Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,7-Dichloro-4-(chloroacetyl)fluorene

Jian-Bo Chu,[a] Guo-Wu Rao[b]* and Jin-Hao Zhao[c]

[a]Department of Pharmacy, Zhejiang Medical College, Hangzhou 310053, People's Republic of China, [b]College of Pharmaceutical Science, Zhejiang University of Technology, Hangzhou,310032, People's Republic of China, and [c]College of Agriculture and Biotechnology, Zhejiang University, Hangzhou 310029, People's Republic of China
Correspondence e-mail: rgw@zjut.edu.cn

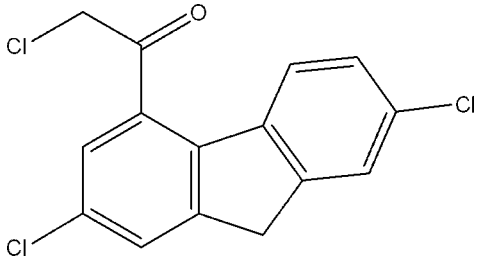
Received 30 June 2009; accepted 11 July 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.174; data-to-parameter ratio = 14.9.

There are two molecules in the asymmetric unit of the title compound, $C_{15}H_9Cl_3O$. The fluorene rings of the two molecules are both coplanar within 066 (3) Å. In the crystal, C—H···O and C—H···Cl hydrogen bonds link the molecules into sheets running parallel to (100).

Related literature

The title compound is an important intermediate in the synthesis of benflumetol, see: Deng *et al.* (2000). Benflumetol conforms structurally and in mode of action to the structure and mode of action of the aryl amino alcohol group of antimalarial drugs, including quinine, mefloquine, and halofantrine, see: Pradines *et al.* (1999). For our ongoing work on structure–activity relationships, see: Rao & Hu (2005, 2006); Hu *et al.* (2004).



Experimental

Crystal data

$C_{15}H_9Cl_3O$
M_r = 311.57
Triclinic, $P\overline{1}$
a = 7.607 (6) Å
b = 13.227 (10) Å
c = 14.957 (11) Å
α = 64.942 (9)°
β = 81.653 (10)°
γ = 76.433 (10)°
V = 1323.5 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 298 K
0.25 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.849, T_{max} = 0.935
6098 measured reflections
5096 independent reflections
3419 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.174
S = 0.96
5096 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1	0.93	2.37	2.998 (4)	124
C15—H15B···Cl6	0.97	2.80	3.678 (5)	151
C21—H21···O2	0.93	2.45	3.086 (5)	126
C35—H35A···O1^{i}	0.97	2.45	3.261 (5)	140

Symmetry code: (i) $x-1, y, z$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work is supported by the Open Foundation of Zhejiang Provincial Top Key Pharmaceutical Discipline (No. 20060611) and the Department of Education of Zhejiang Province of China (No. 20060806).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2225).

References

Deng, R. X., Zhong, J. X., Zhao, D. C. & Wang, J. (2000). *Yaoxue Xuebao*, **35**, 22–25.
Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Hu, W. X., Rao, G. W. & Sun, Y. Q. (2004). *Bioorg. Med. Chem. Lett.* **14**, 1177–1181.
Pradines, B., Tall, A., Fusai, T., Spiegel, A., Hienne, R., Rogier, C., Trape, J. F., Le Bras, J. & Parzy, D. (1999). *Antimicrob. Agents Chemother.* **43**, 418–420.
Rao, G. W. & Hu, W. X. (2005). *Bioorg. Med. Chem. Lett.* **15**, 3174–3176.
Rao, G. W. & Hu, W. X. (2006). *Bioorg. Med. Chem. Lett.* **16**, 3702–3705.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2009). E**65**, o2009 [doi:10.1107/S1600536809027287]

2,7-Dichloro-4-(chloroacetyl)fluorene

Jian-Bo Chu, Guo-Wu Rao and Jin-Hao Zhao

S1. Comment

Benflumetol is a racemic fluorene derivative. It conforms to the structure and reactivity of the aryl amino alcohol group of antimalarial drugs, including quinine, mefloquine, and halofantrine (Pradines *et al.*, 1999). 2,7-Dichloro-4-chloroacetyl fluorene, (I), is an important intermediate in the synthesis of benflumetol (Deng *et al.*, 2000). In a continuation of our work on the structure-activity relationships (Rao *et al.*, 2004, 2005, 2006) we have obtained a colourless crystalline compound as the product of the reaction of 2-chloroacetyl chloride and 2,7-dichloro-9*H*-fluorene. The structural characterization of our product, (I), was performed by single-crystal X-ray diffraction.

