Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1,6,11,18,24,27,33,51,54,60-Decakis(trifluoromethyl)-1,6,11,18,24,27,33,51,54,60-decahydro($C_{60}$-$I_h$)[5,6]fullerene

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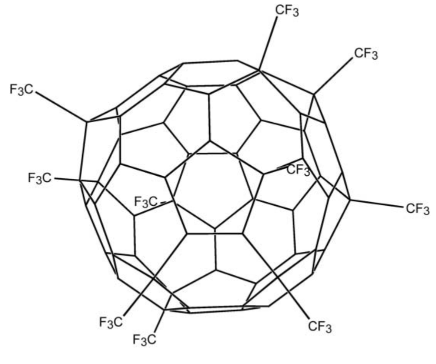
Received 26 May 2007; accepted 28 May 2007

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.051; $wR$ factor = 0.122; data-to-parameter ratio = 11.9.

The title compound, $C_{70}F_{30}$, is one of six isomers of $C_{60}(CF_3)_{10}$ that have now been isolated. The fullerene molecule has an idealized $I_h$ $C_{60}$ core with the ten $CF_3$ groups arranged in an asymmetric fashion on two ribbons of edge-sharing $C_6(CF_3)_2$ hexagons, a *para–para–para–meta–para* ribbon and a *para–meta–para* ribbon, giving an overall $p^3mp,pmp$ structure. 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 2.568 (3) to 2.682 (3) Å.

## Related literature

For related literature, see: Kareev *et al.* (2005); Kareev, Lebedkin, Miller, Anderson, Strauss & Boltalina (2006); Kareev, Lebedkin, Popov, Miller, Anderson, Strauss & Boltalina (2006); Kareev, Shustova, Newell, Miller, Anderson, Strauss & Boltalina (2006); Olmstead *et al.* (2003); Popov *et al.* (2007); Powell *et al.* (2002); Shustova *et al.* (2006); Troyanov *et al.* (2006).




## Experimental

*Crystal data*

$C_{70}F_{30}$
$M_r$ = 1410.70
Triclinic, $P\bar{1}$
$a$ = 11.0257 (4) Å
$b$ = 11.4172 (4) Å
$c$ = 20.4527 (7) Å
$\alpha$ = 82.369 (2)°
$\beta$ = 77.010 (2)°
$\gamma$ = 65.543 (2)°
$V$ = 2281.36 (14) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 296 (2) K
0.20 × 0.15 × 0.07 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000) $T_{min}$ = 0.959, $T_{max}$ = 0.986
77789 measured reflections
10733 independent reflections
6553 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.071

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.122
$S$ = 1.03
10733 reflections
901 parameters
$\Delta\rho_{max}$ = 0.37 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2000); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the US National Science Foundation and the Civilian Research and Development Foundation for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2158).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o3129 [ **doi:10.1107/S1600536807026128** ]

# 1,6,11,18,24,27,33,51,54,60-Decakis(trifluoromethyl)-1,6,11,18,24,27,33,51,54,60-decahydro($C_{60}$-$I_h$)[5,6]fullerene

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

## Comment

Recently reported high-temperature reactions of $C_{60}$ with $CF_3I$ have yielded five $C_{60}(CF_3)_{10}$ derivatives, (I)–(V) with thermodynamically stable addition patterns that are asymmetric or dissymetric 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 new member of this set of isomers, the title compound, (VI), has been prepared and we report its crystal structure here.

The structure of (VI), Fig. 1, comprises an idealized $I_h$ $C_{60}$ core with ten $sp^3$ carbon atoms at positions 1, 6, 11, 18, 24, 27, 33, 51, 54, and 60 (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* and *para-meta-para* ribbons of edge-sharing $C_6(CF_3)_2$ hexagons (*i.e.*, a $p^3$mp,pmp overall addition pattern; see Schlegel diagram in Fig. 1). 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 the recently published structures of three other isomers of $C_{60}(CF_3)_{10}$ (see below), there are F···F intramolecular contacts between pairs of neighboring $CF_3$ groups that range from 2.565 (1) to 2.727 (1) Å.

There are now six isomers of $C_{60}(CF_3)_{10}$ that have been prepared at high temperature, isolated, and characterized. Fluorine-19 NMR spectroscopy has shown that one isomer, (I), has the ten $CF_3$ groups arranged on a ribbon of seven *meta*- and *para*-$C_6(CF_3)_2$ edge-sharing hexagons plus an isolated *para*-$C_6(CF_3)_2$ (Kareev *et al.*, 2005). The other four, $C_1$-$p^3$mpmpmp-$C_{60}(CF_3)_{10}$, (II) (Kareev, Lebedkin, Miller *et al.*, 2006), $C_1$-pm$p^3$mpmp-$C_{60}(CF_3)_{10}$, (III) (Kareev *et al.*, 2005), $C_2$-$[p^3m^2(\text{loop})]^2$– $C_{60}(CF_3)_{10}$, (IV) (Kareev, Lebedkin, Popov, *et al.*, 2006), and $C_1$-pmpmpmpmp-$C_{60}(CF_3)_{10}$, (V) (Popov *et al.*, 2007), have been structurally characterized by single-crystal X-ray diffraction. For comparison, Schlegel diagrams for the six isomers are shown in Fig. 2, arranged according to their DFT relative energies (Popov *et al.*, 2007). The pm$p^3$mpmp ribbon in (III) forms a loop in which two of the *meta*-$C_6(CF_3)_2$ hexagons have a common C($sp^2$)-C($sp^2$) bond (C2—C12). The structure of (IV) is significantly different than the other two isomers in that every $CF_3$ group has two $CF_3$ nearest neighbors (*i.e.*, there are no "terminal" $CF_3$ groups). Instead, it has two symmetry-related $p^3m^2$ loops of five edge-sharing $C_6(CF_3)_2$ hexagons that are joined by a C($sp^2$)-C($sp^2$) bond that is common to one of the *meta*-$C_6(CF_3)_2$ hexagons in each loop.

The four shortest cage C—C bonds in (VI) are C4—C5, 1.350 (4) Å, C7—C8, 1.351 (3) Å, C9—C10, 1.359 (3) Å, and C52—C53, 1.348 (4) 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, three of these bonds, C4—C5, C9—C10, and C52—C53, 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).

The structure of (VI), predicted to be the most stable isomer of $C_{60}(CF_3)_{10}$, demonstrates a new type of addition pattern for fullerene$(CF_3)_n$ derivatives with n = 4–12, two independent ribbons of edge-sharing $C_6(CF_3)_2$ hexagons, to go along with the other six types of addition patterns that have been observed, a single ribbon (*e.g.*, (II)), a ribbon plus an isolated *para*-$C_6(CF_3)_2$ hexagon (Kareev, Shustova, Newell *et al.*, 2006), a single loop of $C_6(CF_3)_2$ hexagons (Troyanov *et al.*, 2006), two loops (*e.g.*, (IV)), a loop plus an isolated hexagon (Shustova *et al.*, 2006), and a loop plus a ribbon (Shustova *et al.*, 2006).

## Experimental

The synthesis of (VI) was carried out by heating $C_{60}$ in a stream of $CF_3I$ at 460 °C as previously described (Kareev *et al.*, 2005). Crystals of the HPLC-purified compound were grown by slow evaporation of a saturated benzene solution.

