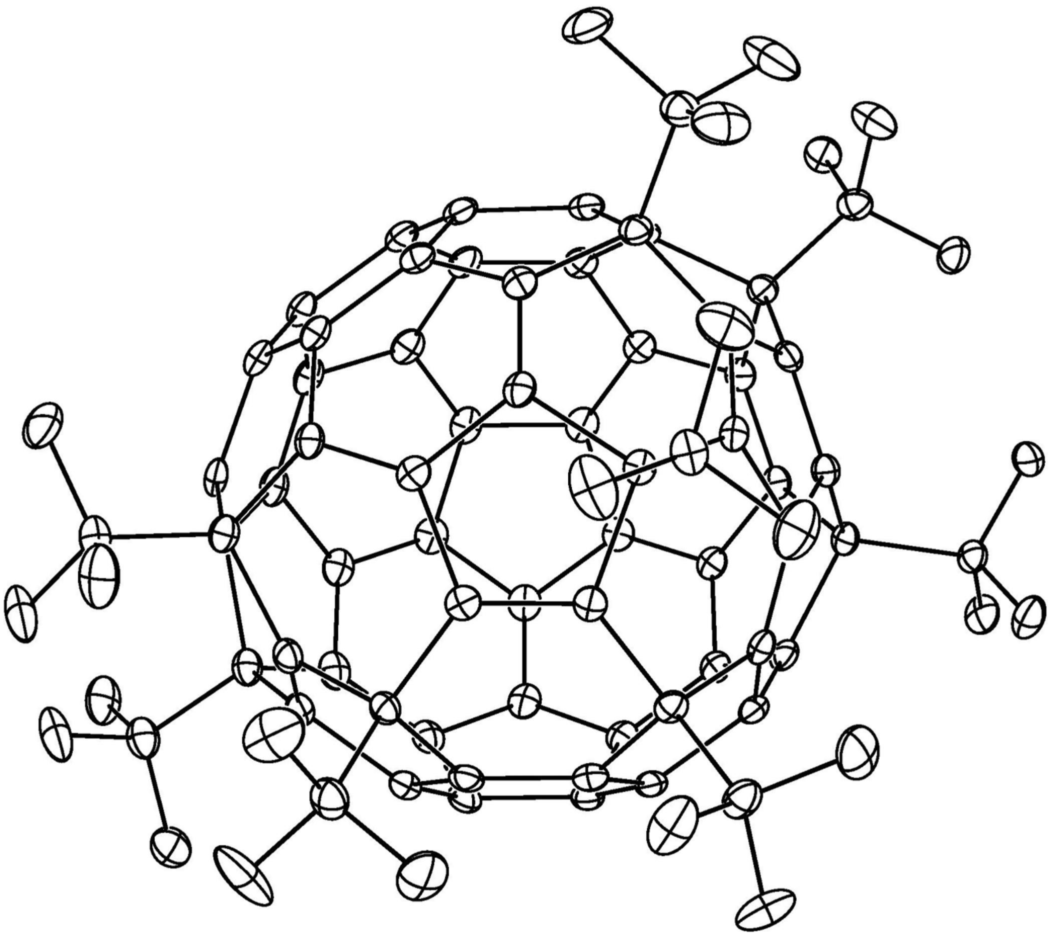

Fig. 2

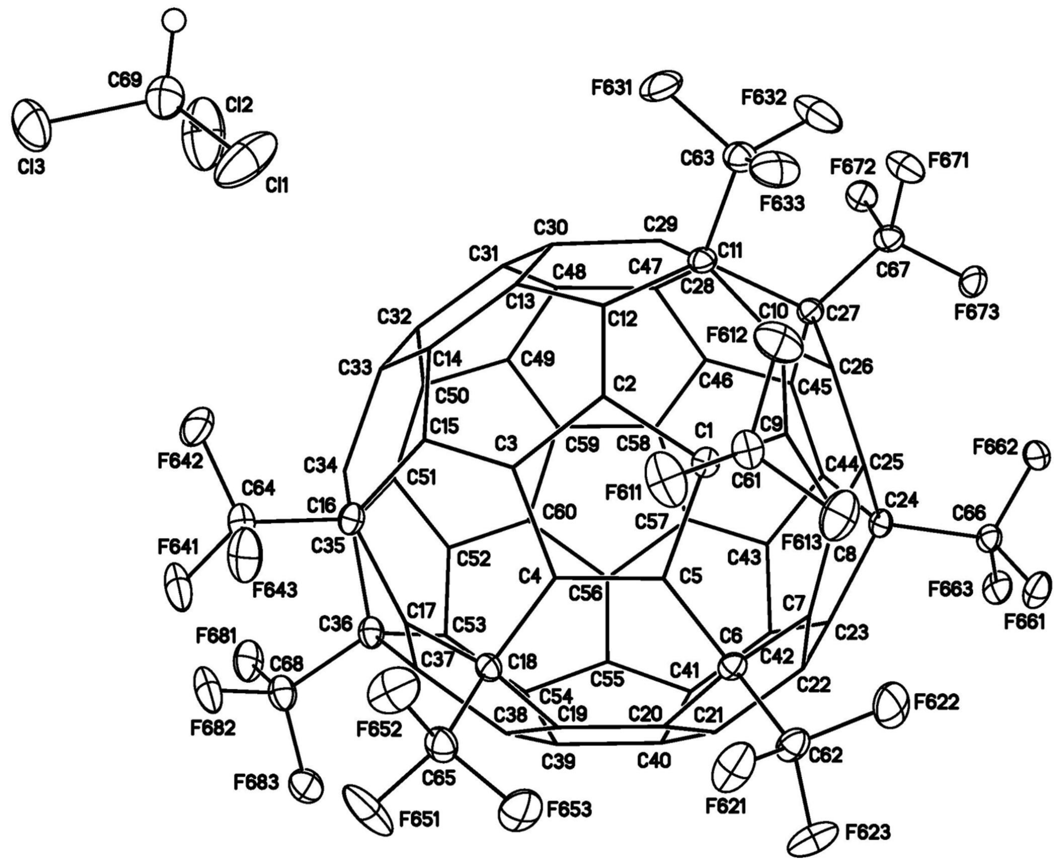
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