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1,3,7,10,14,17,21,28,31,42,52,55-Dodecakis(trifluoromethyl)-1,3,7,10,14,17,21,28,31,42,52,55-dodecahydro(C_{60}-I_h)[5,6]fullerene

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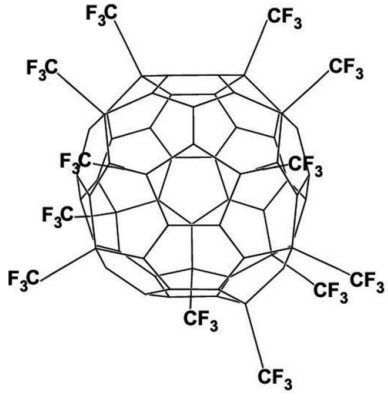
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.058; wR factor = 0.160; data-to-parameter ratio = 10.3.

The title compound, $C_{72}F_{36}$, is one of four isomers of $C_{60}(CF_3)_{12}$ for which crystal structures have been obtained. The fullerene molecule has an idealized I_h C_{60} core with the 12 CF_3 groups arranged in an asymmetric fashion on two ribbons of edge-sharing $C_6(CF_3)_2$ hexagons, a *para–meta–para–para–para–meta–para* ribbon and a *para–meta–para* ribbon, giving an overall *pmp*^{3}*mp*,*pmp* structure. There are no cage C*sp*^{3}—C*sp*^{3} bonds. The F atoms of two CF_3 groups are disordered over two positions; the site occupancy factors are 0.85/0.15 and 0.73/0.27. There are intramolecular F···F contacts between pairs of CF_3 groups on the same hexagon that range from 2.521 (3) to 2.738 (4) Å.

Related literature

For related literature, see: Kareev *et al.* (2005, 2007); Omelyanyuk *et al.* (2007); Popov *et al.* (2007); Powell *et al.* (2002); Troyanov *et al.* (2006).



Experimental

Crystal data

$C_{72}F_{36}$
M_r = 1548.72
Monoclinic, $P2_1/n$
a = 12.2475 (2) Å
b = 20.0326 (4) Å
c = 20.3782 (4) Å
β = 90.288 (1)°
V = 4999.71 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 (1) K
0.13 × 0.10 × 0.08 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.973, T_{max} = 0.982
123040 measured reflections
10625 independent reflections
6628 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.160
S = 1.03
10625 reflections
1030 parameters
24 restraints
$\Delta\rho_{max}$ = 0.47 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: OM2195).

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1,3,7,10,14,17,21,28,31,42,52,55-Dodecakis(trifluoromethyl)-1,3,7,10,14,17,21,28,31,42,52,55-dodecahydro(C_{60}–I_h)[5,6]fullerene

Natalia B. Shustova, Oren P. Anderson, Olga V. Boltalina, Steven H. Strauss and Ivan E. Kareev

S1. Comment

Four isomers of $C_{60}(CF_3)_{12}$ have now been isolated and characterized by X-ray structure crystallography (Troyanov *et al.*, 2006; Kareev *et al.*, 2007; Popov *et al.*, 2007; Omelyanyuk *et al.*, 2007).

The structure of C_1-pmp^{3}mp,pmp-$C_{60}(CF_3)_{12}$ has an idealized I_h C_{60} core with twelve sp^3 carbon atoms at positions 1,3,7,10,14,17,21,28,31,42,52,and 55 (Powell *et al.*, 2002), each of which is attached to a CF_3 group. The cage sp^3 carbon atoms are not adjacent to one another. The CF_3 groups are arranged on a *para-meta-para-para-para-meta-para* ribbon and a *para-meta-para* ribbon of edge-sharing $C_6(CF_3)_2$ hexagons (*i.e.*, a pmp^{3}mp,pmp overall addition pattern; see Schlegel diagram in Figure 1).

The two CF_3 groups attached to C1 and C7 are disordered (F atom occupancies are 73:27 for the CF_3 group attached to C1 and 85:15 for the CF_3 group attached to C7). Only the 73/85 set of the two disordered pairs is shown in the figures. As in all other published structures of fullerene$(CF_3)_n$ compounds, there are F···F intramolecular contacts between pairs of neighboring CF_3 groups. The range of F—F distances that do not involve the disordered CF_3 groups is from 2.521 (3) to 2.738 (4) Å. The range of C—F distances that do not involve the disordered CF_3 groups is from 1.301 (5) to 1.341 (5) Å.

S2. Experimental

The synthesis of C_1-pmp^{3}mp,pmp-$C_{60}(CF_3)_{12}$ was carried out by heating of C_{60} in the stream of CF_3I at 500 °C during two hours as previously described (Kareev *et al.*, 2005). The red crystals of the HPLC-purified compound were grown by slow evaporation of toluene/heptane saturated solution.

S3. Refinement

The maximum (0.47 e/Å^3) and minimum (-0.32 e/Å^3) residual electron density peaks were located 0.98 Å from F_{693} and 0.81 Å from F_{633}.

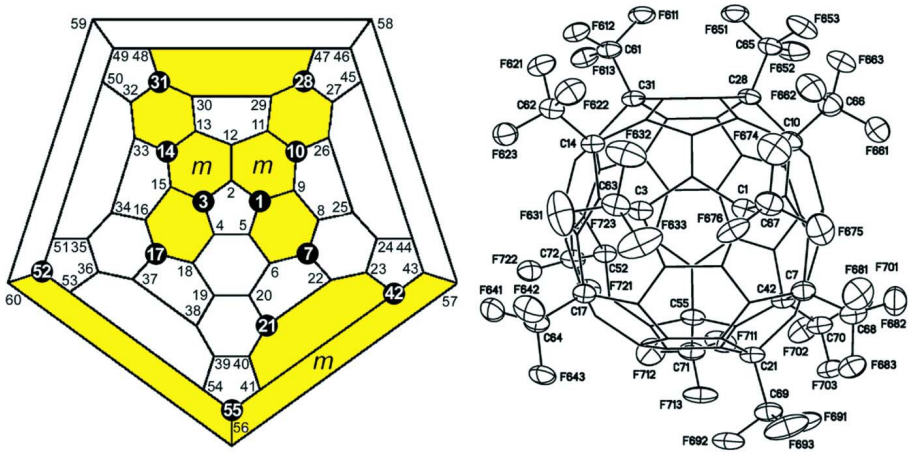

Figure 1

(Left) Schlegel diagram of 1,3,7,10,14,17,21,28,31,42,52,55-$C_{60}(CF_3)_{12}$ showing the IUPAC lowest-locants for the cage carbon atoms to which the CF_3 groups are attached. (Right) The molecular structure of 1,3,7,10,14,17,21,28,31,42,52,55-$C_{60}(CF_3)_{12}$. Displacement ellipsoids for selected atoms are shown at the 50% probability level.