## Figures

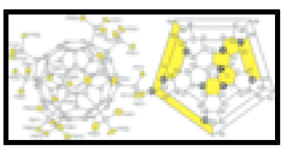

Fig. 1. Left: The molecular structure of (VI) (50% probability ellipsoids; F611 is attached to C61, F621 is attached to C62, *etc*.). Right: Schlegel diagram of (VI), showing the $C_{60}$ core carbon atom numbers (each core carbon atom bearing a $CF_3$ group is depicted as a black circle) and the $p^3mp$ and pmp ribbons 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).

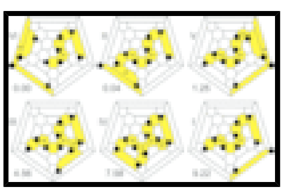

Fig. 2. Schlegel diagrams of (I)–(VI) showing the location of the $CF_3$ groups as black circles, the IUPAC lowest-locant numbers for the cage carbon atoms to which they are attached, the ribbons or loops of *meta*- and *para*-$C_6(CF_3)_2$ edge-sharing hexagons (*meta*-$C_6(CF_3)_2$ hexagons are indicated by the letter m), and the DFT-predicted relative energies.

## 1,6,11,18,24,27,33,51,54,60-Decakis(trifluoromethyl)- 1,6,11,18,24,27,33,51,54,60-decahydro($C_{60}$—$I_h$)[5,6]fullerene

*Crystal data*

| | |
|---|---|
| $C_{70}F_{30}$ | $V$ = 2281.36 (14) Å$^3$ |
| $M_r$ = 1410.70 | $Z$ = 2 |
| Triclinic, $P\bar{1}$ | $F_{000}$ = 1380 |
| Hall symbol: -P 1 | $D_x$ = 2.054 Mg m$^{-3}$ |
| $a$ = 11.0257 (4) Å | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| $b$ = 11.4172 (4) Å | μ = 0.21 mm$^{-1}$ |
| $c$ = 20.4527 (7) Å | $T$ = 296 (2) K |
| α = 82.369 (2)° | Plate, red |
| β = 77.010 (2)° | 0.20 × 0.15 × 0.07 mm |
| γ = 65.543 (2)° | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 10733 independent reflections |
| Radiation source: fine-focus sealed tube | 6553 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.071$ |
| Detector resolution: 0 pixels mm$^{-1}$ | $\theta_{max} = 27.9°$ |
| $T = 100(2)$ K | $\theta_{min} = 2.0°$ |
| φ and ω scans | $h = -14 \rightarrow 14$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $k = -15 \rightarrow 15$ |
| $T_{min} = 0.959$, $T_{max} = 0.986$ | $l = -26 \rightarrow 26$ |
| 77789 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.051$ | $w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 1.012P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.122$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.03$ | $\Delta\rho_{max} = 0.37$ e Å$^{-3}$ |
| 10733 reflections | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |
| 901 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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 | 0.2417 (2) | 0.7966 (2) | 0.34912 (13) | 0.0167 (5) |
| C2 | 0.2516 (2) | 0.7634 (2) | 0.27679 (12) | 0.0157 (5) |
| C3 | 0.2495 (2) | 0.8705 (2) | 0.23314 (13) | 0.0173 (6) |
| C4 | 0.2609 (2) | 0.9648 (2) | 0.27116 (13) | 0.0162 (5) |
| C5 | 0.2671 (2) | 0.9221 (2) | 0.33561 (13) | 0.0168 (6) |
| C6 | 0.3388 (2) | 0.9626 (2) | 0.37893 (13) | 0.0177 (6) |

| | | | | |
|---|---|---|---|---|
| C7 | 0.4466 (2) | 0.8404 (2) | 0.40600 (12) | 0.0169 (6) |
| C8 | 0.4474 (2) | 0.7213 (2) | 0.40838 (12) | 0.0162 (5) |
| C9 | 0.3574 (2) | 0.6916 (2) | 0.37692 (12) | 0.0162 (5) |
| C10 | 0.4272 (3) | 0.5707 (2) | 0.35399 (12) | 0.0162 (5) |
| C11 | 0.3963 (3) | 0.5230 (2) | 0.29636 (13) | 0.0176 (6) |
| C12 | 0.3211 (2) | 0.6414 (2) | 0.25287 (13) | 0.0162 (5) |
| C13 | 0.3861 (3) | 0.6252 (2) | 0.18461 (13) | 0.0175 (6) |
| C14 | 0.3740 (2) | 0.7309 (2) | 0.14025 (12) | 0.0166 (6) |
| C15 | 0.3069 (2) | 0.8550 (2) | 0.16543 (13) | 0.0167 (6) |
| C16 | 0.3800 (2) | 0.9347 (2) | 0.13014 (13) | 0.0166 (6) |
| C17 | 0.3899 (2) | 1.0259 (2) | 0.16422 (13) | 0.0168 (6) |
| C18 | 0.3072 (2) | 1.0677 (2) | 0.23469 (13) | 0.0178 (6) |
| C19 | 0.4165 (2) | 1.0723 (2) | 0.26848 (13) | 0.0169 (6) |
| C20 | 0.4315 (3) | 1.0228 (2) | 0.33214 (13) | 0.0189 (6) |
| C21 | 0.5635 (3) | 0.9656 (2) | 0.34854 (13) | 0.0173 (6) |
| C22 | 0.5765 (3) | 0.8555 (2) | 0.39425 (12) | 0.0180 (6) |
| C23 | 0.6973 (3) | 0.7512 (2) | 0.39117 (12) | 0.0177 (6) |
| C24 | 0.7061 (3) | 0.6125 (2) | 0.41016 (13) | 0.0184 (6) |
| C25 | 0.5740 (2) | 0.6062 (2) | 0.40545 (12) | 0.0169 (6) |
| C26 | 0.5631 (3) | 0.5161 (2) | 0.37195 (12) | 0.0168 (5) |
| C27 | 0.6828 (3) | 0.4085 (2) | 0.33531 (13) | 0.0185 (6) |
| C28 | 0.6564 (3) | 0.4076 (2) | 0.26429 (13) | 0.0183 (6) |
| C29 | 0.5305 (3) | 0.4583 (2) | 0.24692 (13) | 0.0175 (6) |
| C30 | 0.5150 (3) | 0.5120 (2) | 0.18045 (13) | 0.0172 (6) |
| C31 | 0.6259 (3) | 0.5114 (2) | 0.13233 (12) | 0.0173 (6) |
| C32 | 0.6174 (3) | 0.6223 (2) | 0.08498 (12) | 0.0174 (6) |
| C33 | 0.4824 (2) | 0.7288 (2) | 0.07731 (12) | 0.0165 (5) |
| C34 | 0.4910 (3) | 0.8593 (2) | 0.08202 (12) | 0.0168 (6) |
| C35 | 0.6130 (3) | 0.8730 (2) | 0.07202 (12) | 0.0160 (5) |
| C36 | 0.6250 (3) | 0.9616 (2) | 0.10971 (13) | 0.0166 (5) |
| C37 | 0.5142 (3) | 1.0392 (2) | 0.15430 (13) | 0.0173 (6) |
| C38 | 0.5328 (3) | 1.0666 (2) | 0.21882 (13) | 0.0173 (6) |
| C39 | 0.6600 (3) | 1.0195 (2) | 0.23429 (13) | 0.0176 (6) |
| C40 | 0.6768 (3) | 0.9647 (2) | 0.30016 (13) | 0.0189 (6) |
| C41 | 0.8032 (3) | 0.8540 (2) | 0.29596 (13) | 0.0188 (6) |
| C42 | 0.8110 (3) | 0.7479 (2) | 0.34053 (13) | 0.0186 (6) |
| C43 | 0.8836 (2) | 0.6200 (2) | 0.31604 (13) | 0.0182 (6) |
| C44 | 0.8164 (3) | 0.5385 (2) | 0.35195 (13) | 0.0192 (6) |
| C45 | 0.8045 (2) | 0.4494 (2) | 0.31806 (13) | 0.0191 (6) |
| C46 | 0.8588 (2) | 0.4371 (2) | 0.24768 (13) | 0.0178 (6) |
| C47 | 0.7705 (3) | 0.4108 (2) | 0.21537 (13) | 0.0183 (6) |
| C48 | 0.7565 (2) | 0.4596 (2) | 0.14998 (13) | 0.0168 (6) |
| C49 | 0.8269 (3) | 0.5382 (2) | 0.11544 (13) | 0.0180 (6) |
| C50 | 0.7365 (3) | 0.6373 (2) | 0.07528 (12) | 0.0165 (6) |
| C51 | 0.7523 (2) | 0.7629 (2) | 0.05412 (13) | 0.0179 (6) |
| C52 | 0.8333 (2) | 0.7879 (2) | 0.10011 (13) | 0.0174 (6) |
| C53 | 0.7617 (2) | 0.9049 (2) | 0.12601 (12) | 0.0169 (6) |
| C54 | 0.7919 (3) | 0.9537 (2) | 0.18355 (13) | 0.0189 (6) |
| C55 | 0.8700 (3) | 0.8365 (2) | 0.22661 (13) | 0.0185 (6) |

