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C_{60} 1,1,2,2-tetrachloroethylene tetrasolvate

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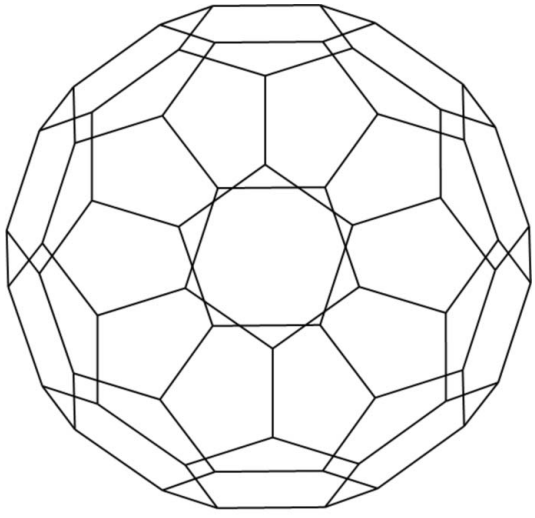
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.019 Å; disorder in solvent or counterion; R factor = 0.105; wR factor = 0.265; data-to-parameter ratio = 9.6.

In the title complex, $C_{60}\cdot 4C_2Cl_4$, the C_{60} molecule is located on an inversion centre and there are two tetrachloroethylene (TCE) molecules in the asymmetric unit. Both TCE molecules show positional disorder, with occupancy ratios of 0.75:0.25 and 0.56:0.44. Four fullerene C atoms form short contacts [3.208 (17) and 3.223 (17) Å] with the centres of the TCE double bonds, indicating that C_{60}–solvent interactions are largely π–π in nature.

Related literature

For related literature on inclusion compounds of C_{60} with various guest molecules, see: Balch & Olmstead (1999) and references cited therein; Olmstead *et al.* (2000); Hardie *et al.* (2003); Bond (2003); Litvinov *et al.* (2003); Soldatov *et al.* (2001); Dodrick *et al.* (2005).



$4\,Cl_2C{=}{=}CCl_2$

Experimental

Crystal data

$C_{60}\cdot 4C_2Cl_4$
M_r = 1383.88
Triclinic, $P\overline{1}$
a = 10.049 (5) Å
b = 10.168 (5) Å
c = 13.412 (5) Å
α = 70.484 (5)°
β = 68.508 (5)°
γ = 79.834 (5)°
V = 1199.6 (10) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 173 (2) K
0.3 × 0.2 × 0.2 mm

Data collection

Bruker Kappa APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.759, T_{max} = 0.830
11755 measured reflections
4047 independent reflections
3502 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.105
$wR(F^2)$ = 0.265
S = 1.11
4047 reflections
420 parameters
34 restraints
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2113).

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C_{60} 1,1,2,2-tetrachloroethylene tetrasolvate

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S1. Comment

C_{60} is located around inversion centre and there are two symmetry independent 1,1,2,2-tetrachloroethylene (TCE) solvent molecules in the asymmetric unit. The *ORTEP* drawing of the title compound is shown in Fig. 1. In the C_{60} molecule inter-pentagonal bond distances are in the range 1.3947 (17)–1.414 (15) Å while the intra-pentagonal bond distances are in the range 1.364 (19)–1.55 (2) Å. Such a variation in bond lengths is possibly due to the librational motion of the C_{60} molecule in the crystal. Similar variations of bond lengths were observed in some other C_{60} co-crystals (Dodrick *et al.*, 2005). The C_{60} and TCE molecules show intermolecular π-π interactions (Fig. 2). The short contacts between the fullerene C2 atom and the centre of the ethylene C33A—C34A bond, and C22 atom and the centre of the ethylene C31A —C32A bond are of 3.208 (17) and 3.223 (17) Å, respectively. Additionally, short contacts are observed between Cl atoms of TCE and C_{60} (Cl7···C14^{i} 3.419 (14) Å, Cl5···Cl4 = 3.491 (4) Å; symmetry code: (i) *x*, -1 + *y*, *z*]. The solvent molecules and C_{60} are located in alternating layers parallel to the (001) plane. The shortest C_{60}···C_{60} contacts are: C27···C29^{i} 3.690 (14) Å and C9···C11^{ii} 3.447 (14) Å [symmetry code: (i) 2 - *x*, 1 - *y*, -*z*, (ii) 1 - *x*, -*y*, -*z*]

S2. Experimental

C_{60} sample was purchased from Sigma-Aldrich and used as received. The solvents for crystallization, 1,1,2,2-tetrachloroethylene (TCE) and methanol were of purity >99% and were purchased from E. Merck (Germany). Crystals of the C_{60}. 4(CCl_4) were grown by diffusion of methanol into a solution of C_{60} in TCE over a period of five days. Upon removal from the mother liquor the crystals were unstable anad therefore were mounted at 0°C.