The two essentially identical molecules form the asymmetric unit of (I) (Fig. 1). The two independent molecules are roughly parallel to each other, with a head-to-head orientation. The molecular structure is built up from three fused ring, two of which are six-membered and one five-membered. In both molecules, the three rings in the fluorene are coplanar with the largest deviation from the planes being 0.0664 (27) Å for atom C9 and 0.0656 (28)Å for atom C29, respectively. In both molecules, the dihedral angle between the two planes of the fluorene ring is 35.59 (6)°. The torsion angles for substituted $COCH_2Cl$ (O1/C14/C15/Cl3 and O2/C34/C35/Cl6) are -8.4 (5) and 31.8 (5)^o, respectively.

The crystal packing of (I) is defined by C—H···O and C—H···Cl hydrogen bonds that link the molecules into sheets running parallel to the (100) plane (Table 1, Fig. 2).

S2. Experimental

The title compound was prepared from 2-chloroacetyl chloride and 2,7-dichloro-9*H*-fluorene according to the procedure of Deng *et al.* (2000). A solution of the compound in ethanol was concentrated gradually at room temperature to afford colourless prisms (m.p. 398–399 K).

S3. Refinement

H atoms were included in calculated positions and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 times the equivalent isotropic displacement parameters of their parent atoms and C—H distances were restrained to 0.97 Å for methylene H atoms, 0.93 Å for aromatic H atoms.

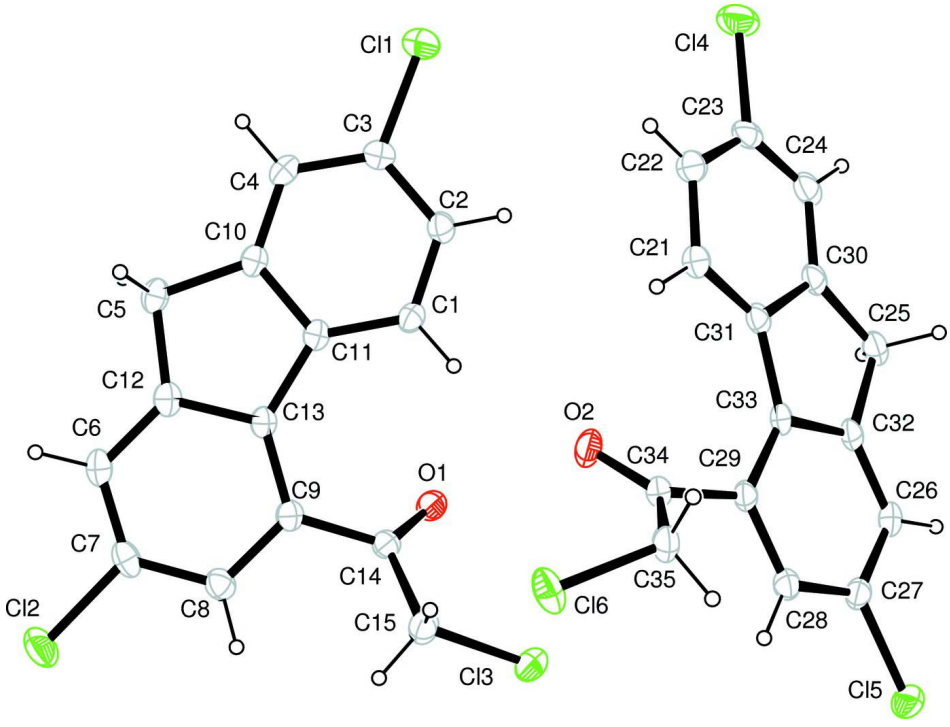


Figure 1

The structure of (I) showing the atom-labelling scheme. Ellipsoids are drawn at the 30% probability level.