| | | | | |
|---|---|---|---|---|
| C56 | 0.9363 (2) | 0.7156 (2) | 0.20313 (13) | 0.0183 (6) |
| C57 | 0.9411 (2) | 0.6057 (2) | 0.24838 (13) | 0.0187 (6) |
| C58 | 0.9285 (2) | 0.5115 (2) | 0.21303 (13) | 0.0188 (6) |
| C59 | 0.9144 (2) | 0.5601 (2) | 0.14573 (13) | 0.0190 (6) |
| C60 | 0.9458 (2) | 0.6816 (2) | 0.13085 (13) | 0.0192 (6) |
| C61 | 0.7442 (3) | 0.5715 (3) | 0.47912 (14) | 0.0239 (6) |
| C62 | 0.7206 (3) | 0.2761 (3) | 0.37207 (14) | 0.0234 (6) |
| C63 | 0.3201 (3) | 0.4339 (3) | 0.31551 (13) | 0.0226 (6) |
| C64 | 0.1010 (3) | 0.8192 (3) | 0.39247 (13) | 0.0204 (6) |
| C65 | 0.2467 (3) | 1.0509 (3) | 0.43616 (14) | 0.0230 (6) |
| C66 | 0.1864 (3) | 1.1957 (2) | 0.22957 (13) | 0.0203 (6) |
| C67 | 0.8628 (3) | 1.0456 (3) | 0.15876 (14) | 0.0247 (6) |
| C68 | 1.0902 (3) | 0.6488 (3) | 0.09045 (13) | 0.0222 (6) |
| C69 | 0.8119 (3) | 0.7730 (3) | −0.02073 (14) | 0.0226 (6) |
| C70 | 0.4339 (3) | 0.7203 (2) | 0.01389 (14) | 0.0214 (6) |
| F611 | 0.76569 (16) | 0.44873 (15) | 0.49619 (8) | 0.0308 (4) |
| F612 | 0.85722 (16) | 0.58620 (16) | 0.48205 (8) | 0.0319 (4) |
| F613 | 0.64501 (16) | 0.64363 (15) | 0.52626 (7) | 0.0314 (4) |
| F621 | 0.74936 (18) | 0.27710 (15) | 0.43163 (8) | 0.0381 (4) |
| F622 | 0.62194 (17) | 0.23418 (15) | 0.38229 (9) | 0.0390 (4) |
| F623 | 0.82980 (17) | 0.18848 (15) | 0.33644 (8) | 0.0383 (4) |
| F631 | 0.39635 (16) | 0.31892 (14) | 0.33950 (8) | 0.0296 (4) |
| F632 | 0.20746 (15) | 0.48301 (15) | 0.36110 (8) | 0.0295 (4) |
| F633 | 0.28378 (18) | 0.41388 (16) | 0.26113 (8) | 0.0371 (4) |
| F642 | 0.06714 (15) | 0.72019 (15) | 0.39106 (8) | 0.0298 (4) |
| F641 | 0.09679 (15) | 0.83392 (17) | 0.45607 (8) | 0.0327 (4) |
| F643 | 0.00523 (14) | 0.92366 (15) | 0.37012 (8) | 0.0312 (4) |
| F651 | 0.19299 (17) | 0.98964 (16) | 0.48593 (8) | 0.0382 (4) |
| F652 | 0.31852 (17) | 1.09449 (18) | 0.46359 (9) | 0.0426 (5) |
| F653 | 0.14744 (18) | 1.15135 (17) | 0.41575 (8) | 0.0463 (5) |
| F661 | 0.12361 (15) | 1.24453 (14) | 0.28967 (7) | 0.0274 (4) |
| F662 | 0.22418 (15) | 1.28328 (13) | 0.19096 (7) | 0.0243 (4) |
| F663 | 0.09553 (15) | 1.17960 (14) | 0.20141 (8) | 0.0287 (4) |
| F671 | 0.97937 (16) | 0.99175 (16) | 0.11674 (8) | 0.0357 (4) |
| F672 | 0.78381 (17) | 1.15036 (15) | 0.12711 (8) | 0.0342 (4) |
| F673 | 0.88955 (17) | 1.08596 (16) | 0.21035 (8) | 0.0338 (4) |
| F681 | 1.11860 (16) | 0.75255 (16) | 0.07779 (9) | 0.0374 (4) |
| F682 | 1.18111 (15) | 0.56230 (16) | 0.12451 (8) | 0.0333 (4) |
| F683 | 1.10892 (16) | 0.59912 (18) | 0.03215 (8) | 0.0391 (4) |
| F691 | 0.92556 (16) | 0.67079 (16) | −0.04011 (8) | 0.0365 (4) |
| F692 | 0.72486 (16) | 0.78140 (15) | −0.05850 (7) | 0.0290 (4) |
| F693 | 0.84067 (17) | 0.87724 (16) | −0.03585 (8) | 0.0335 (4) |
| F701 | 0.52725 (16) | 0.70742 (16) | −0.04165 (7) | 0.0305 (4) |
| F702 | 0.39998 (15) | 0.61870 (14) | 0.01983 (7) | 0.0250 (4) |
| F703 | 0.32346 (15) | 0.82544 (14) | 0.00445 (8) | 0.0263 (4) |