S3. Refinement

The C_{60} molecule was refined without any restraints. Both TCE molecules were disordered and showed two approximately perpendicular orientations with overlapping Cl atoms (the ratio of occupancies 0.75:0.25 and 0.56:0.44). Since one of the disordered TCE molecules showed occupancies very close to 0.75 and 0.25 these values were fixed at the final stages of the refinement. The restraints were imposed on C—C and C—Cl bond lengths of the TCE molecules and anisotropic displacement parameters of C31A, C32A and C34A atoms. The residual peak of 1.25 e Å^{-3} is located at 1.06 Å from the C5 atom of C_{60} indicating that in addition to large librational motion the C_{60} molecule can be also partially disordered. The high residual values, R1=0.105 and wR1=0.259 are most probably due to disorder of the TCE and C_{60} molecules.

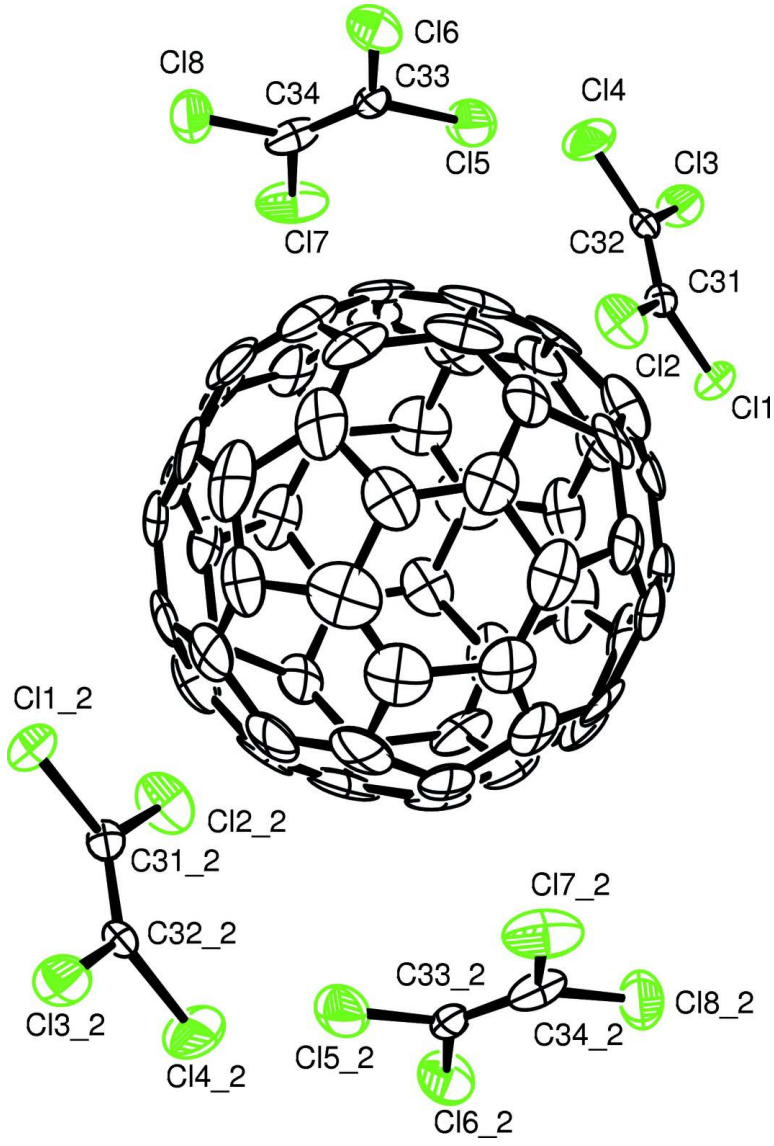

Figure 1

ORTEP diagram of the title compound showing 50% probability displacement ellipsoids. Labels for C_{60} were omitted. The TCE molecules in minor occupancies are not shown. Symmetry code for the atoms not from the asymmetric unit(_2): 2 - *x*, -*y*, -*z*).

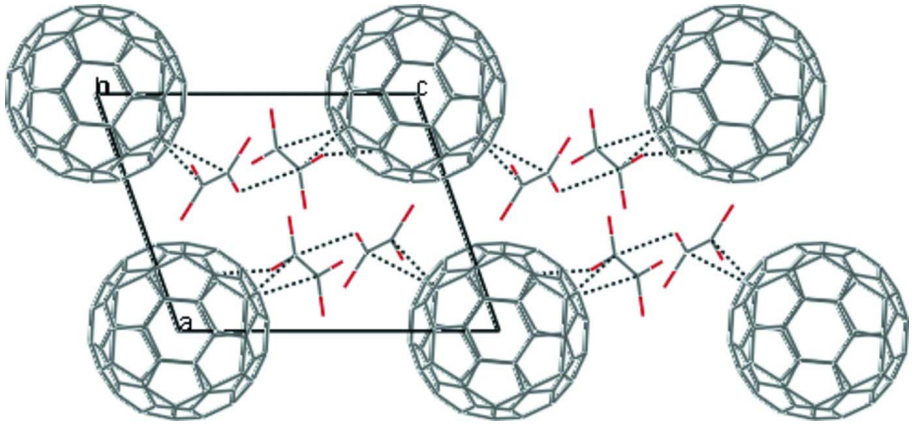

Figure 2

View of the crystal packing in the title compound along the *b* axis.