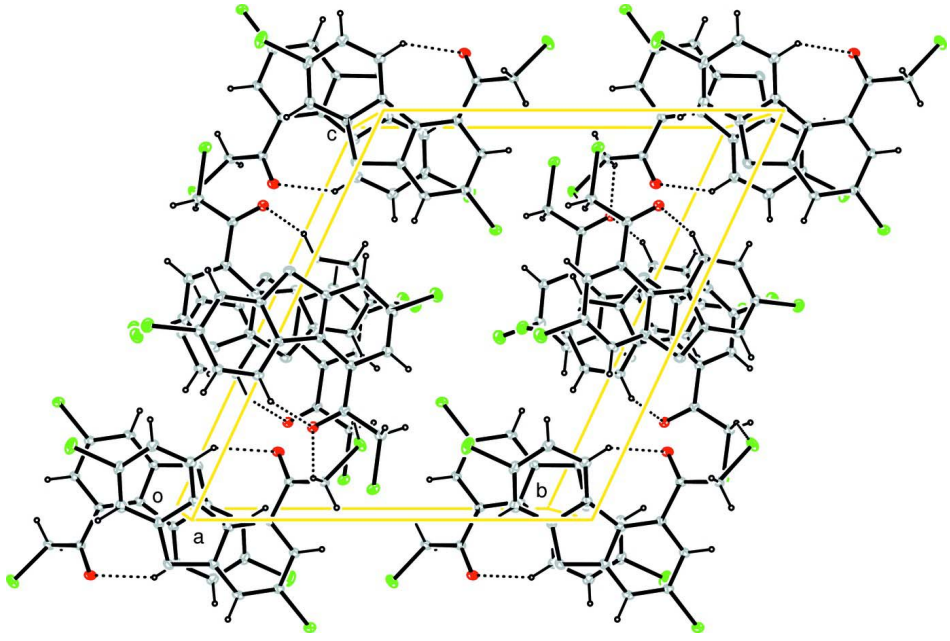


Figure 2

The crystal packing of (I) showing the C—H···O and C—H···Cl hydrogen bonds.

2,7-Dichloro-4-(chloroacetyl)fluorene

Crystal data

$C_{15}H_9Cl_3O$
$M_r = 311.57$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.607$ (6) Å
$b = 13.227$ (10) Å
$c = 14.957$ (11) Å
$\alpha = 64.942$ (9)°
$\beta = 81.653$ (10)°
$\gamma = 76.433$ (10)°
$V = 1323.5$ (17) Å^3
$Z = 4$
$F(000) = 632$
$D_x = 1.564$ Mg m^{-3}
Melting point = 398–399 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 868 reflections
$\theta = 2.7$–$23.5°$
$\mu = 0.68$ mm^{-1}
$T = 298$ K
Prismatic, colorless
0.25 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.849$, $T_{max} = 0.935$
6098 measured reflections
5096 independent reflections
3419 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.5°$
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 14$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.174$
$S = 0.96$
5096 reflections
343 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1131P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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}
Cl1	0.38813 (15)	1.35826 (8)	0.52879 (8)	0.0682 (3)
Cl2	1.12004 (16)	0.64244 (10)	0.44936 (9)	0.0768 (4)
Cl3	0.74877 (16)	0.60526 (8)	0.91826 (7)	0.0685 (3)