*Atomic displacement parameters ($Å^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0127 (13) | 0.0197 (14) | 0.0188 (14) | −0.0072 (11) | −0.0034 (11) | −0.0011 (11) |
| C2 | 0.0083 (12) | 0.0215 (14) | 0.0201 (14) | −0.0083 (11) | −0.0034 (11) | −0.0006 (11) |
| C3 | 0.0083 (12) | 0.0192 (14) | 0.0246 (15) | −0.0046 (10) | −0.0045 (11) | −0.0021 (11) |
| C4 | 0.0063 (12) | 0.0167 (13) | 0.0216 (15) | −0.0015 (10) | 0.0008 (10) | −0.0035 (11) |
| C5 | 0.0091 (12) | 0.0160 (13) | 0.0241 (15) | −0.0038 (10) | −0.0021 (11) | −0.0021 (11) |
| C6 | 0.0150 (13) | 0.0174 (13) | 0.0200 (14) | −0.0062 (11) | −0.0008 (11) | −0.0037 (11) |
| C7 | 0.0149 (13) | 0.0220 (14) | 0.0145 (13) | −0.0078 (11) | −0.0013 (11) | −0.0038 (11) |
| C8 | 0.0150 (13) | 0.0199 (14) | 0.0138 (13) | −0.0077 (11) | −0.0013 (10) | −0.0007 (10) |
| C9 | 0.0157 (13) | 0.0194 (14) | 0.0168 (14) | −0.0111 (11) | −0.0025 (11) | 0.0017 (11) |
| C10 | 0.0186 (14) | 0.0161 (13) | 0.0158 (13) | −0.0103 (11) | −0.0026 (11) | 0.0032 (10) |
| C11 | 0.0174 (14) | 0.0147 (13) | 0.0221 (14) | −0.0079 (11) | −0.0032 (11) | −0.0011 (11) |
| C12 | 0.0116 (13) | 0.0207 (14) | 0.0226 (14) | −0.0118 (11) | −0.0057 (11) | 0.0007 (11) |
| C13 | 0.0162 (13) | 0.0198 (14) | 0.0219 (14) | −0.0107 (11) | −0.0070 (11) | −0.0014 (11) |
| C14 | 0.0156 (13) | 0.0208 (14) | 0.0184 (14) | −0.0099 (11) | −0.0077 (11) | −0.0001 (11) |
| C15 | 0.0104 (13) | 0.0179 (13) | 0.0237 (15) | −0.0051 (10) | −0.0075 (11) | −0.0013 (11) |
| C16 | 0.0140 (13) | 0.0187 (13) | 0.0190 (14) | −0.0072 (11) | −0.0080 (11) | 0.0042 (11) |
| C17 | 0.0127 (13) | 0.0143 (13) | 0.0206 (14) | −0.0026 (10) | −0.0055 (11) | 0.0025 (10) |
| C18 | 0.0149 (13) | 0.0150 (13) | 0.0233 (15) | −0.0052 (11) | −0.0050 (11) | 0.0001 (11) |
| C19 | 0.0150 (13) | 0.0099 (12) | 0.0257 (15) | −0.0040 (10) | −0.0041 (11) | −0.0027 (11) |
| C20 | 0.0173 (14) | 0.0145 (13) | 0.0260 (15) | −0.0066 (11) | −0.0013 (11) | −0.0087 (11) |
| C21 | 0.0176 (14) | 0.0171 (13) | 0.0217 (14) | −0.0096 (11) | −0.0046 (11) | −0.0051 (11) |
| C22 | 0.0191 (14) | 0.0241 (14) | 0.0146 (13) | −0.0112 (12) | −0.0027 (11) | −0.0056 (11) |
| C23 | 0.0174 (14) | 0.0232 (14) | 0.0174 (14) | −0.0106 (11) | −0.0081 (11) | −0.0011 (11) |
| C24 | 0.0138 (13) | 0.0242 (14) | 0.0183 (14) | −0.0074 (11) | −0.0053 (11) | −0.0013 (11) |
| C25 | 0.0150 (13) | 0.0201 (14) | 0.0173 (14) | −0.0085 (11) | −0.0058 (11) | 0.0030 (11) |
| C26 | 0.0175 (14) | 0.0177 (13) | 0.0153 (13) | −0.0087 (11) | −0.0034 (11) | 0.0051 (10) |
| C27 | 0.0176 (14) | 0.0168 (13) | 0.0219 (14) | −0.0075 (11) | −0.0048 (11) | 0.0002 (11) |
| C28 | 0.0219 (14) | 0.0106 (12) | 0.0232 (15) | −0.0063 (11) | −0.0071 (12) | 0.0003 (10) |
| C29 | 0.0216 (14) | 0.0117 (13) | 0.0226 (15) | −0.0105 (11) | −0.0032 (12) | −0.0008 (11) |
| C30 | 0.0186 (14) | 0.0140 (13) | 0.0225 (14) | −0.0090 (11) | −0.0042 (11) | −0.0033 (11) |
| C31 | 0.0208 (14) | 0.0151 (13) | 0.0175 (14) | −0.0068 (11) | −0.0056 (11) | −0.0041 (10) |
| C32 | 0.0184 (14) | 0.0172 (13) | 0.0179 (14) | −0.0079 (11) | −0.0018 (11) | −0.0053 (11) |
| C33 | 0.0151 (13) | 0.0181 (13) | 0.0161 (13) | −0.0057 (11) | −0.0036 (11) | −0.0013 (10) |
| C34 | 0.0179 (14) | 0.0174 (13) | 0.0159 (14) | −0.0068 (11) | −0.0073 (11) | 0.0024 (10) |
| C35 | 0.0178 (14) | 0.0140 (13) | 0.0148 (13) | −0.0062 (10) | −0.0041 (11) | 0.0051 (10) |
| C36 | 0.0168 (13) | 0.0162 (13) | 0.0192 (14) | −0.0104 (11) | −0.0033 (11) | 0.0038 (10) |
| C37 | 0.0180 (14) | 0.0124 (13) | 0.0216 (14) | −0.0066 (11) | −0.0046 (11) | 0.0022 (11) |
| C38 | 0.0199 (14) | 0.0096 (12) | 0.0228 (14) | −0.0068 (11) | −0.0029 (11) | −0.0008 (10) |
| C39 | 0.0194 (14) | 0.0155 (13) | 0.0223 (15) | −0.0112 (11) | −0.0031 (11) | −0.0022 (11) |
| C40 | 0.0198 (14) | 0.0176 (14) | 0.0263 (15) | −0.0122 (11) | −0.0060 (12) | −0.0057 (11) |
| C41 | 0.0145 (13) | 0.0249 (14) | 0.0245 (15) | −0.0129 (11) | −0.0076 (11) | −0.0022 (12) |
| C42 | 0.0135 (13) | 0.0255 (15) | 0.0215 (14) | −0.0101 (11) | −0.0078 (11) | −0.0011 (11) |
| C43 | 0.0093 (13) | 0.0229 (14) | 0.0240 (15) | −0.0061 (11) | −0.0083 (11) | 0.0014 (11) |
| C44 | 0.0139 (13) | 0.0224 (14) | 0.0194 (14) | −0.0036 (11) | −0.0082 (11) | 0.0016 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C45 | 0.0119 (13) | 0.0175 (13) | 0.0243 (15) | −0.0009 (11) | −0.0083 (11) | 0.0026 (11) |
| C46 | 0.0136 (13) | 0.0117 (13) | 0.0226 (15) | 0.0000 (10) | −0.0035 (11) | 0.0006 (11) |
| C47 | 0.0178 (14) | 0.0091 (12) | 0.0248 (15) | −0.0008 (10) | −0.0055 (12) | −0.0026 (11) |
| C48 | 0.0163 (13) | 0.0129 (13) | 0.0197 (14) | −0.0033 (11) | −0.0035 (11) | −0.0037 (10) |
| C49 | 0.0150 (13) | 0.0174 (13) | 0.0187 (14) | −0.0032 (11) | −0.0013 (11) | −0.0053 (11) |
| C50 | 0.0178 (14) | 0.0162 (13) | 0.0142 (13) | −0.0047 (11) | −0.0021 (11) | −0.0048 (10) |
| C51 | 0.0142 (13) | 0.0201 (14) | 0.0201 (14) | −0.0077 (11) | −0.0029 (11) | −0.0012 (11) |
| C52 | 0.0137 (13) | 0.0224 (14) | 0.0178 (14) | −0.0115 (11) | 0.0009 (11) | 0.0014 (11) |
| C53 | 0.0145 (13) | 0.0210 (14) | 0.0171 (14) | −0.0112 (11) | −0.0004 (11) | 0.0021 (11) |
| C54 | 0.0159 (13) | 0.0193 (14) | 0.0251 (15) | −0.0105 (11) | −0.0037 (11) | −0.0016 (11) |
| C55 | 0.0136 (13) | 0.0255 (15) | 0.0233 (15) | −0.0142 (11) | −0.0053 (11) | 0.0013 (11) |
| C56 | 0.0082 (13) | 0.0235 (14) | 0.0256 (15) | −0.0079 (11) | −0.0045 (11) | −0.0014 (11) |
| C57 | 0.0071 (12) | 0.0196 (14) | 0.0277 (15) | −0.0027 (10) | −0.0042 (11) | −0.0028 (11) |
| C58 | 0.0087 (12) | 0.0186 (14) | 0.0249 (15) | −0.0004 (11) | −0.0044 (11) | −0.0027 (11) |
| C59 | 0.0096 (13) | 0.0190 (14) | 0.0240 (15) | −0.0025 (11) | 0.0004 (11) | −0.0030 (11) |
| C60 | 0.0114 (13) | 0.0225 (14) | 0.0241 (15) | −0.0065 (11) | −0.0036 (11) | −0.0028 (11) |
| C61 | 0.0186 (15) | 0.0280 (16) | 0.0243 (16) | −0.0080 (12) | −0.0062 (12) | 0.0013 (12) |
| C62 | 0.0253 (15) | 0.0199 (14) | 0.0247 (16) | −0.0088 (12) | −0.0060 (12) | 0.0010 (12) |
| C63 | 0.0284 (16) | 0.0252 (15) | 0.0214 (15) | −0.0177 (13) | −0.0059 (13) | 0.0003 (12) |
| C64 | 0.0160 (14) | 0.0245 (15) | 0.0206 (15) | −0.0073 (12) | −0.0049 (11) | −0.0008 (11) |
| C65 | 0.0221 (15) | 0.0214 (15) | 0.0258 (16) | −0.0086 (12) | −0.0038 (12) | −0.0035 (12) |
| C66 | 0.0175 (14) | 0.0203 (14) | 0.0230 (15) | −0.0078 (11) | −0.0038 (12) | −0.0002 (12) |
| C67 | 0.0225 (15) | 0.0303 (16) | 0.0272 (16) | −0.0165 (13) | −0.0034 (13) | −0.0026 (13) |
| C68 | 0.0165 (14) | 0.0268 (15) | 0.0232 (15) | −0.0090 (12) | −0.0035 (12) | 0.0008 (12) |
| C69 | 0.0187 (14) | 0.0215 (15) | 0.0257 (16) | −0.0066 (12) | −0.0034 (12) | −0.0008 (12) |
| C70 | 0.0201 (14) | 0.0199 (14) | 0.0260 (16) | −0.0095 (12) | −0.0051 (12) | 0.0000 (12) |
| F611 | 0.0380 (10) | 0.0272 (9) | 0.0290 (9) | −0.0125 (8) | −0.0150 (8) | 0.0069 (7) |
| F612 | 0.0239 (9) | 0.0477 (11) | 0.0315 (9) | −0.0188 (8) | −0.0144 (7) | 0.0040 (8) |
| F613 | 0.0297 (9) | 0.0385 (10) | 0.0221 (9) | −0.0084 (8) | −0.0057 (7) | −0.0049 (7) |
| F621 | 0.0600 (12) | 0.0261 (9) | 0.0295 (10) | −0.0140 (9) | −0.0216 (9) | 0.0063 (7) |
| F622 | 0.0401 (11) | 0.0271 (9) | 0.0567 (12) | −0.0209 (8) | −0.0176 (9) | 0.0149 (8) |
| F623 | 0.0407 (10) | 0.0186 (9) | 0.0365 (10) | 0.0028 (8) | −0.0011 (8) | 0.0020 (7) |
| F631 | 0.0359 (10) | 0.0206 (9) | 0.0370 (10) | −0.0171 (8) | −0.0074 (8) | 0.0037 (7) |
| F632 | 0.0235 (9) | 0.0322 (9) | 0.0370 (10) | −0.0189 (7) | 0.0011 (8) | 0.0000 (7) |
| F633 | 0.0585 (12) | 0.0481 (11) | 0.0296 (10) | −0.0434 (10) | −0.0159 (9) | 0.0040 (8) |
| F642 | 0.0199 (8) | 0.0326 (9) | 0.0419 (10) | −0.0176 (7) | −0.0008 (7) | −0.0029 (8) |
| F641 | 0.0221 (9) | 0.0543 (11) | 0.0219 (9) | −0.0162 (8) | 0.0015 (7) | −0.0086 (8) |
| F643 | 0.0131 (8) | 0.0317 (9) | 0.0407 (10) | −0.0046 (7) | −0.0026 (7) | 0.0058 (8) |
| F651 | 0.0439 (11) | 0.0340 (10) | 0.0306 (10) | −0.0176 (8) | 0.0139 (8) | −0.0090 (8) |
| F652 | 0.0374 (10) | 0.0561 (12) | 0.0432 (11) | −0.0252 (9) | 0.0053 (8) | −0.0320 (9) |
| F653 | 0.0426 (11) | 0.0359 (11) | 0.0331 (10) | 0.0149 (8) | −0.0095 (9) | −0.0101 (8) |
| F661 | 0.0238 (9) | 0.0227 (9) | 0.0260 (9) | −0.0008 (7) | −0.0010 (7) | −0.0037 (7) |
| F662 | 0.0270 (9) | 0.0166 (8) | 0.0272 (9) | −0.0066 (7) | −0.0058 (7) | 0.0006 (7) |
| F663 | 0.0218 (9) | 0.0218 (8) | 0.0433 (10) | −0.0049 (7) | −0.0153 (8) | −0.0010 (7) |
| F671 | 0.0310 (10) | 0.0389 (10) | 0.0427 (11) | −0.0246 (8) | 0.0071 (8) | −0.0078 (8) |
| F672 | 0.0416 (10) | 0.0272 (9) | 0.0425 (10) | −0.0223 (8) | −0.0142 (8) | 0.0095 (8) |
| F673 | 0.0378 (10) | 0.0403 (10) | 0.0387 (10) | −0.0293 (9) | −0.0082 (8) | −0.0045 (8) |
| F681 | 0.0198 (9) | 0.0309 (10) | 0.0591 (12) | −0.0140 (8) | 0.0033 (8) | 0.0004 (8) |
| F682 | 0.0128 (8) | 0.0401 (10) | 0.0383 (10) | −0.0047 (7) | −0.0026 (7) | 0.0036 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F683 | 0.0230 (9) | 0.0627 (12) | 0.0328 (10) | −0.0190 (9) | 0.0053 (8) | −0.0176 (9) |
| F691 | 0.0265 (9) | 0.0357 (10) | 0.0288 (10) | 0.0025 (8) | 0.0030 (7) | −0.0042 (8) |
| F692 | 0.0293 (9) | 0.0423 (10) | 0.0204 (9) | −0.0186 (8) | −0.0073 (7) | 0.0010 (7) |
| F693 | 0.0423 (10) | 0.0378 (10) | 0.0286 (9) | −0.0283 (9) | −0.0001 (8) | 0.0013 (7) |
| F701 | 0.0265 (9) | 0.0475 (11) | 0.0211 (9) | −0.0190 (8) | −0.0014 (7) | −0.0043 (7) |
| F702 | 0.0282 (9) | 0.0240 (8) | 0.0287 (9) | −0.0136 (7) | −0.0088 (7) | −0.0033 (7) |
| F703 | 0.0255 (9) | 0.0251 (9) | 0.0312 (9) | −0.0100 (7) | −0.0131 (7) | 0.0024 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C9 | 1.505 (3) | C36—C37 | 1.388 (3) |
| C1—C64 | 1.539 (4) | C36—C53 | 1.470 (3) |
| C1—C2 | 1.545 (3) | C37—C38 | 1.472 (4) |
| C1—C5 | 1.549 (3) | C38—C39 | 1.373 (4) |
| C2—C12 | 1.377 (3) | C39—C40 | 1.426 (4) |
| C2—C3 | 1.410 (4) | C39—C54 | 1.543 (4) |
| C3—C15 | 1.389 (4) | C40—C41 | 1.437 (4) |
| C3—C4 | 1.469 (3) | C41—C42 | 1.401 (4) |
| C4—C5 | 1.350 (4) | C41—C55 | 1.441 (4) |
| C4—C18 | 1.513 (4) | C42—C43 | 1.438 (4) |
| C5—C6 | 1.532 (3) | C43—C57 | 1.387 (4) |
| C6—C65 | 1.533 (4) | C43—C44 | 1.449 (4) |
| C6—C7 | 1.544 (3) | C44—C45 | 1.368 (4) |
| C6—C20 | 1.550 (4) | C45—C46 | 1.431 (4) |
| C7—C8 | 1.351 (3) | C46—C58 | 1.397 (4) |
| C7—C22 | 1.475 (4) | C46—C47 | 1.435 (4) |
| C8—C9 | 1.462 (3) | C47—C48 | 1.395 (4) |
| C8—C25 | 1.464 (3) | C48—C49 | 1.439 (4) |
| C9—C10 | 1.359 (3) | C49—C59 | 1.373 (4) |
| C10—C26 | 1.477 (3) | C49—C50 | 1.461 (3) |
| C10—C11 | 1.519 (3) | C50—C51 | 1.511 (4) |
| C11—C63 | 1.532 (4) | C51—C69 | 1.534 (4) |
| C11—C29 | 1.542 (4) | C51—C52 | 1.556 (3) |
| C11—C12 | 1.546 (3) | C52—C53 | 1.348 (4) |
| C12—C13 | 1.416 (4) | C52—C60 | 1.519 (4) |
| C13—C14 | 1.389 (4) | C53—C54 | 1.520 (4) |
| C13—C30 | 1.466 (3) | C54—C67 | 1.525 (4) |
| C14—C15 | 1.405 (3) | C54—C55 | 1.543 (4) |
| C14—C33 | 1.542 (4) | C55—C56 | 1.361 (4) |
| C15—C16 | 1.473 (4) | C56—C57 | 1.447 (4) |
| C16—C17 | 1.380 (3) | C56—C60 | 1.548 (4) |
| C16—C34 | 1.421 (4) | C57—C58 | 1.439 (4) |
| C17—C37 | 1.408 (4) | C58—C59 | 1.431 (4) |
| C17—C18 | 1.539 (4) | C59—C60 | 1.541 (4) |
| C18—C66 | 1.527 (3) | C60—C68 | 1.534 (4) |
| C18—C19 | 1.539 (3) | C61—F611 | 1.333 (3) |
| C19—C20 | 1.366 (4) | C61—F612 | 1.339 (3) |
| C19—C38 | 1.430 (4) | C61—F613 | 1.340 (3) |
| C20—C21 | 1.425 (4) | C62—F622 | 1.326 (3) |