(I)

Crystal data

$C_{60}\cdot 4C_2Cl_4$
$M_r = 1383.88$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.049\ (5)$ Å
$b = 10.168\ (5)$ Å
$c = 13.412\ (5)$ Å
$\alpha = 70.484\ (5)°$
$\beta = 68.508\ (5)°$
$\gamma = 79.834\ (5)°$
$V = 1199.6\ (10)$ Å^3
$Z = 1$
$F(000) = 680$
$D_x = 1.916$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9670 reflections
$\theta = 2.2–28.4°$
$\mu = 0.97$ mm^{-1}
$T = 173$ K
Plate, brown
0.3 × 0.2 × 0.2 mm

Data collection

Bruker APEX2 Kappa diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.759$, $T_{max} = 0.830$
11755 measured reflections
4047 independent reflections
3502 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -11\rightarrow11$
$k = -12\rightarrow11$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.105$
$wR(F^2) = 0.265$
$S = 1.11$
4047 reflections
420 parameters
34 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 20.5574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.25$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.7872 (12)	0.2020 (11)	0.1752 (10)	0.048 (3)	
C2	0.8649 (12)	0.1051 (13)	0.2458 (9)	0.050 (3)	
C3	0.8346 (14)	−0.0347 (13)	0.2881 (8)	0.053 (3)	
C4	0.7301 (14)	−0.0837 (17)	0.2621 (11)	0.069 (4)	
C5	0.6574 (12)	−0.0048 (16)	0.2046 (11)	0.069 (4)	
C6	0.6836 (10)	0.1484 (11)	0.1574 (9)	0.044 (3)	
C7	0.6674 (10)	0.1949 (11)	0.0509 (10)	0.043 (2)	
C8	0.6353 (9)	0.0806 (11)	0.0226 (9)	0.038 (2)	
C9	0.6293 (9)	−0.0449 (12)	0.1128 (11)	0.051 (3)	
C10	0.6808 (12)	−0.1691 (13)	0.0941 (14)	0.068 (4)	
C11	0.6954 (10)	0.0755 (11)	−0.0878 (9)	0.043 (3)	
C12	1.2500 (12)	0.0616 (14)	0.1058 (11)	0.055 (3)	
C13	1.2598 (12)	0.1767 (11)	0.0131 (12)	0.051 (3)	
C14	0.7609 (12)	−0.2663 (12)	0.1663 (12)	0.062 (4)	
C15	0.7816 (13)	−0.2274 (11)	0.2465 (9)	0.052 (3)	
C16	0.9231 (17)	−0.2585 (12)	0.2626 (9)	0.063 (4)	
C17	0.9541 (18)	−0.1434 (13)	0.2871 (8)	0.064 (4)	
C18	1.0919 (15)	−0.1027 (16)	0.2459 (9)	0.064 (4)	
C19	1.1206 (14)	0.0448 (15)	0.2018 (10)	0.057 (3)	
C20	1.0097 (15)	0.1432 (14)	0.2030 (10)	0.059 (3)	
C21	1.2117 (14)	−0.1785 (12)	0.1725 (11)	0.060 (3)	
C22	1.1800 (13)	−0.2823 (11)	0.1474 (10)	0.052 (3)	
C23	1.0266 (11)	−0.3278 (10)	0.1968 (9)	0.043 (2)	
C24	0.7594 (10)	0.2949 (10)	−0.0361 (9)	0.041 (2)	
C25	1.0019 (12)	−0.3678 (9)	0.1130 (10)	0.045 (3)	
C26	0.8641 (12)	0.3473 (10)	−0.0120 (12)	0.053 (3)	
C27	0.8788 (13)	0.3009 (11)	0.0902 (10)	0.049 (3)	
C28	1.0212 (15)	0.2708 (13)	0.1026 (12)	0.061 (3)	
C29	1.1246 (13)	0.3373 (10)	−0.0941 (10)	0.049 (3)	
C30	1.1358 (17)	0.2883 (12)	0.0146 (12)	0.065 (4)	
C31	1.3841 (11)	0.4523 (10)	0.2363 (7)	0.027 (3)	0.82 (2)
C32	1.3342 (11)	0.4954 (11)	0.3232 (7)	0.029 (3)	0.82 (2)
C31A	1.306 (2)	0.430 (3)	0.3017 (15)	0.013 (10)	0.18 (2)
C32A	1.406 (2)	0.515 (3)	0.2605 (15)	0.007 (9)	0.18 (2)
C33	0.7666 (10)	0.1574 (11)	0.4919 (11)	0.030 (5)	0.56 (3)