O1	0.8430 (4)	0.81774 (19)	0.77151 (16)	0.0514 (6)
C1	0.5934 (5)	1.0272 (3)	0.6453 (2)	0.0436 (8)
H1	0.5919	0.9673	0.7072	0.052*
C2	0.5018 (5)	1.1346 (3)	0.6318 (2)	0.0462 (8)
H2	0.4382	1.1474	0.6853	0.055*
C3	0.5023 (5)	1.2242 (3)	0.5401 (2)	0.0469 (8)
C4	0.5926 (5)	1.2073 (3)	0.4590 (2)	0.0468 (8)
H4	0.5919	1.2675	0.3971	0.056*
C5	0.7849 (5)	1.0590 (3)	0.3956 (2)	0.0462 (8)
H5A	0.7058	1.0706	0.3453	0.055*
H5B	0.8851	1.0978	0.3641	0.055*
C6	0.9522 (5)	0.8548 (3)	0.4220 (3)	0.0503 (9)
H6	0.9899	0.8749	0.3557	0.060*
C7	0.9956 (5)	0.7454 (3)	0.4890 (3)	0.0530 (9)
C8	0.9454 (5)	0.7127 (3)	0.5885 (3)	0.0489 (8)
H8	0.9759	0.6370	0.6322	0.059*
C9	0.8482 (4)	0.7941 (3)	0.6235 (2)	0.0408 (7)
C10	0.6833 (4)	1.0998 (3)	0.4718 (2)	0.0403 (7)
C11	0.6891 (4)	1.0092 (3)	0.5647 (2)	0.0381 (7)
C12	0.8510 (4)	0.9354 (3)	0.4544 (2)	0.0436 (8)
C13	0.7963 (4)	0.9061 (3)	0.5552 (2)	0.0384 (7)
C14	0.8187 (4)	0.7600 (3)	0.7319 (2)	0.0419 (7)
C15	0.7535 (6)	0.6491 (3)	0.7895 (3)	0.0588 (10)
H15A	0.8323	0.5903	0.7719	0.071*
H15B	0.6327	0.6574	0.7704	0.071*
Cl4	0.11626 (18)	1.38515 (8)	0.82118 (10)	0.0877 (4)
Cl5	0.41632 (16)	0.54224 (8)	1.28292 (6)	0.0645 (3)
Cl6	0.26609 (15)	0.64588 (9)	0.81998 (8)	0.0681 (3)
O2	0.3758 (4)	0.8383 (2)	0.84044 (17)	0.0593 (7)
C21	0.1871 (5)	1.0602 (3)	0.8631 (3)	0.0507 (8)
H21	0.1806	1.0196	0.8263	0.061*
C22	0.1468 (5)	1.1780 (3)	0.8212 (3)	0.0566 (9)
H22	0.1113	1.2170	0.7564	0.068*
C23	0.1596 (5)	1.2369 (3)	0.8761 (3)	0.0534 (9)
C24	0.2074 (5)	1.1838 (3)	0.9724 (3)	0.0553 (9)
H24	0.2157	1.2255	1.0079	0.066*
C25	0.2907 (5)	0.9899 (3)	1.1187 (3)	0.0512 (9)
H25A	0.1947	1.0019	1.1656	0.061*
H25B	0.4023	1.0013	1.1339	0.061*
C26	0.3527 (5)	0.7703 (3)	1.1986 (2)	0.0467 (8)
H26	0.3686	0.7666	1.2605	0.056*
C27	0.3686 (5)	0.6728 (3)	1.1837 (2)	0.0466 (8)
C28	0.3466 (5)	0.6773 (3)	1.0921 (2)	0.0448 (8)
H28	0.3586	0.6101	1.0838	0.054*
C29	0.3065 (4)	0.7813 (3)	1.0120 (2)	0.0404 (7)
C30	0.2427 (5)	1.0668 (3)	1.0149 (3)	0.0461 (8)
C31	0.2373 (4)	1.0032 (3)	0.9603 (2)	0.0417 (7)
C32	0.3128 (4)	0.8733 (3)	1.1198 (2)	0.0431 (8)