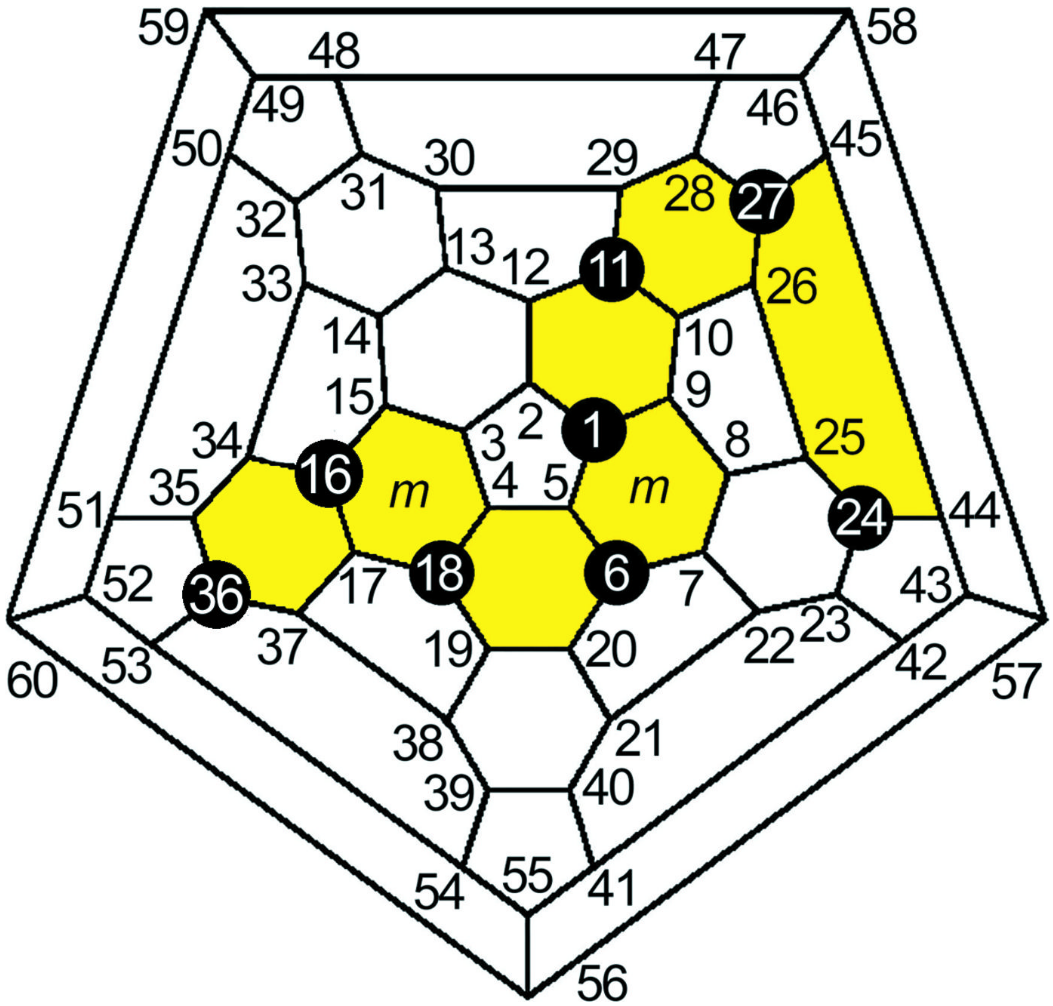
Fig. 3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