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|---|---|---|---|
| C21—C40 | 1.405 (4) | C62—F621 | 1.328 (3) |
| C21—C22 | 1.440 (4) | C62—F623 | 1.335 (3) |
| C22—C23 | 1.366 (4) | C63—F632 | 1.329 (3) |
| C23—C42 | 1.425 (4) | C63—F631 | 1.331 (3) |
| C23—C24 | 1.548 (4) | C63—F633 | 1.339 (3) |
| C24—C25 | 1.512 (3) | C64—F641 | 1.322 (3) |
| C24—C61 | 1.521 (4) | C64—F643 | 1.333 (3) |
| C24—C44 | 1.541 (4) | C64—F642 | 1.335 (3) |
| C25—C26 | 1.367 (3) | C65—F653 | 1.313 (3) |
| C26—C27 | 1.506 (3) | C65—F651 | 1.326 (3) |
| C27—C62 | 1.531 (4) | C65—F652 | 1.338 (3) |
| C27—C28 | 1.546 (4) | C66—F661 | 1.334 (3) |
| C27—C45 | 1.550 (4) | C66—F662 | 1.335 (3) |
| C28—C29 | 1.375 (4) | C66—F663 | 1.346 (3) |
| C28—C47 | 1.431 (4) | C67—F671 | 1.326 (3) |
| C29—C30 | 1.432 (4) | C67—F672 | 1.339 (3) |
| C30—C31 | 1.385 (4) | C67—F673 | 1.340 (3) |
| C31—C48 | 1.423 (3) | C68—F681 | 1.326 (3) |
| C31—C32 | 1.472 (4) | C68—F683 | 1.326 (3) |
| C32—C50 | 1.361 (4) | C68—F682 | 1.333 (3) |
| C32—C33 | 1.509 (3) | C69—F692 | 1.328 (3) |
| C33—C70 | 1.539 (4) | C69—F691 | 1.333 (3) |
| C33—C34 | 1.547 (3) | C69—F693 | 1.335 (3) |
| C34—C35 | 1.386 (4) | C70—F701 | 1.329 (3) |
| C35—C36 | 1.414 (3) | C70—F703 | 1.339 (3) |
| C35—C51 | 1.531 (3) | C70—F702 | 1.342 (3) |
| C9—C1—C64 | 114.0 (2) | C38—C39—C40 | 118.5 (2) |
| C9—C1—C2 | 107.7 (2) | C38—C39—C54 | 123.6 (2) |
| C64—C1—C2 | 111.8 (2) | C40—C39—C54 | 109.8 (2) |
| C9—C1—C5 | 109.8 (2) | C21—C40—C39 | 120.0 (2) |
| C64—C1—C5 | 111.9 (2) | C21—C40—C41 | 120.1 (2) |
| C2—C1—C5 | 100.83 (19) | C39—C40—C41 | 109.2 (2) |
| C12—C2—C3 | 119.2 (2) | C42—C41—C40 | 118.9 (2) |
| C12—C2—C1 | 123.8 (2) | C42—C41—C55 | 120.9 (2) |
| C3—C2—C1 | 108.9 (2) | C40—C41—C55 | 109.2 (2) |
| C15—C3—C2 | 120.8 (2) | C41—C42—C23 | 120.8 (2) |
| C15—C3—C4 | 121.3 (2) | C41—C42—C43 | 119.3 (2) |
| C2—C3—C4 | 108.0 (2) | C23—C42—C43 | 109.5 (2) |
| C5—C4—C3 | 110.7 (2) | C57—C43—C42 | 118.8 (2) |
| C5—C4—C18 | 125.9 (2) | C57—C43—C44 | 121.1 (2) |
| C3—C4—C18 | 120.3 (2) | C42—C43—C44 | 108.8 (2) |
| C4—C5—C6 | 122.8 (2) | C45—C44—C43 | 119.6 (2) |
| C4—C5—C1 | 109.9 (2) | C45—C44—C24 | 122.8 (2) |
| C6—C5—C1 | 123.8 (2) | C43—C44—C24 | 109.2 (2) |
| C5—C6—C65 | 116.1 (2) | C44—C45—C46 | 119.8 (2) |
| C5—C6—C7 | 108.8 (2) | C44—C45—C27 | 124.1 (2) |
| C65—C6—C7 | 110.8 (2) | C46—C45—C27 | 109.0 (2) |
| C5—C6—C20 | 108.5 (2) | C58—C46—C45 | 121.2 (2) |
| C65—C6—C20 | 111.2 (2) | C58—C46—C47 | 119.2 (2) |