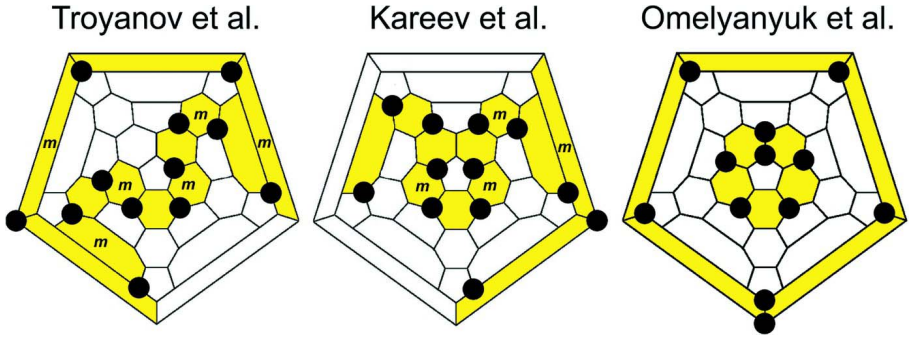

Figure 2

Schlegel diagrams for the three other isomers of $C_{60}(CF_3)_{12}$.

1,3,7,10,14,17,21,28,31,42,52,55-Dodecakis(trifluoromethyl)- 1,3,7,10,14,17,21,28,31,42,52,55-dodecahydro(C_{60}—I_h)[5,6]fullerene

Crystal data

$C_{72}F_{36}$
M_r = 1548.72
Monoclinic, $P2_1/n$
a = 12.2475 (2) Å
b = 20.0326 (4) Å
c = 20.3782 (4) Å
β = 90.288 (1)°
V = 4999.71 (16) Å^3
Z = 4

$F(000)$ = 3024
D_x = 2.057 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9667 reflections
θ = 1.9–26.7°
μ = 0.22 mm^{-1}
T = 100 K
Plate, red
0.13 × 0.10 × 0.08 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube

Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
φ and ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.973, T_{max} = 0.982
123040 measured reflections
10625 independent reflections
6628 reflections with $I > 2\sigma(I)$

R_{int} = 0.079
θ_{max} = 26.7°, θ_{min} = 1.9°
h = −15→15
k = −25→25
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.160
S = 1.03
10625 reflections
1030 parameters
24 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 8.0347P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Experimental. none

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.4855 (3)	0.67541 (16)	0.32301 (18)	0.0281 (8)	
C2	0.5362 (3)	0.65158 (16)	0.25856 (18)	0.0261 (8)	
C3	0.4941 (3)	0.69245 (16)	0.19950 (18)	0.0270 (8)	
C4	0.3812 (3)	0.71086 (15)	0.22733 (18)	0.0263 (8)	
C5	0.3759 (3)	0.70147 (16)	0.29550 (18)	0.0265 (8)	
C6	0.2766 (3)	0.69039 (16)	0.32575 (19)	0.0288 (8)	
C7	0.2638 (3)	0.64990 (17)	0.38908 (19)	0.0309 (8)	
C8	0.3618 (3)	0.60429 (18)	0.39386 (18)	0.0291 (8)	
C9	0.4609 (3)	0.61651 (18)	0.36757 (18)	0.0304 (8)	
C10	0.5318 (3)	0.55292 (17)	0.37014 (19)	0.0296 (8)	
C11	0.5710 (3)	0.53723 (17)	0.30263 (18)	0.0272 (8)	
C12	0.5744 (3)	0.58830 (16)	0.25145 (18)	0.0255 (8)	
C13	0.5778 (3)	0.55262 (16)	0.18887 (18)	0.0256 (8)	
C14	0.5478 (3)	0.58606 (16)	0.12551 (18)	0.0261 (8)	
C15	0.4761 (3)	0.64757 (15)	0.14044 (17)	0.0243 (7)	
C16	0.3820 (3)	0.64371 (16)	0.10646 (17)	0.0257 (8)	
C17	0.2825 (3)	0.68634 (16)	0.11813 (18)	0.0267 (8)	
C18	0.2864 (3)	0.70968 (15)	0.18978 (19)	0.0275 (8)	
C19	0.1856 (3)	0.69632 (15)	0.22081 (18)	0.0258 (8)	

C20	0.1806 (3)	0.68786 (16)	0.28802 (19)	0.0281 (8)
C21	0.0902 (3)	0.64666 (17)	0.32089 (19)	0.0296 (8)
C22	0.1577 (3)	0.61088 (17)	0.37402 (18)	0.0288 (8)
C23	0.1516 (3)	0.54476 (17)	0.38277 (18)	0.0286 (8)
C24	0.2478 (3)	0.50418 (17)	0.40167 (18)	0.0299 (8)
C25	0.3489 (3)	0.53305 (17)	0.40760 (18)	0.0296 (8)
C26	0.4460 (3)	0.49969 (18)	0.38851 (19)	0.0305 (8)
C27	0.4398 (3)	0.43805 (16)	0.35908 (18)	0.0291 (8)
C28	0.5176 (3)	0.41480 (17)	0.30469 (19)	0.0287 (8)
C29	0.5666 (3)	0.47649 (17)	0.27315 (19)	0.0272 (8)
C30	0.5707 (3)	0.48579 (16)	0.20122 (18)	0.0250 (8)
C31	0.5270 (3)	0.43556 (16)	0.15223 (19)	0.0287 (8)
C32	0.4551 (3)	0.47340 (17)	0.10231 (18)	0.0268 (8)
C33	0.4661 (3)	0.54056 (17)	0.08970 (17)	0.0263 (8)
C34	0.3720 (3)	0.57849 (16)	0.07406 (17)	0.0258 (8)
C35	0.2707 (3)	0.54783 (16)	0.06645 (17)	0.0267 (8)
C36	0.1713 (3)	0.58109 (17)	0.08977 (18)	0.0274 (8)
C37	0.1775 (3)	0.64362 (16)	0.11863 (18)	0.0272 (8)
C38	0.1177 (3)	0.65612 (16)	0.17592 (18)	0.0268 (8)
C39	0.0511 (3)	0.60700 (17)	0.20200 (19)	0.0277 (8)
C40	0.0458 (3)	0.59568 (17)	0.27249 (19)	0.0284 (8)
C41	0.0289 (3)	0.53056 (17)	0.2855 (2)	0.0303 (8)
C42	0.0679 (3)	0.49851 (17)	0.34864 (19)	0.0300 (8)
C43	0.1407 (3)	0.43805 (16)	0.3320 (2)	0.0300 (8)
C44	0.2397 (3)	0.44086 (16)	0.37059 (19)	0.0295 (8)
C45	0.3354 (3)	0.40920 (16)	0.34837 (19)	0.0289 (8)
C46	0.3330 (3)	0.37552 (16)	0.28586 (19)	0.0290 (8)
C47	0.4370 (3)	0.38438 (15)	0.25475 (19)	0.0280 (8)
C48	0.4406 (3)	0.39327 (15)	0.18807 (19)	0.0265 (8)
C49	0.3412 (3)	0.39306 (16)	0.15049 (19)	0.0291 (8)
C50	0.3505 (3)	0.44281 (16)	0.09845 (19)	0.0283 (8)
C51	0.2605 (3)	0.47880 (17)	0.07770 (18)	0.0285 (8)
C52	0.1432 (3)	0.46134 (17)	0.09818 (19)	0.0295 (8)
C53	0.0984 (3)	0.53129 (17)	0.11393 (18)	0.0280 (8)
C54	0.0390 (3)	0.54503 (17)	0.17000 (19)	0.0295 (8)
C55	0.0065 (3)	0.49235 (17)	0.2208 (2)	0.0316 (9)
C56	0.0844 (3)	0.43415 (16)	0.2148 (2)	0.0292 (8)
C57	0.1400 (3)	0.40745 (16)	0.2726 (2)	0.0298 (8)
C58	0.2379 (3)	0.37374 (15)	0.2490 (2)	0.0284 (8)
C59	0.2419 (3)	0.38264 (15)	0.18070 (19)	0.0287 (8)
C60	0.1450 (3)	0.42110 (16)	0.1605 (2)	0.0293 (8)
C61	0.6113 (3)	0.39149 (17)	0.1164 (2)	0.0319 (9)
C62	0.6463 (3)	0.60561 (17)	0.08318 (19)	0.0304 (8)
C63	0.5671 (3)	0.75369 (17)	0.1838 (2)	0.0321 (9)
C64	0.2726 (3)	0.74343 (17)	0.0683 (2)	0.0332 (9)
C65	0.5998 (3)	0.36236 (18)	0.3293 (2)	0.0343 (9)
C66	0.6245 (3)	0.5595 (2)	0.4209 (2)	0.0370 (9)
C67	0.5543 (3)	0.73045 (18)	0.3590 (2)	0.0359 (9)