C34	0.6841 (11)	0.2472 (11)	0.4454 (12)	0.039 (5)	0.56 (3)
C33A	0.7762 (13)	0.2488 (14)	0.4439 (16)	0.039 (7)	0.44 (3)
C34A	0.677 (2)	0.162 (2)	0.4950 (19)	0.034 (6)	0.44 (3)
Cl1	1.5322 (2)	0.5188 (2)	0.12839 (19)	0.0357 (6)	
Cl2	1.2994 (3)	0.3299 (3)	0.2202 (2)	0.0484 (7)	
Cl3	1.4140 (3)	0.6192 (3)	0.3386 (2)	0.0425 (6)	
Cl4	1.1832 (3)	0.4285 (3)	0.4339 (2)	0.0566 (8)	
Cl5	0.9370 (3)	0.2011 (4)	0.4666 (2)	0.0569 (8)	
Cl6	0.7062 (3)	−0.0017 (3)	0.5858 (2)	0.0535 (7)	
Cl7	0.7431 (4)	0.4076 (3)	0.3547 (2)	0.0615 (9)	
Cl8	0.5146 (3)	0.2052 (3)	0.4689 (2)	0.0565 (8)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.053 (7)	0.072 (8)	0.036 (6)	0.006 (6)	−0.008 (5)	−0.043 (6)
C3	0.073 (8)	0.064 (8)	0.012 (4)	−0.005 (6)	0.002 (5)	−0.016 (5)
C6	0.026 (5)	0.042 (6)	0.042 (6)	0.015 (4)	0.011 (4)	−0.021 (5)
C7	0.023 (5)	0.039 (6)	0.065 (7)	0.019 (4)	−0.015 (5)	−0.023 (5)
C8	0.014 (4)	0.046 (6)	0.058 (6)	0.003 (4)	−0.017 (4)	−0.018 (5)
C9	0.007 (4)	0.054 (7)	0.077 (8)	−0.007 (4)	−0.004 (5)	−0.009 (6)
C10	0.026 (6)	0.055 (8)	0.114 (12)	−0.025 (5)	−0.015 (7)	−0.011 (8)
C12	0.040 (6)	0.088 (9)	0.069 (8)	−0.008 (6)	−0.035 (6)	−0.041 (7)
C13	0.039 (6)	0.040 (6)	0.090 (9)	−0.015 (5)	−0.037 (6)	−0.018 (6)
C14	0.038 (6)	0.043 (6)	0.079 (9)	−0.033 (5)	−0.015 (6)	0.024 (6)
C15	0.053 (7)	0.031 (5)	0.035 (6)	−0.016 (5)	0.019 (5)	0.006 (4)
C17	0.121 (12)	0.055 (7)	0.017 (5)	−0.007 (7)	−0.032 (6)	0.001 (5)
C19	0.067 (8)	0.082 (9)	0.054 (7)	0.002 (7)	−0.044 (7)	−0.036 (7)
C20	0.089 (10)	0.066 (8)	0.052 (7)	0.003 (7)	−0.042 (7)	−0.039 (6)
C21	0.072 (8)	0.040 (6)	0.076 (9)	0.003 (6)	−0.055 (7)	0.003 (6)
C22	0.063 (7)	0.041 (6)	0.051 (7)	0.027 (5)	−0.045 (6)	0.000 (5)
C23	0.048 (6)	0.026 (5)	0.042 (6)	−0.001 (4)	−0.020 (5)	0.010 (4)
C24	0.032 (5)	0.024 (5)	0.063 (7)	0.015 (4)	−0.019 (5)	−0.011 (4)
C25	0.053 (6)	0.009 (4)	0.061 (7)	−0.007 (4)	−0.015 (5)	0.004 (4)
C26	0.050 (6)	0.017 (5)	0.090 (9)	0.011 (4)	−0.019 (6)	−0.025 (5)
C27	0.060 (7)	0.035 (6)	0.063 (7)	0.009 (5)	−0.019 (6)	−0.037 (5)
C28	0.080 (9)	0.053 (7)	0.080 (9)	−0.008 (6)	−0.031 (8)	−0.048 (7)
C29	0.065 (8)	0.019 (5)	0.065 (7)	−0.014 (5)	−0.031 (6)	0.003 (5)
C30	0.096 (10)	0.040 (6)	0.079 (9)	−0.036 (7)	−0.034 (8)	−0.020 (6)
C31	0.028 (6)	0.023 (5)	0.028 (6)	−0.005 (4)	−0.009 (5)	−0.001 (4)
C32	0.028 (6)	0.034 (6)	0.027 (6)	0.002 (5)	−0.014 (5)	−0.010 (5)
C31A	0.014 (11)	0.013 (11)	0.014 (11)	0.000 (5)	−0.004 (6)	−0.005 (6)
C32A	0.008 (10)	0.007 (10)	0.006 (11)	0.000 (5)	−0.001 (6)	−0.003 (5)
C33	0.023 (10)	0.039 (11)	0.024 (9)	0.009 (9)	−0.004 (8)	−0.012 (8)
C34	0.051 (13)	0.024 (10)	0.025 (10)	−0.008 (9)	0.008 (9)	−0.006 (8)
C33A	0.042 (15)	0.046 (15)	0.030 (13)	−0.012 (13)	−0.006 (12)	−0.015 (11)
C34A	0.019 (11)	0.028 (12)	0.037 (13)	−0.007 (10)	0.010 (10)	−0.007 (10)
Cl1	0.0277 (11)	0.0402 (13)	0.0334 (12)	−0.0031 (9)	−0.0002 (9)	−0.0140 (10)