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| C7—C6—C20 | 100.25 (19) | C45—C46—C47 | 109.5 (2) |
| C8—C7—C22 | 119.4 (2) | C48—C47—C28 | 121.0 (2) |
| C8—C7—C6 | 123.9 (2) | C48—C47—C46 | 119.3 (2) |
| C22—C7—C6 | 109.5 (2) | C28—C47—C46 | 109.2 (2) |
| C7—C8—C9 | 123.2 (2) | C47—C48—C31 | 119.5 (2) |
| C7—C8—C25 | 121.1 (2) | C47—C48—C49 | 120.7 (2) |
| C9—C8—C25 | 107.2 (2) | C31—C48—C49 | 107.3 (2) |
| C10—C9—C8 | 107.5 (2) | C59—C49—C48 | 119.7 (2) |
| C10—C9—C1 | 125.7 (2) | C59—C49—C50 | 122.9 (2) |
| C8—C9—C1 | 121.4 (2) | C48—C49—C50 | 107.3 (2) |
| C9—C10—C26 | 109.3 (2) | C32—C50—C49 | 109.2 (2) |
| C9—C10—C11 | 123.7 (2) | C32—C50—C51 | 124.7 (2) |
| C26—C10—C11 | 122.6 (2) | C49—C50—C51 | 121.0 (2) |
| C10—C11—C63 | 116.4 (2) | C50—C51—C35 | 108.0 (2) |
| C10—C11—C29 | 108.2 (2) | C50—C51—C69 | 113.4 (2) |
| C63—C11—C29 | 110.7 (2) | C35—C51—C69 | 110.5 (2) |
| C10—C11—C12 | 108.1 (2) | C50—C51—C52 | 110.5 (2) |
| C63—C11—C12 | 111.4 (2) | C35—C51—C52 | 101.25 (19) |
| C29—C11—C12 | 100.8 (2) | C69—C51—C52 | 112.5 (2) |
| C2—C12—C13 | 119.8 (2) | C53—C52—C60 | 123.2 (2) |
| C2—C12—C11 | 123.1 (2) | C53—C52—C51 | 109.6 (2) |
| C13—C12—C11 | 110.0 (2) | C60—C52—C51 | 123.7 (2) |
| C14—C13—C12 | 120.9 (2) | C52—C53—C36 | 110.6 (2) |
| C14—C13—C30 | 120.5 (2) | C52—C53—C54 | 125.4 (2) |
| C12—C13—C30 | 108.7 (2) | C36—C53—C54 | 120.7 (2) |
| C13—C14—C15 | 118.8 (2) | C53—C54—C67 | 112.0 (2) |
| C13—C14—C33 | 123.1 (2) | C53—C54—C39 | 110.2 (2) |
| C15—C14—C33 | 110.6 (2) | C67—C54—C39 | 110.4 (2) |
| C3—C15—C14 | 120.0 (2) | C53—C54—C55 | 108.4 (2) |
| C3—C15—C16 | 120.1 (2) | C67—C54—C55 | 114.2 (2) |
| C14—C15—C16 | 108.4 (2) | C39—C54—C55 | 101.0 (2) |
| C17—C16—C34 | 121.0 (2) | C56—C55—C41 | 119.8 (2) |
| C17—C16—C15 | 119.9 (2) | C56—C55—C54 | 122.6 (2) |
| C34—C16—C15 | 108.8 (2) | C41—C55—C54 | 109.1 (2) |
| C16—C17—C37 | 119.6 (2) | C55—C56—C57 | 119.6 (2) |
| C16—C17—C18 | 123.3 (2) | C55—C56—C60 | 124.3 (2) |
| C37—C17—C18 | 110.4 (2) | C57—C56—C60 | 109.1 (2) |
| C4—C18—C66 | 111.0 (2) | C43—C57—C58 | 119.1 (2) |
| C4—C18—C17 | 110.8 (2) | C43—C57—C56 | 121.5 (2) |
| C66—C18—C17 | 110.1 (2) | C58—C57—C56 | 108.8 (2) |
| C4—C18—C19 | 108.5 (2) | C46—C58—C59 | 120.9 (2) |
| C66—C18—C19 | 115.2 (2) | C46—C58—C57 | 119.2 (2) |
| C17—C18—C19 | 100.76 (19) | C59—C58—C57 | 109.0 (2) |
| C20—C19—C38 | 120.0 (2) | C49—C59—C58 | 119.9 (2) |
| C20—C19—C18 | 122.4 (2) | C49—C59—C60 | 123.5 (2) |
| C38—C19—C18 | 109.9 (2) | C58—C59—C60 | 109.9 (2) |
| C19—C20—C21 | 119.6 (2) | C52—C60—C68 | 115.8 (2) |
| C19—C20—C6 | 124.6 (2) | C52—C60—C59 | 109.4 (2) |
| C21—C20—C6 | 109.4 (2) | C68—C60—C59 | 110.6 (2) |