C68	0.2572 (3)	0.69083 (19)	0.4531 (2)	0.0383 (10)	
C69	−0.0057 (3)	0.69122 (18)	0.3437 (2)	0.0368 (9)	
C70	−0.0227 (3)	0.47745 (19)	0.3963 (2)	0.0373 (9)	
C71	−0.1144 (3)	0.47384 (19)	0.2125 (2)	0.0384 (10)	
C72	0.0861 (3)	0.42380 (18)	0.0419 (2)	0.0370 (9)	
F611	0.66741 (18)	0.35333 (10)	0.15730 (12)	0.0434 (6)	
F612	0.68207 (17)	0.42821 (10)	0.08279 (11)	0.0373 (5)	
F613	0.56072 (18)	0.35232 (10)	0.07283 (12)	0.0410 (6)	
F621	0.70069 (18)	0.55188 (10)	0.06297 (12)	0.0403 (6)	
F622	0.71669 (18)	0.64290 (11)	0.11774 (12)	0.0442 (6)	
F623	0.61639 (17)	0.63995 (10)	0.03062 (11)	0.0384 (5)	
F631	0.5620 (2)	0.77039 (14)	0.12184 (13)	0.0643 (8)	
F632	0.67022 (18)	0.74309 (11)	0.19896 (14)	0.0543 (7)	
F633	0.5364 (2)	0.80616 (11)	0.21872 (15)	0.0622 (8)	
F641	0.2722 (2)	0.71984 (11)	0.00726 (11)	0.0434 (6)	
F642	0.35450 (18)	0.78687 (10)	0.07388 (12)	0.0454 (6)	
F643	0.17957 (18)	0.77742 (10)	0.07661 (11)	0.0380 (5)	
F651	0.66163 (19)	0.33893 (11)	0.28142 (12)	0.0473 (6)	
F652	0.54784 (19)	0.31059 (11)	0.35540 (14)	0.0556 (7)	
F653	0.6656 (2)	0.38666 (12)	0.37444 (13)	0.0544 (7)	
F661	0.58658 (19)	0.58067 (12)	0.47871 (11)	0.0444 (6)	
F662	0.69862 (18)	0.60371 (12)	0.40074 (12)	0.0466 (6)	
F663	0.67566 (18)	0.50196 (11)	0.43147 (12)	0.0450 (6)	
F691	−0.0706 (2)	0.66045 (12)	0.38405 (16)	0.0645 (8)	
F692	−0.0640 (3)	0.71067 (16)	0.29227 (15)	0.0817 (10)	
F693	0.0276 (2)	0.74630 (12)	0.37154 (17)	0.0721 (9)	
F701	0.0194 (2)	0.45074 (11)	0.45045 (12)	0.0495 (6)	
F702	−0.0892 (2)	0.43242 (12)	0.36954 (14)	0.0561 (7)	
F703	−0.08363 (18)	0.52964 (11)	0.41401 (12)	0.0437 (6)	
F711	−0.14409 (19)	0.42251 (12)	0.24751 (15)	0.0563 (7)	
F712	−0.1373 (2)	0.45961 (14)	0.15034 (14)	0.0615 (8)	
F713	−0.17832 (17)	0.52528 (11)	0.22916 (14)	0.0541 (7)	
F721	−0.01828 (17)	0.40987 (11)	0.05478 (12)	0.0436 (6)	
F722	0.08801 (18)	0.45966 (11)	−0.01372 (11)	0.0404 (6)	
F723	0.13747 (19)	0.36623 (11)	0.03010 (13)	0.0477 (6)	
F671	0.6544 (3)	0.7341 (2)	0.3353 (2)	0.0493 (10)	0.85
F672	0.5621 (3)	0.71815 (17)	0.42302 (16)	0.0482 (8)	0.85
F673	0.5079 (3)	0.79036 (15)	0.35302 (19)	0.0495 (9)	0.85
F683	0.1721 (7)	0.7319 (5)	0.4531 (3)	0.053 (3)	0.73 (3)
F682	0.2451 (8)	0.6501 (3)	0.5031 (3)	0.0484 (18)	0.73 (3)
F681	0.3460 (6)	0.7265 (3)	0.4605 (4)	0.052 (2)	0.73 (3)
F674	0.6599 (14)	0.7149 (12)	0.3663 (12)	0.053 (7)	0.15
F675	0.5137 (17)	0.7459 (8)	0.4186 (8)	0.052 (6)	0.15
F676	0.5494 (15)	0.7873 (8)	0.3230 (8)	0.038 (5)	0.15
F685	0.229 (4)	0.7544 (8)	0.4420 (7)	0.071 (8)	0.27 (3)
F684	0.187 (3)	0.6685 (15)	0.4960 (12)	0.087 (11)	0.27 (3)
F686	0.3519 (15)	0.697 (2)	0.4868 (17)	0.098 (13)	0.27 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0258 (19)	0.0214 (17)	0.037 (2)	−0.0020 (14)	−0.0058 (16)	−0.0025 (15)
C2	0.0190 (17)	0.0234 (17)	0.036 (2)	−0.0072 (14)	−0.0026 (15)	0.0017 (15)
C3	0.0206 (18)	0.0193 (16)	0.041 (2)	−0.0019 (14)	0.0005 (16)	0.0006 (15)
C4	0.0258 (19)	0.0122 (15)	0.041 (2)	−0.0026 (13)	−0.0005 (16)	−0.0027 (14)
C5	0.0254 (19)	0.0169 (16)	0.037 (2)	−0.0008 (14)	−0.0038 (16)	−0.0061 (14)
C6	0.028 (2)	0.0185 (16)	0.040 (2)	0.0029 (14)	0.0015 (17)	−0.0076 (15)
C7	0.029 (2)	0.0241 (18)	0.040 (2)	0.0020 (15)	0.0007 (17)	−0.0018 (16)
C8	0.030 (2)	0.0291 (18)	0.029 (2)	−0.0012 (15)	−0.0023 (16)	−0.0019 (15)
C9	0.028 (2)	0.0295 (19)	0.034 (2)	−0.0001 (15)	−0.0045 (17)	−0.0017 (16)
C10	0.0224 (19)	0.0288 (18)	0.038 (2)	−0.0013 (15)	−0.0034 (16)	0.0037 (16)
C11	0.0141 (17)	0.0282 (18)	0.039 (2)	0.0015 (14)	−0.0035 (15)	0.0041 (16)
C12	0.0144 (16)	0.0233 (17)	0.039 (2)	−0.0023 (13)	−0.0025 (15)	0.0029 (15)
C13	0.0143 (16)	0.0242 (17)	0.038 (2)	0.0012 (13)	0.0008 (15)	0.0008 (15)
C14	0.0204 (18)	0.0190 (16)	0.039 (2)	−0.0008 (14)	0.0011 (16)	−0.0006 (15)
C15	0.0222 (18)	0.0178 (16)	0.033 (2)	−0.0009 (13)	0.0020 (15)	0.0026 (14)
C16	0.0245 (19)	0.0201 (16)	0.032 (2)	−0.0001 (14)	−0.0006 (16)	0.0026 (14)
C17	0.0251 (19)	0.0190 (16)	0.036 (2)	−0.0007 (14)	−0.0017 (16)	−0.0016 (14)
C18	0.0267 (19)	0.0114 (15)	0.044 (2)	0.0018 (13)	−0.0010 (17)	0.0023 (14)
C19	0.0234 (18)	0.0120 (15)	0.042 (2)	0.0041 (13)	−0.0020 (16)	0.0007 (14)
C20	0.0255 (19)	0.0179 (16)	0.041 (2)	0.0040 (14)	−0.0005 (17)	−0.0027 (15)
C21	0.0217 (18)	0.0215 (17)	0.046 (2)	0.0045 (14)	0.0030 (17)	0.0014 (16)
C22	0.0234 (19)	0.0249 (17)	0.038 (2)	0.0026 (15)	0.0047 (16)	−0.0039 (15)
C23	0.0243 (19)	0.0265 (18)	0.035 (2)	0.0022 (15)	0.0077 (16)	0.0009 (15)
C24	0.029 (2)	0.0268 (18)	0.034 (2)	0.0008 (15)	0.0035 (16)	0.0068 (15)
C25	0.029 (2)	0.0273 (18)	0.032 (2)	0.0038 (15)	−0.0023 (16)	0.0035 (15)
C26	0.0256 (19)	0.0311 (19)	0.035 (2)	0.0030 (15)	−0.0038 (16)	0.0105 (16)
C27	0.028 (2)	0.0218 (17)	0.038 (2)	0.0042 (15)	−0.0001 (17)	0.0108 (15)
C28	0.0211 (18)	0.0233 (17)	0.042 (2)	0.0041 (14)	−0.0001 (16)	0.0080 (15)
C29	0.0147 (17)	0.0248 (17)	0.042 (2)	0.0032 (14)	−0.0013 (16)	0.0052 (15)
C30	0.0114 (16)	0.0209 (16)	0.043 (2)	0.0005 (13)	0.0009 (15)	0.0039 (15)
C31	0.0212 (18)	0.0206 (16)	0.044 (2)	0.0035 (14)	0.0038 (17)	0.0020 (15)
C32	0.0192 (18)	0.0249 (17)	0.036 (2)	0.0020 (14)	0.0013 (16)	−0.0038 (15)
C33	0.0219 (18)	0.0263 (18)	0.031 (2)	−0.0013 (14)	0.0042 (15)	−0.0010 (15)
C34	0.0272 (19)	0.0203 (16)	0.030 (2)	0.0016 (14)	−0.0014 (16)	0.0004 (14)
C35	0.0274 (19)	0.0246 (17)	0.028 (2)	0.0001 (15)	−0.0044 (16)	−0.0042 (15)
C36	0.0221 (18)	0.0252 (17)	0.035 (2)	0.0013 (14)	−0.0087 (16)	0.0003 (15)
C37	0.0217 (18)	0.0188 (16)	0.041 (2)	0.0040 (14)	−0.0099 (16)	0.0043 (15)
C38	0.0209 (18)	0.0205 (16)	0.039 (2)	0.0082 (14)	−0.0050 (16)	−0.0006 (15)
C39	0.0154 (17)	0.0245 (17)	0.043 (2)	0.0036 (14)	−0.0036 (16)	−0.0015 (16)
C40	0.0153 (17)	0.0251 (18)	0.045 (2)	0.0028 (14)	0.0011 (16)	−0.0017 (16)
C41	0.0122 (17)	0.0249 (18)	0.054 (2)	0.0007 (14)	0.0053 (16)	0.0013 (16)
C42	0.0216 (19)	0.0227 (17)	0.046 (2)	0.0035 (14)	0.0046 (17)	−0.0001 (16)
C43	0.0229 (19)	0.0197 (16)	0.047 (2)	−0.0028 (14)	0.0055 (17)	0.0084 (16)
C44	0.0269 (19)	0.0203 (17)	0.041 (2)	0.0024 (15)	0.0057 (17)	0.0091 (15)
C45	0.0225 (19)	0.0201 (16)	0.044 (2)	0.0032 (14)	0.0042 (17)	0.0116 (16)