Cl2	0.0645 (17)	0.0344 (13)	0.0625 (17)	−0.0119 (12)	−0.0345 (14)	−0.0150 (12)
Cl3	0.0450 (14)	0.0485 (14)	0.0442 (14)	−0.0097 (11)	−0.0119 (11)	−0.0262 (11)
Cl4	0.0426 (15)	0.074 (2)	0.0378 (14)	−0.0217 (14)	0.0055 (11)	−0.0085 (13)
Cl5	0.0457 (16)	0.086 (2)	0.0461 (16)	−0.0226 (15)	−0.0169 (13)	−0.0166 (15)
Cl6	0.0653 (18)	0.0400 (14)	0.0425 (15)	−0.0036 (12)	−0.0213 (13)	0.0076 (11)
Cl7	0.104 (3)	0.0280 (13)	0.0343 (14)	−0.0175 (14)	−0.0051 (15)	0.0002 (10)
Cl8	0.0380 (14)	0.0658 (18)	0.0538 (17)	0.0013 (13)	−0.0180 (12)	−0.0021 (14)
C16	0.111 (11)	0.041 (6)	0.022 (5)	−0.027 (7)	−0.020 (6)	0.017 (5)
C5	0.028 (6)	0.092 (10)	0.047 (7)	−0.001 (6)	0.020 (5)	−0.007 (7)
C1	0.046 (6)	0.043 (6)	0.061 (7)	0.017 (5)	−0.009 (5)	−0.041 (6)
C11	0.028 (5)	0.052 (6)	0.054 (6)	−0.004 (4)	−0.033 (5)	−0.001 (5)
C18	0.078 (9)	0.100 (11)	0.028 (6)	0.001 (8)	−0.043 (6)	−0.010 (6)
C4	0.044 (7)	0.100 (11)	0.040 (7)	−0.015 (7)	0.016 (6)	−0.019 (7)

Geometric parameters (Å, º)

C2—C3	1.386 (17)	C23—C25	1.426 (16)
C2—C20	1.426 (17)	C24—C22^{i}	1.432 (16)
C2—C1	1.457 (16)	C24—C26	1.433 (16)
C3—C4	1.429 (19)	C25—C29^{i}	1.350 (16)
C3—C17	1.482 (19)	C25—C26^{i}	1.505 (16)
C6—C1	1.382 (16)	C26—C27	1.348 (17)
C6—C7	1.408 (15)	C26—C25^{i}	1.505 (16)
C6—C5	1.504 (18)	C27—C1	1.396 (16)
C7—C24	1.414 (15)	C27—C28	1.468 (17)
C7—C8	1.454 (14)	C28—C30	1.299 (19)
C8—C11	1.394 (15)	C29—C25^{i}	1.350 (16)
C8—C9	1.427 (15)	C29—C30	1.415 (17)
C9—C10	1.347 (17)	C29—C14^{i}	1.463 (19)
C9—C5	1.55 (2)	C31—C32	1.280 (2)
C10—C13^{i}	1.364 (19)	C31—Cl1	1.699 (10)
C10—C14	1.487 (18)	C31—Cl2	1.735 (10)
C12—C13	1.379 (18)	C32—Cl3	1.709 (10)
C12—C19	1.443 (17)	C32—Cl4	1.735 (10)
C12—C11^{i}	1.471 (16)	C31A—C32A	1.282 (2)
C13—C10^{i}	1.364 (19)	C31A—Cl2	1.747 (9)
C13—C30	1.529 (19)	C31A—Cl4	1.748 (9)
C14—C15	1.354 (19)	C32A—Cl3	1.751 (9)
C14—C29^{i}	1.463 (19)	C32A—Cl1	1.751 (9)
C15—C16	1.480 (19)	C33—C34	1.281 (2)
C15—C4	1.517 (19)	C33—Cl5	1.728 (8)
C17—C18	1.372 (19)	C33—Cl6	1.731 (8)
C17—C16	1.427 (17)	C34—Cl8	1.720 (8)
C19—C20	1.360 (18)	C34—Cl7	1.726 (8)
C19—C18	1.454 (19)	C33A—C34A	1.281 (2)
C20—C28	1.510 (19)	C33A—Cl5	1.711 (9)
C21—C22	1.327 (17)	C33A—Cl7	1.721 (9)
C21—C11^{i}	1.426 (16)	C34A—Cl8	1.75 (2)