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| C40—C21—C20 | 120.1 (2) | C52—C60—C56 | 109.2 (2) |
| C40—C21—C22 | 119.3 (2) | C68—C60—C56 | 110.4 (2) |
| C20—C21—C22 | 110.7 (2) | C59—C60—C56 | 100.3 (2) |
| C23—C22—C21 | 120.7 (2) | F611—C61—F612 | 107.2 (2) |
| C23—C22—C7 | 121.5 (2) | F611—C61—F613 | 107.5 (2) |
| C21—C22—C7 | 106.9 (2) | F612—C61—F613 | 107.4 (2) |
| C22—C23—C42 | 120.1 (2) | F611—C61—C24 | 112.7 (2) |
| C22—C23—C24 | 122.5 (2) | F612—C61—C24 | 111.5 (2) |
| C42—C23—C24 | 109.6 (2) | F613—C61—C24 | 110.3 (2) |
| C25—C24—C61 | 113.7 (2) | F622—C62—F621 | 107.3 (2) |
| C25—C24—C44 | 108.4 (2) | F622—C62—F623 | 107.0 (2) |
| C61—C24—C44 | 114.4 (2) | F621—C62—F623 | 107.3 (2) |
| C25—C24—C23 | 109.3 (2) | F622—C62—C27 | 112.3 (2) |
| C61—C24—C23 | 109.4 (2) | F621—C62—C27 | 111.9 (2) |
| C44—C24—C23 | 100.8 (2) | F623—C62—C27 | 110.7 (2) |
| C26—C25—C8 | 107.7 (2) | F632—C63—F631 | 107.8 (2) |
| C26—C25—C24 | 125.0 (2) | F632—C63—F633 | 107.3 (2) |
| C8—C25—C24 | 122.1 (2) | F631—C63—F633 | 107.0 (2) |
| C25—C26—C10 | 108.2 (2) | F632—C63—C11 | 112.6 (2) |
| C25—C26—C27 | 123.9 (2) | F631—C63—C11 | 112.2 (2) |
| C10—C26—C27 | 123.4 (2) | F633—C63—C11 | 109.8 (2) |
| C26—C27—C62 | 115.3 (2) | F641—C64—F643 | 108.2 (2) |
| C26—C27—C28 | 107.9 (2) | F641—C64—F642 | 107.1 (2) |
| C62—C27—C28 | 112.6 (2) | F643—C64—F642 | 107.0 (2) |
| C26—C27—C45 | 107.9 (2) | F641—C64—C1 | 111.9 (2) |
| C62—C27—C45 | 111.2 (2) | F643—C64—C1 | 111.0 (2) |
| C28—C27—C45 | 100.8 (2) | F642—C64—C1 | 111.4 (2) |
| C29—C28—C47 | 119.1 (2) | F653—C65—F651 | 108.2 (2) |
| C29—C28—C27 | 124.9 (2) | F653—C65—F652 | 107.7 (2) |
| C47—C28—C27 | 109.2 (2) | F651—C65—F652 | 105.5 (2) |
| C28—C29—C30 | 120.1 (2) | F653—C65—C6 | 112.5 (2) |
| C28—C29—C11 | 124.1 (2) | F651—C65—C6 | 112.3 (2) |
| C30—C29—C11 | 109.4 (2) | F652—C65—C6 | 110.2 (2) |
| C31—C30—C29 | 121.0 (2) | F661—C66—F662 | 108.0 (2) |
| C31—C30—C13 | 119.6 (2) | F661—C66—F663 | 108.0 (2) |
| C29—C30—C13 | 108.7 (2) | F662—C66—F663 | 107.0 (2) |
| C30—C31—C48 | 119.3 (2) | F661—C66—C18 | 111.9 (2) |
| C30—C31—C32 | 121.4 (2) | F662—C66—C18 | 111.6 (2) |
| C48—C31—C32 | 107.8 (2) | F663—C66—C18 | 110.1 (2) |
| C50—C32—C31 | 108.4 (2) | F671—C67—F672 | 107.8 (2) |
| C50—C32—C33 | 124.9 (2) | F671—C67—F673 | 107.4 (2) |
| C31—C32—C33 | 121.2 (2) | F672—C67—F673 | 107.2 (2) |
| C32—C33—C70 | 113.3 (2) | F671—C67—C54 | 112.7 (2) |
| C32—C33—C14 | 110.3 (2) | F672—C67—C54 | 110.8 (2) |
| C70—C33—C14 | 110.1 (2) | F673—C67—C54 | 110.8 (2) |
| C32—C33—C34 | 108.4 (2) | F681—C68—F683 | 107.7 (2) |
| C70—C33—C34 | 113.5 (2) | F681—C68—F682 | 107.7 (2) |
| C14—C33—C34 | 100.45 (19) | F683—C68—F682 | 107.0 (2) |
| C35—C34—C16 | 119.2 (2) | F681—C68—C60 | 111.1 (2) |