C46	0.0251 (19)	0.0140 (15)	0.048 (2)	0.0012 (14)	0.0061 (17)	0.0075 (15)
C47	0.0221 (18)	0.0126 (15)	0.049 (2)	0.0041 (13)	0.0039 (17)	0.0043 (15)
C48	0.0209 (18)	0.0144 (15)	0.044 (2)	0.0031 (13)	0.0050 (16)	−0.0012 (15)
C49	0.030 (2)	0.0123 (15)	0.045 (2)	0.0028 (14)	0.0000 (17)	−0.0057 (15)
C50	0.0262 (19)	0.0205 (16)	0.038 (2)	0.0005 (14)	0.0016 (16)	−0.0096 (15)
C51	0.028 (2)	0.0245 (17)	0.033 (2)	−0.0007 (15)	−0.0023 (16)	−0.0049 (15)
C52	0.0221 (18)	0.0239 (17)	0.043 (2)	−0.0032 (14)	−0.0028 (16)	−0.0049 (16)
C53	0.0207 (18)	0.0229 (17)	0.040 (2)	−0.0018 (14)	−0.0100 (17)	−0.0016 (15)
C54	0.0155 (17)	0.0265 (18)	0.046 (2)	0.0022 (14)	−0.0073 (17)	0.0005 (16)
C55	0.0210 (19)	0.0239 (17)	0.050 (2)	0.0014 (15)	−0.0040 (17)	−0.0033 (16)
C56	0.0207 (18)	0.0176 (16)	0.049 (2)	−0.0057 (14)	−0.0013 (17)	−0.0015 (15)
C57	0.0226 (19)	0.0173 (16)	0.049 (2)	−0.0031 (14)	0.0066 (17)	0.0028 (16)
C58	0.0220 (18)	0.0126 (15)	0.051 (2)	−0.0026 (13)	0.0027 (17)	0.0032 (15)
C59	0.0242 (19)	0.0125 (15)	0.049 (2)	−0.0029 (14)	−0.0005 (17)	−0.0038 (15)
C60	0.0224 (18)	0.0172 (16)	0.048 (2)	−0.0056 (14)	−0.0052 (17)	−0.0070 (16)
C61	0.0238 (19)	0.0213 (17)	0.051 (2)	0.0021 (15)	0.0038 (18)	0.0029 (17)
C62	0.0258 (19)	0.0238 (17)	0.042 (2)	−0.0010 (15)	−0.0019 (17)	0.0010 (16)
C63	0.029 (2)	0.0204 (17)	0.047 (3)	−0.0020 (15)	−0.0047 (18)	−0.0001 (16)
C64	0.032 (2)	0.0247 (18)	0.043 (2)	0.0020 (16)	−0.0024 (18)	−0.0010 (16)
C65	0.026 (2)	0.0307 (19)	0.046 (2)	0.0053 (16)	−0.0017 (19)	0.0082 (18)
C66	0.033 (2)	0.038 (2)	0.040 (2)	−0.0013 (18)	0.0011 (19)	0.0016 (18)
C67	0.036 (2)	0.0260 (19)	0.046 (3)	0.0007 (17)	−0.005 (2)	−0.0014 (18)
C68	0.031 (2)	0.037 (2)	0.047 (3)	0.0044 (18)	0.002 (2)	−0.0036 (19)
C69	0.031 (2)	0.0223 (18)	0.057 (3)	0.0032 (16)	0.005 (2)	−0.0009 (18)
C70	0.027 (2)	0.030 (2)	0.055 (3)	0.0034 (17)	0.0069 (19)	0.0010 (19)
C71	0.025 (2)	0.028 (2)	0.062 (3)	−0.0004 (16)	−0.002 (2)	−0.0018 (19)
C72	0.030 (2)	0.0283 (19)	0.053 (3)	−0.0001 (16)	−0.0042 (19)	−0.0043 (18)
F611	0.0351 (13)	0.0351 (12)	0.0601 (15)	0.0167 (10)	0.0077 (11)	0.0090 (11)
F612	0.0268 (11)	0.0299 (11)	0.0552 (15)	−0.0001 (9)	0.0107 (10)	0.0003 (10)
F613	0.0332 (12)	0.0303 (11)	0.0596 (15)	−0.0014 (10)	0.0070 (11)	−0.0124 (11)
F621	0.0335 (12)	0.0294 (11)	0.0582 (15)	0.0038 (9)	0.0150 (11)	0.0024 (10)
F622	0.0295 (12)	0.0463 (13)	0.0568 (15)	−0.0131 (10)	0.0028 (11)	−0.0060 (11)
F623	0.0353 (12)	0.0332 (11)	0.0469 (14)	0.0025 (10)	0.0066 (10)	0.0107 (10)
F631	0.081 (2)	0.0622 (17)	0.0494 (16)	−0.0450 (15)	−0.0112 (14)	0.0190 (13)
F632	0.0266 (13)	0.0378 (13)	0.099 (2)	−0.0113 (10)	−0.0084 (13)	0.0184 (13)
F633	0.0525 (16)	0.0208 (11)	0.113 (2)	−0.0118 (11)	0.0281 (16)	−0.0185 (13)
F641	0.0544 (15)	0.0365 (12)	0.0393 (13)	0.0126 (11)	−0.0003 (11)	0.0032 (10)
F642	0.0408 (14)	0.0290 (11)	0.0665 (17)	−0.0070 (10)	−0.0039 (12)	0.0125 (11)
F643	0.0389 (13)	0.0260 (11)	0.0491 (14)	0.0120 (9)	−0.0011 (11)	0.0040 (10)
F651	0.0361 (13)	0.0443 (13)	0.0614 (16)	0.0199 (11)	0.0063 (12)	0.0104 (12)
F652	0.0367 (14)	0.0359 (13)	0.094 (2)	0.0083 (11)	0.0104 (13)	0.0347 (13)
F653	0.0512 (15)	0.0426 (14)	0.0690 (17)	0.0148 (12)	−0.0237 (14)	0.0061 (12)
F661	0.0415 (14)	0.0528 (14)	0.0388 (14)	0.0036 (11)	−0.0072 (11)	−0.0017 (11)
F662	0.0346 (13)	0.0507 (14)	0.0544 (15)	−0.0133 (11)	−0.0103 (11)	0.0043 (12)
F663	0.0346 (13)	0.0448 (13)	0.0555 (15)	0.0086 (10)	−0.0135 (11)	0.0074 (11)
F691	0.0446 (15)	0.0362 (13)	0.113 (2)	0.0098 (11)	0.0424 (16)	0.0128 (14)
F692	0.074 (2)	0.098 (2)	0.073 (2)	0.0656 (19)	−0.0051 (17)	−0.0033 (17)
F693	0.0493 (16)	0.0376 (14)	0.129 (3)	−0.0004 (12)	0.0221 (17)	−0.0352 (16)