C21—C18	1.524 (19)	C34A—Cl6	1.75 (2)
C22—C24^{i}	1.432 (16)	C5—C4	1.251 (19)
C22—C23	1.525 (16)	C11—C21^{i}	1.426 (16)
C23—C16	1.358 (17)	C11—C12^{i}	1.471 (16)
C3—C2—C20	120.2 (11)	C27—C26—C24	121.6 (11)
C3—C2—C1	119.0 (11)	C27—C26—C25^{i}	117.9 (11)
C20—C2—C1	108.6 (11)	C24—C26—C25^{i}	108.2 (10)
C2—C3—C4	120.7 (12)	C26—C27—C1	118.9 (11)
C2—C3—C17	119.2 (12)	C26—C27—C28	121.0 (11)
C4—C3—C17	107.2 (11)	C1—C27—C28	108.6 (11)
C1—C6—C7	119.7 (10)	C30—C28—C27	120.3 (13)
C1—C6—C5	121.1 (11)	C30—C28—C20	121.0 (13)
C7—C6—C5	107.4 (11)	C27—C28—C20	106.3 (11)
C6—C7—C24	118.8 (10)	C25^{i}—C29—C30	123.2 (12)
C6—C7—C8	111.1 (9)	C25^{i}—C29—C14^{i}	117.5 (11)
C24—C7—C8	117.6 (10)	C30—C29—C14^{i}	108.4 (11)
C11—C8—C9	119.7 (10)	C28—C30—C29	120.3 (14)
C11—C8—C7	118.9 (9)	C28—C30—C13	119.0 (12)
C9—C8—C7	109.3 (10)	C29—C30—C13	107.8 (12)
C10—C9—C8	121.5 (12)	C32—C31—Cl1	121.3 (8)
C10—C9—C5	120.3 (12)	C32—C31—Cl2	121.7 (8)
C8—C9—C5	106.4 (10)	Cl1—C31—Cl2	117.0 (5)
C9—C10—C13^{i}	119.8 (13)	C31—C32—Cl3	122.2 (9)
C9—C10—C14	117.8 (14)	C31—C32—Cl4	121.7 (9)
C13^{i}—C10—C14	110.6 (12)	Cl3—C32—Cl4	116.0 (5)
C13—C12—C19	119.7 (12)	C32A—C31A—Cl2	117.9 (7)
C13—C12—C11^{i}	118.3 (11)	C32A—C31A—Cl4	116.8 (7)
C19—C12—C11^{i}	109.1 (11)	Cl2—C31A—Cl4	125.3 (7)
C10^{i}—C13—C12	123.0 (12)	C31A—C32A—Cl3	119.1 (7)
C10^{i}—C13—C30	107.0 (11)	C31A—C32A—Cl1	118.2 (7)
C12—C13—C30	119.8 (12)	Cl3—C32A—Cl1	122.7 (6)
C15—C14—C29^{i}	121.7 (11)	C34—C33—Cl5	119.1 (7)
C15—C14—C10	119.8 (13)	C34—C33—Cl6	121.0 (7)
C29^{i}—C14—C10	106.2 (12)	Cl5—C33—Cl6	119.8 (5)
C14—C15—C16	119.4 (11)	C33—C34—Cl8	119.7 (7)
C14—C15—C4	121.6 (12)	C33—C34—Cl7	120.9 (7)
C16—C15—C4	105.7 (11)	Cl8—C34—Cl7	119.3 (5)
C18—C17—C16	119.9 (14)	C34A—C33A—Cl5	118.4 (14)
C18—C17—C3	119.0 (12)	C34A—C33A—Cl7	119.0 (14)
C16—C17—C3	109.9 (13)	Cl5—C33A—Cl7	122.6 (7)
C20—C19—C12	120.6 (13)	C33A—C34A—Cl8	119.4 (17)
C20—C19—C18	119.7 (12)	C33A—C34A—Cl6	120.8 (17)
C12—C19—C18	108.0 (11)	Cl8—C34A—Cl6	119.8 (7)
C19—C20—C2	121.4 (12)	C23—C16—C17	121.5 (13)
C19—C20—C28	119.8 (13)	C23—C16—C15	117.9 (11)
C2—C20—C28	106.7 (11)	C17—C16—C15	108.4 (12)
C22—C21—C11^{i}	120.2 (13)	C4—C5—C6	118.8 (15)

C22—C21—C18	119.0 (12)	C4—C5—C9	122.0 (14)
C11^{i}—C21—C18	107.1 (11)	C6—C5—C9	105.8 (11)
C21—C22—C24^{i}	121.0 (12)	C6—C1—C27	122.1 (11)
C21—C22—C23	119.6 (11)	C6—C1—C2	117.2 (10)
C24^{i}—C22—C23	108.4 (10)	C27—C1—C2	109.7 (10)
C16—C23—C25	121.6 (11)	C8—C11—C21^{i}	121.5 (11)
C16—C23—C22	119.6 (11)	C8—C11—C12^{i}	117.6 (10)
C25—C23—C22	106.5 (9)	C21^{i}—C11—C12^{i}	108.6 (11)
C7—C24—C22^{i}	120.8 (10)	C17—C18—C19	120.6 (13)
C7—C24—C26	118.8 (10)	C17—C18—C21	120.2 (13)
C22^{i}—C24—C26	108.7 (10)	C19—C18—C21	107.1 (11)
C29^{i}—C25—C23	121.9 (11)	C5—C4—C3	123.1 (15)
C29^{i}—C25—C26^{i}	117.2 (11)	C5—C4—C15	118.2 (15)
C23—C25—C26^{i}	108.2 (9)	C3—C4—C15	108.9 (12)