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|---|---|---|---|
| C35—C34—C33 | 122.8 (2) | F683—C68—C60 | 112.5 (2) |
| C16—C34—C33 | 109.7 (2) | F682—C68—C60 | 110.6 (2) |
| C34—C35—C36 | 119.6 (2) | F692—C69—F691 | 106.8 (2) |
| C34—C35—C51 | 124.1 (2) | F692—C69—F693 | 107.2 (2) |
| C36—C35—C51 | 108.8 (2) | F691—C69—F693 | 107.5 (2) |
| C37—C36—C35 | 120.7 (2) | F692—C69—C51 | 111.0 (2) |
| C37—C36—C53 | 121.0 (2) | F691—C69—C51 | 112.4 (2) |
| C35—C36—C53 | 108.1 (2) | F693—C69—C51 | 111.7 (2) |
| C36—C37—C17 | 119.7 (2) | F701—C70—F703 | 107.5 (2) |
| C36—C37—C38 | 120.0 (2) | F701—C70—F702 | 107.2 (2) |
| C17—C37—C38 | 108.8 (2) | F703—C70—F702 | 107.1 (2) |
| C39—C38—C19 | 121.6 (2) | F701—C70—C33 | 113.2 (2) |
| C39—C38—C37 | 120.4 (2) | F703—C70—C33 | 111.1 (2) |
| C19—C38—C37 | 108.2 (2) | F702—C70—C33 | 110.4 (2) |

**Fig. 1**

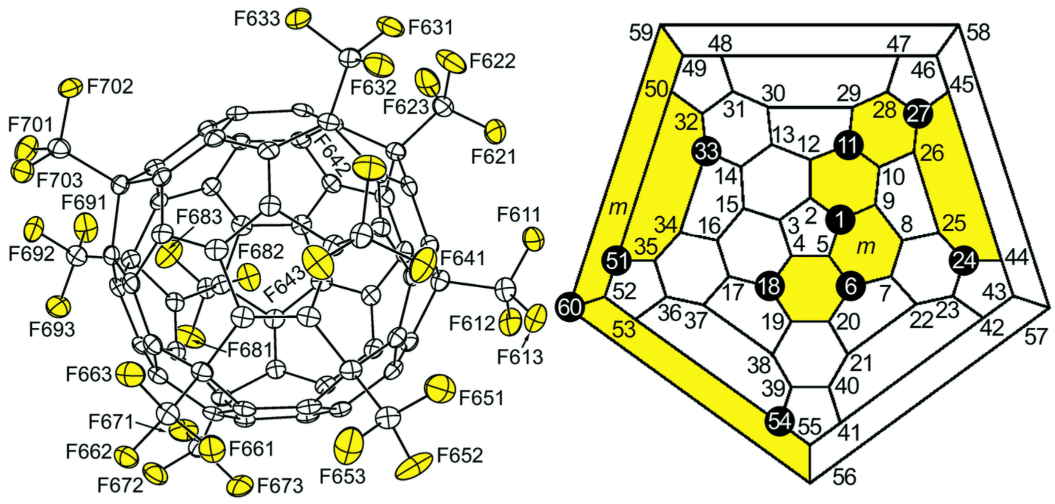
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Fig. 2