F701	0.0457 (15)	0.0439 (14)	0.0593 (16)	0.0109 (11)	0.0173 (13)	0.0149 (12)
F702	0.0404 (14)	0.0476 (14)	0.0804 (19)	−0.0206 (12)	0.0209 (13)	−0.0129 (13)
F703	0.0318 (12)	0.0373 (12)	0.0620 (16)	0.0084 (10)	0.0157 (11)	0.0038 (11)
F711	0.0288 (13)	0.0411 (13)	0.099 (2)	−0.0082 (11)	−0.0040 (13)	0.0223 (14)
F712	0.0333 (14)	0.0794 (19)	0.0718 (19)	−0.0195 (13)	−0.0062 (13)	−0.0171 (15)
F713	0.0206 (12)	0.0375 (13)	0.104 (2)	0.0058 (10)	−0.0067 (13)	−0.0081 (13)
F721	0.0272 (12)	0.0411 (13)	0.0625 (16)	−0.0110 (10)	−0.0054 (11)	−0.0079 (11)
F722	0.0313 (12)	0.0418 (13)	0.0480 (14)	−0.0013 (10)	−0.0068 (10)	−0.0073 (11)
F723	0.0420 (14)	0.0300 (12)	0.0708 (17)	0.0022 (10)	−0.0099 (12)	−0.0172 (11)
F671	0.0317 (18)	0.049 (3)	0.067 (3)	−0.0191 (16)	0.0003 (18)	−0.017 (2)
F672	0.059 (2)	0.044 (2)	0.0416 (19)	−0.0163 (17)	−0.0143 (17)	−0.0033 (16)
F673	0.053 (2)	0.0257 (15)	0.070 (3)	−0.0019 (16)	−0.0240 (19)	−0.0106 (17)
F683	0.060 (4)	0.049 (4)	0.048 (3)	0.024 (3)	0.003 (3)	−0.013 (3)
F682	0.065 (4)	0.045 (2)	0.035 (2)	0.002 (2)	0.000 (2)	−0.0006 (17)
F681	0.053 (3)	0.046 (3)	0.058 (4)	−0.014 (2)	−0.003 (2)	−0.018 (2)
F674	0.044 (12)	0.044 (13)	0.072 (18)	−0.008 (9)	−0.008 (12)	−0.003 (11)
F675	0.084 (16)	0.024 (9)	0.047 (12)	0.011 (9)	−0.008 (11)	−0.014 (8)
F676	0.036 (11)	0.025 (8)	0.052 (13)	−0.006 (7)	0.017 (8)	−0.008 (8)
F685	0.12 (2)	0.039 (7)	0.057 (8)	0.012 (10)	0.021 (9)	−0.003 (5)
F684	0.12 (2)	0.075 (15)	0.065 (11)	−0.039 (16)	0.039 (14)	−0.023 (10)
F686	0.059 (9)	0.15 (3)	0.087 (18)	0.033 (13)	−0.028 (10)	−0.082 (18)