C20—C2—C3—C4	−137.2 (11)	Cl5—C33—C34—Cl8	179.6 (9)
C1—C2—C3—C4	0.8 (15)	Cl6—C33—C34—Cl8	−4 (2)
C20—C2—C3—C17	−0.7 (14)	Cl5—C33—C34—Cl7	2 (2)
C1—C2—C3—C17	137.3 (10)	Cl6—C33—C34—Cl7	178.3 (10)
C1—C6—C7—C24	0.7 (13)	Cl5—C33A—C34A—Cl8	−177.4 (12)
C5—C6—C7—C24	−142.6 (9)	Cl7—C33A—C34A—Cl8	2 (3)
C1—C6—C7—C8	141.9 (9)	Cl5—C33A—C34A—Cl6	0 (3)
C5—C6—C7—C8	−1.4 (10)	Cl7—C33A—C34A—Cl6	179.4 (12)
C6—C7—C8—C11	−142.2 (9)	C32—C31—Cl1—C32A	0 (2)
C24—C7—C8—C11	−0.4 (13)	Cl2—C31—Cl1—C32A	177 (3)
C6—C7—C8—C9	0.3 (10)	C31A—C32A—Cl1—C31	0 (2)
C24—C7—C8—C9	142.0 (9)	Cl3—C32A—Cl1—C31	179 (4)
C11—C8—C9—C10	0.1 (14)	C32—C31—Cl2—C31A	−2 (3)
C7—C8—C9—C10	−141.9 (10)	Cl1—C31—Cl2—C31A	−179 (3)
C11—C8—C9—C5	143.0 (9)	C32A—C31A—Cl2—C31	2 (2)
C7—C8—C9—C5	1.0 (10)	Cl4—C31A—Cl2—C31	180 (5)
C8—C9—C10—C13^{i}	0.0 (15)	C31—C32—Cl3—C32A	1 (3)
C5—C9—C10—C13^{i}	−137.9 (11)	Cl4—C32—Cl3—C32A	180 (3)
C8—C9—C10—C14	139.6 (11)	C31A—C32A—Cl3—C32	−1 (2)
C5—C9—C10—C14	1.7 (15)	Cl1—C32A—Cl3—C32	−180 (4)
C19—C12—C13—C10^{i}	−138.2 (11)	C31—C32—Cl4—C31A	0 (2)
C11^{i}—C12—C13—C10^{i}	−0.8 (15)	Cl3—C32—Cl4—C31A	−179 (3)
C19—C12—C13—C30	2.4 (15)	C32A—C31A—Cl4—C32	0 (2)
C11^{i}—C12—C13—C30	139.8 (10)	Cl2—C31A—Cl4—C32	−178 (5)
C9—C10—C14—C15	−1.0 (15)	C34A—C33A—Cl5—C33	2.6 (16)
C13^{i}—C10—C14—C15	142.1 (11)	Cl7—C33A—Cl5—C33	−177 (3)
C9—C10—C14—C29^{i}	−143.9 (10)	C34—C33—Cl5—C33A	0.4 (18)
C13^{i}—C10—C14—C29^{i}	−0.8 (12)	Cl6—C33—Cl5—C33A	−176 (2)
C29^{i}—C14—C15—C16	−0.6 (15)	C34—C33—Cl6—C34A	−0.7 (18)
C10—C14—C15—C16	−137.7 (11)	Cl5—C33—Cl6—C34A	175 (3)
C29^{i}—C14—C15—C4	134.6 (11)	C33A—C34A—Cl6—C33	−2.6 (17)
C10—C14—C15—C4	−2.5 (16)	Cl8—C34A—Cl6—C33	174 (3)
C2—C3—C17—C18	1.1 (15)	C34A—C33A—Cl7—C34	−1.0 (17)

C4—C3—C17—C18	142.8 (10)	Cl5—C33A—Cl7—C34	179 (3)
C2—C3—C17—C16	−142.6 (10)	C33—C34—Cl7—C33A	−2.1 (18)
C4—C3—C17—C16	−0.9 (12)	Cl8—C34—Cl7—C33A	−179 (3)
C13—C12—C19—C20	−1.9 (15)	C33—C34—Cl8—C34A	3.8 (17)
C11^{i}—C12—C19—C20	−142.7 (10)	Cl7—C34—Cl8—C34A	−179 (3)
C13—C12—C19—C18	141.0 (10)	C33A—C34A—Cl8—C34	−0.7 (18)
C11^{i}—C12—C19—C18	0.2 (11)	Cl6—C34A—Cl8—C34	−178 (3)
C12—C19—C20—C2	138.1 (11)	C25—C23—C16—C17	−137.0 (11)
C18—C19—C20—C2	−0.6 (16)	C22—C23—C16—C17	0.0 (15)
C12—C19—C20—C28	0.6 (15)	C25—C23—C16—C15	1.1 (14)
C18—C19—C20—C28	−138.1 (11)	C22—C23—C16—C15	138.1 (10)
C3—C2—C20—C19	0.5 (15)	C18—C17—C16—C23	−1.6 (16)
C1—C2—C20—C19	−141.3 (10)	C3—C17—C16—C23	141.8 (11)
C3—C2—C20—C28	142.7 (10)	C18—C17—C16—C15	−143.1 (11)
C1—C2—C20—C28	0.9 (11)	C3—C17—C16—C15	0.2 (12)
C11^{i}—C21—C22—C24^{i}	1.4 (16)	C14—C15—C16—C23	−1.2 (14)
C18—C21—C22—C24^{i}	136.9 (11)	C4—C15—C16—C23	−142.6 (10)
C11^{i}—C21—C22—C23	−138.4 (11)	C14—C15—C16—C17	142.0 (10)
C18—C21—C22—C23	−2.8 (15)	C4—C15—C16—C17	0.5 (11)
C21—C22—C23—C16	2.3 (14)	C1—C6—C5—C4	1.0 (16)
C24^{i}—C22—C23—C16	−142.0 (10)	C7—C6—C5—C4	143.6 (11)
C21—C22—C23—C25	145.0 (10)	C1—C6—C5—C9	−140.7 (10)
C24^{i}—C22—C23—C25	0.7 (10)	C7—C6—C5—C9	1.9 (10)
C6—C7—C24—C22^{i}	137.9 (10)	C10—C9—C5—C4	1.5 (17)
C8—C7—C24—C22^{i}	−0.8 (13)	C8—C9—C5—C4	−141.9 (12)
C6—C7—C24—C26	−1.1 (13)	C10—C9—C5—C6	141.7 (10)
C8—C7—C24—C26	−139.9 (9)	C8—C9—C5—C6	−1.8 (10)
C16—C23—C25—C29^{i}	0.8 (15)	C7—C6—C1—C27	−0.6 (14)
C22—C23—C25—C29^{i}	−141.0 (9)	C5—C6—C1—C27	137.6 (10)
C16—C23—C25—C26^{i}	141.4 (10)	C7—C6—C1—C2	−141.0 (9)
C22—C23—C25—C26^{i}	−0.4 (10)	C5—C6—C1—C2	−2.8 (14)
C7—C24—C26—C27	1.6 (14)	C26—C27—C1—C6	1.1 (15)
C22^{i}—C24—C26—C27	−141.9 (10)	C28—C27—C1—C6	−142.7 (9)
C7—C24—C26—C25^{i}	143.1 (9)	C26—C27—C1—C2	144.0 (10)
C22^{i}—C24—C26—C25^{i}	−0.4 (11)	C28—C27—C1—C2	0.2 (11)
C24—C26—C27—C1	−1.6 (15)	C3—C2—C1—C6	1.9 (14)
C25^{i}—C26—C27—C1	−139.5 (10)	C20—C2—C1—C6	144.2 (9)
C24—C26—C27—C28	137.6 (11)	C3—C2—C1—C27	−143.1 (9)
C25^{i}—C26—C27—C28	−0.3 (14)	C20—C2—C1—C27	−0.7 (11)
C26—C27—C28—C30	−0.1 (16)	C9—C8—C11—C21^{i}	−137.7 (10)
C1—C27—C28—C30	142.9 (11)	C7—C8—C11—C21^{i}	0.8 (14)
C26—C27—C28—C20	−142.6 (10)	C9—C8—C11—C12^{i}	0.2 (12)
C1—C27—C28—C20	0.3 (11)	C7—C8—C11—C12^{i}	138.7 (9)
C19—C20—C28—C30	0.0 (16)	C16—C17—C18—C19	138.8 (11)
C2—C20—C28—C30	−142.9 (11)	C3—C17—C18—C19	−1.2 (15)
C19—C20—C28—C27	142.2 (10)	C16—C17—C18—C21	1.0 (16)
C2—C20—C28—C27	−0.8 (11)	C3—C17—C18—C21	−139.1 (11)
C27—C28—C30—C29	0.3 (16)	C20—C19—C18—C17	1.0 (16)

C20—C28—C30—C29	137.3 (12)	C12—C19—C18—C17	−142.3 (10)
C27—C28—C30—C13	−136.5 (11)	C20—C19—C18—C21	143.7 (10)
C20—C28—C30—C13	0.6 (16)	C12—C19—C18—C21	0.4 (11)
C25^{i}—C29—C30—C28	−0.2 (17)	C22—C21—C18—C17	1.3 (16)
C14^{i}—C29—C30—C28	−143.2 (11)	C11^{i}—C21—C18—C17	142.0 (11)
C25^{i}—C29—C30—C13	140.8 (10)	C22—C21—C18—C19	−141.5 (10)
C14^{i}—C29—C30—C13	−2.2 (11)	C11^{i}—C21—C18—C19	−0.8 (11)
C10^{i}—C13—C30—C28	144.3 (11)	C6—C5—C4—C3	1.9 (18)
C12—C13—C30—C28	−1.8 (15)	C9—C5—C4—C3	137.2 (13)
C10^{i}—C13—C30—C29	2.7 (11)	C6—C5—C4—C15	−140.2 (11)
C12—C13—C30—C29	−143.5 (10)	C9—C5—C4—C15	−4.9 (17)
Cl1—C31—C32—Cl3	−1.3 (14)	C2—C3—C4—C5	−2.8 (18)
Cl2—C31—C32—Cl3	−178.3 (6)	C17—C3—C4—C5	−143.9 (12)
Cl1—C31—C32—Cl4	180.0 (6)	C2—C3—C4—C15	142.2 (10)
Cl2—C31—C32—Cl4	3.0 (14)	C17—C3—C4—C15	1.2 (12)
Cl2—C31A—C32A—Cl3	178.6 (19)	C14—C15—C4—C5	5.5 (16)
Cl4—C31A—C32A—Cl3	1 (4)	C16—C15—C4—C5	145.9 (11)
Cl2—C31A—C32A—Cl1	−2 (4)	C14—C15—C4—C3	−141.5 (11)
Cl4—C31A—C32A—Cl1	179.8 (19)	C16—C15—C4—C3	−1.1 (12)

Symmetry code: (i) −*x*+2, −*y*, −*z*.