Geometric parameters (Å, º)

C1—C9	1.520 (5)	C39—C40	1.456 (5)
C1—C2	1.532 (5)	C40—C41	1.347 (5)
C1—C5	1.543 (5)	C41—C42	1.513 (5)
C1—C67	1.567 (5)	C41—C55	1.548 (5)
C2—C12	1.359 (5)	C42—C70	1.538 (5)
C2—C3	1.542 (5)	C42—C43	1.543 (5)
C3—C15	1.518 (5)	C43—C57	1.358 (5)
C3—C4	1.542 (5)	C43—C44	1.442 (5)
C3—C63	1.553 (5)	C44—C45	1.409 (5)
C4—C18	1.387 (5)	C45—C46	1.442 (5)
C4—C5	1.404 (5)	C46—C58	1.383 (5)
C5—C6	1.385 (5)	C46—C47	1.436 (5)
C6—C20	1.402 (5)	C47—C48	1.371 (5)
C6—C7	1.533 (5)	C48—C49	1.435 (5)
C7—C8	1.511 (5)	C49—C59	1.381 (5)
C7—C68	1.543 (5)	C49—C50	1.460 (5)
C7—C22	1.546 (5)	C50—C51	1.381 (5)
C8—C9	1.352 (5)	C51—C52	1.538 (5)
C8—C25	1.463 (5)	C52—C60	1.504 (5)
C9—C10	1.543 (5)	C52—C72	1.538 (5)
C10—C11	1.493 (5)	C52—C53	1.540 (5)
C10—C66	1.537 (5)	C53—C54	1.385 (5)
C10—C26	1.545 (5)	C54—C55	1.532 (5)
C11—C29	1.358 (5)	C55—C56	1.511 (5)

C11—C12	1.462 (5)	C55—C71	1.535 (5)
C12—C13	1.463 (5)	C56—C60	1.361 (5)
C13—C30	1.365 (5)	C56—C57	1.459 (5)
C13—C14	1.499 (5)	C57—C58	1.460 (5)
C14—C33	1.536 (5)	C58—C59	1.404 (5)
C14—C62	1.537 (5)	C59—C60	1.472 (5)
C14—C15	1.545 (5)	C61—F611	1.322 (4)
C15—C16	1.343 (5)	C61—F612	1.329 (4)
C16—C34	1.469 (5)	C61—F613	1.335 (4)
C16—C17	1.508 (5)	C62—F623	1.323 (4)
C17—C64	1.533 (5)	C62—F621	1.332 (4)
C17—C18	1.534 (5)	C62—F622	1.338 (4)
C17—C37	1.545 (5)	C63—F631	1.308 (5)
C18—C19	1.416 (5)	C63—F632	1.315 (4)
C19—C20	1.382 (5)	C63—F633	1.325 (4)
C19—C38	1.473 (5)	C64—F641	1.331 (4)
C20—C21	1.537 (5)	C64—F642	1.332 (4)
C21—C40	1.518 (5)	C64—F643	1.339 (4)
C21—C22	1.536 (5)	C65—F653	1.312 (4)
C21—C69	1.548 (5)	C65—F651	1.324 (5)
C22—C23	1.339 (5)	C65—F652	1.329 (4)
C23—C24	1.481 (5)	C66—F663	1.328 (4)
C23—C42	1.545 (5)	C66—F662	1.335 (4)
C24—C25	1.371 (5)	C66—F661	1.338 (5)
C24—C44	1.421 (5)	C67—F671	1.323 (5)
C25—C26	1.421 (5)	C67—F672	1.331 (5)
C26—C27	1.375 (5)	C67—F673	1.333 (5)
C27—C45	1.419 (5)	C67—F674	1.337 (16)
C27—C28	1.538 (5)	C67—F675	1.350 (14)
C28—C29	1.518 (5)	C67—F676	1.356 (14)
C28—C65	1.538 (5)	C68—F684	1.305 (14)
C28—C47	1.541 (5)	C68—F681	1.309 (7)
C29—C30	1.479 (5)	C68—F682	1.316 (6)
C30—C31	1.513 (5)	C68—F683	1.327 (5)
C31—C32	1.541 (5)	C68—F685	1.336 (11)
C31—C48	1.543 (5)	C68—F686	1.352 (13)
C31—C61	1.545 (5)	C69—F691	1.301 (5)
C32—C33	1.376 (5)	C69—F693	1.305 (4)
C32—C50	1.422 (5)	C69—F692	1.324 (5)
C33—C34	1.415 (5)	C70—F701	1.328 (5)
C34—C35	1.392 (5)	C70—F702	1.331 (5)
C35—C51	1.407 (5)	C70—F703	1.335 (4)
C35—C36	1.469 (5)	C71—F711	1.304 (5)
C36—C37	1.386 (5)	C71—F712	1.327 (5)
C36—C53	1.428 (5)	C71—F713	1.339 (4)
C37—C38	1.404 (5)	C72—F721	1.336 (4)
C38—C39	1.386 (5)	C72—F723	1.336 (4)
C39—C54	1.410 (5)	C72—F722	1.342 (5)

C9—C1—C2	110.7 (3)	C45—C44—C24	119.2 (3)
C9—C1—C5	107.7 (3)	C45—C44—C43	120.4 (3)
C2—C1—C5	98.6 (3)	C24—C44—C43	109.5 (3)
C9—C1—C67	112.0 (3)	C44—C45—C27	121.2 (3)
C2—C1—C67	113.7 (3)	C44—C45—C46	118.8 (3)
C5—C1—C67	113.4 (3)	C27—C45—C46	109.9 (3)
C12—C2—C1	121.5 (3)	C58—C46—C47	120.6 (4)
C12—C2—C3	121.7 (3)	C58—C46—C45	120.3 (3)
C1—C2—C3	111.6 (3)	C47—C46—C45	108.6 (3)
C15—C3—C4	107.8 (3)	C48—C47—C46	119.1 (3)
C15—C3—C2	110.6 (3)	C48—C47—C28	125.4 (3)
C4—C3—C2	97.9 (3)	C46—C47—C28	108.9 (3)
C15—C3—C63	112.7 (3)	C47—C48—C49	119.8 (3)
C4—C3—C63	113.9 (3)	C47—C48—C31	124.5 (3)
C2—C3—C63	112.9 (3)	C49—C48—C31	109.3 (3)
C18—C4—C5	120.1 (3)	C59—C49—C48	120.6 (3)
C18—C4—C3	122.9 (3)	C59—C49—C50	119.9 (3)
C5—C4—C3	112.2 (3)	C48—C49—C50	108.4 (3)
C6—C5—C4	120.5 (3)	C51—C50—C32	120.6 (3)
C6—C5—C1	123.3 (3)	C51—C50—C49	120.9 (3)
C4—C5—C1	111.1 (3)	C32—C50—C49	109.1 (3)
C5—C6—C20	119.9 (3)	C50—C51—C35	119.4 (3)
C5—C6—C7	123.6 (3)	C50—C51—C52	122.9 (3)
C20—C6—C7	110.7 (3)	C35—C51—C52	110.6 (3)
C8—C7—C6	106.9 (3)	C60—C52—C72	111.9 (3)
C8—C7—C68	108.2 (3)	C60—C52—C51	110.0 (3)
C6—C7—C68	115.9 (3)	C72—C52—C51	109.3 (3)
C8—C7—C22	111.9 (3)	C60—C52—C53	108.4 (3)
C6—C7—C22	100.9 (3)	C72—C52—C53	116.0 (3)
C68—C7—C22	112.9 (3)	C51—C52—C53	100.6 (3)
C9—C8—C25	110.5 (3)	C54—C53—C36	118.5 (3)
C9—C8—C7	125.4 (3)	C54—C53—C52	122.8 (3)
C25—C8—C7	121.1 (3)	C36—C53—C52	109.8 (3)
C8—C9—C1	124.0 (3)	C53—C54—C39	120.1 (3)
C8—C9—C10	110.1 (3)	C53—C54—C55	124.0 (3)
C1—C9—C10	123.2 (3)	C39—C54—C55	108.7 (3)
C11—C10—C66	113.5 (3)	C56—C55—C54	108.1 (3)
C11—C10—C9	109.0 (3)	C56—C55—C71	114.4 (3)
C66—C10—C9	111.5 (3)	C54—C55—C71	110.2 (3)
C11—C10—C26	107.5 (3)	C56—C55—C41	109.9 (3)
C66—C10—C26	113.4 (3)	C54—C55—C41	100.9 (3)
C9—C10—C26	101.2 (3)	C71—C55—C41	112.3 (3)
C29—C11—C12	108.2 (3)	C60—C56—C57	109.4 (3)
C29—C11—C10	125.8 (3)	C60—C56—C55	124.1 (3)
C12—C11—C10	121.4 (3)	C57—C56—C55	120.7 (3)
C2—C12—C11	124.5 (3)	C43—C57—C56	123.7 (3)
C2—C12—C13	124.1 (3)	C43—C57—C58	120.1 (3)

C11—C12—C13	106.3 (3)	C56—C57—C58	106.5 (3)
C30—C13—C12	108.4 (3)	C46—C58—C59	120.1 (3)
C30—C13—C14	125.6 (3)	C46—C58—C57	120.0 (3)
C12—C13—C14	121.6 (3)	C59—C58—C57	107.5 (3)
C13—C14—C33	107.5 (3)	C49—C59—C58	119.7 (3)
C13—C14—C62	114.1 (3)	C49—C59—C60	120.4 (3)
C33—C14—C62	113.4 (3)	C58—C59—C60	108.2 (3)
C13—C14—C15	108.9 (3)	C56—C60—C59	108.4 (3)
C33—C14—C15	101.3 (3)	C56—C60—C52	125.3 (3)
C62—C14—C15	110.9 (3)	C59—C60—C52	121.7 (3)
C16—C15—C3	124.3 (3)	F611—C61—F612	107.9 (3)
C16—C15—C14	109.9 (3)	F611—C61—F613	108.5 (3)
C3—C15—C14	123.2 (3)	F612—C61—F613	106.6 (3)
C15—C16—C34	110.6 (3)	F611—C61—C31	112.2 (3)
C15—C16—C17	125.3 (3)	F612—C61—C31	111.5 (3)
C34—C16—C17	120.6 (3)	F613—C61—C31	109.9 (3)
C16—C17—C64	112.3 (3)	F623—C62—F621	107.9 (3)
C16—C17—C18	107.5 (3)	F623—C62—F622	108.1 (3)
C64—C17—C18	113.9 (3)	F621—C62—F622	107.0 (3)
C16—C17—C37	111.2 (3)	F623—C62—C14	111.8 (3)
C64—C17—C37	110.8 (3)	F621—C62—C14	111.2 (3)
C18—C17—C37	100.6 (3)	F622—C62—C14	110.6 (3)
C4—C18—C19	119.1 (3)	F631—C63—F632	108.0 (3)
C4—C18—C17	123.5 (3)	F631—C63—F633	107.6 (3)
C19—C18—C17	110.1 (3)	F632—C63—F633	106.1 (3)
C20—C19—C18	120.6 (3)	F631—C63—C3	112.1 (3)
C20—C19—C38	121.4 (3)	F632—C63—C3	112.2 (3)
C18—C19—C38	108.5 (3)	F633—C63—C3	110.5 (3)
C19—C20—C6	119.9 (3)	F641—C64—F642	108.1 (3)
C19—C20—C21	122.2 (3)	F641—C64—F643	107.4 (3)
C6—C20—C21	112.6 (3)	F642—C64—F643	107.3 (3)
C40—C21—C22	109.5 (3)	F641—C64—C17	110.7 (3)
C40—C21—C20	109.5 (3)	F642—C64—C17	112.0 (3)
C22—C21—C20	99.9 (3)	F643—C64—C17	111.1 (3)
C40—C21—C69	108.3 (3)	F653—C65—F651	107.3 (3)
C22—C21—C69	117.6 (3)	F653—C65—F652	107.6 (3)
C20—C21—C69	111.7 (3)	F651—C65—F652	107.1 (3)
C23—C22—C21	121.7 (3)	F653—C65—C28	112.0 (3)
C23—C22—C7	121.4 (3)	F651—C65—C28	112.1 (3)
C21—C22—C7	110.7 (3)	F652—C65—C28	110.4 (3)
C22—C23—C24	122.2 (3)	F663—C66—F662	107.7 (3)
C22—C23—C42	124.8 (3)	F663—C66—F661	107.3 (3)
C24—C23—C42	108.3 (3)	F662—C66—F661	107.4 (3)
C25—C24—C44	118.5 (3)	F663—C66—C10	112.4 (3)
C25—C24—C23	120.5 (3)	F662—C66—C10	110.5 (3)
C44—C24—C23	108.7 (3)	F661—C66—C10	111.2 (3)
C24—C25—C26	122.3 (3)	F671—C67—F672	107.9 (4)
C24—C25—C8	119.5 (3)	F671—C67—F673	108.2 (4)

C26—C25—C8	108.4 (3)	F672—C67—F673	106.6 (4)
C27—C26—C25	119.8 (3)	F671—C67—F674	32.4 (9)
C27—C26—C10	123.4 (3)	F672—C67—F674	77.5 (10)
C25—C26—C10	108.3 (3)	F673—C67—F674	129.1 (11)
C26—C27—C45	118.8 (3)	F671—C67—F675	131.5 (10)
C26—C27—C28	123.6 (3)	F672—C67—F675	35.5 (8)
C45—C27—C28	109.1 (3)	F673—C67—F675	73.5 (8)
C29—C28—C65	115.8 (3)	F674—C67—F675	108.3 (13)
C29—C28—C27	107.8 (3)	F671—C67—F676	78.1 (8)
C65—C28—C27	112.3 (3)	F672—C67—F676	133.6 (8)
C29—C28—C47	107.2 (3)	F673—C67—F676	34.6 (6)
C65—C28—C47	111.2 (3)	F674—C67—F676	107.1 (12)
C27—C28—C47	101.4 (3)	F675—C67—F676	106.2 (10)
C11—C29—C30	108.9 (3)	F671—C67—C1	111.4 (3)
C11—C29—C28	123.9 (3)	F672—C67—C1	111.4 (3)
C30—C29—C28	122.5 (3)	F673—C67—C1	111.3 (3)
C13—C30—C29	108.0 (3)	F674—C67—C1	113.9 (12)
C13—C30—C31	123.6 (3)	F675—C67—C1	112.5 (9)
C29—C30—C31	123.8 (3)	F676—C67—C1	108.4 (9)
C30—C31—C32	107.9 (3)	F684—C68—F681	131.0 (12)
C30—C31—C48	107.1 (3)	F684—C68—F682	36.0 (19)
C32—C31—C48	101.1 (3)	F681—C68—F682	110.2 (4)
C30—C31—C61	117.2 (3)	F684—C68—F683	72.3 (18)
C32—C31—C61	110.5 (3)	F681—C68—F683	108.3 (5)
C48—C31—C61	111.8 (3)	F682—C68—F683	107.0 (4)
C33—C32—C50	120.0 (3)	F684—C68—F685	105.9 (10)
C33—C32—C31	123.2 (3)	F681—C68—F685	73.2 (17)
C50—C32—C31	109.6 (3)	F682—C68—F685	133.8 (9)
C32—C33—C34	119.1 (3)	F683—C68—F685	37.9 (14)
C32—C33—C14	123.7 (3)	F684—C68—F686	104.8 (11)
C34—C33—C14	108.5 (3)	F681—C68—F686	35 (2)
C35—C34—C33	120.8 (3)	F682—C68—F686	76 (2)
C35—C34—C16	121.0 (3)	F683—C68—F686	127.7 (10)
C33—C34—C16	108.1 (3)	F685—C68—F686	102.2 (11)
C34—C35—C51	119.7 (3)	F684—C68—C7	114.9 (8)
C34—C35—C36	120.2 (3)	F681—C68—C7	109.9 (4)
C51—C35—C36	108.6 (3)	F682—C68—C7	109.4 (4)
C37—C36—C53	121.2 (3)	F683—C68—C7	112.0 (4)
C37—C36—C35	120.3 (3)	F685—C68—C7	112.2 (7)
C53—C36—C35	108.4 (3)	F686—C68—C7	115.6 (8)
C36—C37—C38	119.1 (3)	F691—C69—F693	108.5 (4)
C36—C37—C17	122.8 (3)	F691—C69—F692	108.1 (4)
C38—C37—C17	110.2 (3)	F693—C69—F692	105.2 (3)
C39—C38—C37	120.2 (3)	F691—C69—C21	112.5 (3)
C39—C38—C19	118.8 (3)	F693—C69—C21	112.5 (3)
C37—C38—C19	108.6 (3)	F692—C69—C21	109.8 (3)
C38—C39—C54	120.6 (3)	F701—C70—F702	107.6 (3)
C38—C39—C40	121.2 (3)	F701—C70—F703	107.9 (3)

C54—C39—C40	108.3 (3)	F702—C70—F703	107.5 (3)
C41—C40—C39	110.6 (3)	F701—C70—C42	110.9 (3)
C41—C40—C21	125.3 (4)	F702—C70—C42	111.6 (3)
C39—C40—C21	121.2 (3)	F703—C70—C42	111.2 (3)
C40—C41—C42	122.0 (3)	F711—C71—F712	107.1 (3)
C40—C41—C55	109.8 (3)	F711—C71—F713	107.6 (3)
C42—C41—C55	124.6 (3)	F712—C71—F713	106.6 (3)
C41—C42—C70	115.4 (3)	F711—C71—C55	113.7 (3)
C41—C42—C43	109.1 (3)	F712—C71—C55	110.8 (3)
C70—C42—C43	110.1 (3)	F713—C71—C55	110.6 (3)
C41—C42—C23	109.5 (3)	F721—C72—F723	107.9 (3)
C70—C42—C23	111.1 (3)	F721—C72—F722	107.4 (3)
C43—C42—C23	100.7 (3)	F723—C72—F722	107.5 (3)
C57—C43—C44	120.3 (3)	F721—C72—C52	112.8 (3)
C57—C43—C42	123.3 (3)	F723—C72—C52	110.1 (3)
C44—C43—C42	109.6 (3)	F722—C72—C52	111.0 (3)