C33	0.2860 (4)	0.8817 (3)	1.0262 (2)	0.0400 (7)
C34	0.3009 (5)	0.7782 (3)	0.9140 (2)	0.0432 (8)
C35	0.1889 (5)	0.6998 (3)	0.9112 (2)	0.0503 (9)
H35A	0.0648	0.7405	0.8994	0.060*
H35B	0.1890	0.6364	0.9754	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0712 (7)	0.0497 (5)	0.0737 (7)	0.0006 (5)	−0.0030 (5)	−0.0222 (5)
Cl2	0.0728 (8)	0.0785 (7)	0.0839 (8)	−0.0045 (6)	0.0218 (6)	−0.0507 (6)
Cl3	0.0938 (9)	0.0535 (5)	0.0483 (5)	−0.0204 (5)	0.0077 (5)	−0.0116 (4)
O1	0.0671 (18)	0.0449 (13)	0.0426 (13)	−0.0150 (12)	−0.0028 (11)	−0.0162 (11)
C1	0.045 (2)	0.0457 (18)	0.0358 (17)	−0.0127 (15)	0.0024 (14)	−0.0115 (14)
C2	0.043 (2)	0.051 (2)	0.0451 (19)	−0.0108 (15)	0.0053 (15)	−0.0218 (16)
C3	0.044 (2)	0.0435 (18)	0.054 (2)	−0.0081 (15)	−0.0047 (16)	−0.0193 (16)
C4	0.050 (2)	0.0472 (19)	0.0362 (17)	−0.0163 (16)	−0.0021 (15)	−0.0066 (14)
C5	0.043 (2)	0.060 (2)	0.0384 (17)	−0.0213 (16)	0.0038 (14)	−0.0190 (15)
C6	0.047 (2)	0.068 (2)	0.0434 (19)	−0.0190 (17)	0.0103 (15)	−0.0300 (18)
C7	0.039 (2)	0.069 (2)	0.062 (2)	−0.0100 (17)	0.0099 (16)	−0.041 (2)
C8	0.044 (2)	0.0499 (19)	0.055 (2)	−0.0104 (16)	0.0046 (16)	−0.0243 (16)
C9	0.0338 (18)	0.0481 (18)	0.0427 (17)	−0.0126 (14)	0.0025 (13)	−0.0194 (14)
C10	0.0360 (18)	0.0502 (18)	0.0377 (17)	−0.0173 (15)	0.0014 (13)	−0.0171 (14)
C11	0.0341 (18)	0.0473 (17)	0.0363 (16)	−0.0149 (14)	0.0004 (13)	−0.0171 (14)
C12	0.0333 (19)	0.060 (2)	0.0445 (18)	−0.0183 (15)	0.0038 (14)	−0.0246 (16)
C13	0.0339 (18)	0.0483 (18)	0.0381 (16)	−0.0161 (14)	0.0034 (13)	−0.0198 (14)
C14	0.0335 (18)	0.0433 (17)	0.0435 (18)	−0.0041 (14)	−0.0001 (14)	−0.0148 (15)
C15	0.074 (3)	0.058 (2)	0.048 (2)	−0.026 (2)	0.0118 (18)	−0.0220 (17)
Cl4	0.0814 (9)	0.0455 (6)	0.1137 (10)	−0.0057 (5)	0.0130 (7)	−0.0201 (6)
Cl5	0.0920 (8)	0.0550 (5)	0.0389 (5)	−0.0111 (5)	−0.0018 (5)	−0.0140 (4)
Cl6	0.0670 (7)	0.0870 (7)	0.0757 (7)	−0.0203 (5)	0.0155 (5)	−0.0601 (6)
O2	0.081 (2)	0.0623 (15)	0.0380 (13)	−0.0298 (14)	0.0168 (12)	−0.0212 (12)
C21	0.045 (2)	0.055 (2)	0.049 (2)	−0.0091 (16)	0.0083 (15)	−0.0218 (17)
C22	0.046 (2)	0.054 (2)	0.058 (2)	−0.0065 (17)	0.0090 (17)	−0.0156 (18)
C23	0.035 (2)	0.0398 (18)	0.075 (3)	−0.0065 (14)	0.0175 (17)	−0.0202 (18)
C24	0.045 (2)	0.054 (2)	0.070 (3)	−0.0129 (17)	0.0195 (18)	−0.0344 (19)
C25	0.051 (2)	0.060 (2)	0.053 (2)	−0.0159 (17)	0.0136 (16)	−0.0355 (17)
C26	0.046 (2)	0.063 (2)	0.0339 (17)	−0.0135 (17)	0.0067 (14)	−0.0238 (16)
C27	0.049 (2)	0.0513 (19)	0.0378 (18)	−0.0147 (16)	0.0075 (14)	−0.0167 (15)
C28	0.049 (2)	0.0480 (18)	0.0399 (18)	−0.0103 (15)	0.0048 (14)	−0.0222 (15)
C29	0.0381 (19)	0.0473 (17)	0.0365 (16)	−0.0106 (14)	0.0091 (13)	−0.0198 (14)
C30	0.0359 (19)	0.0514 (19)	0.055 (2)	−0.0129 (15)	0.0160 (15)	−0.0285 (16)
C31	0.0313 (18)	0.0479 (18)	0.0475 (19)	−0.0103 (14)	0.0116 (14)	−0.0239 (15)
C32	0.0358 (19)	0.0544 (19)	0.0451 (18)	−0.0145 (15)	0.0143 (14)	−0.0279 (16)
C33	0.0318 (18)	0.0523 (18)	0.0374 (17)	−0.0116 (14)	0.0113 (13)	−0.0220 (14)
C34	0.044 (2)	0.0453 (17)	0.0377 (17)	−0.0058 (15)	0.0055 (14)	−0.0181 (14)
C35	0.057 (2)	0.061 (2)	0.0386 (18)	−0.0169 (18)	0.0086 (15)	−0.0269 (16)

Geometric parameters (Å, º)

Cl1—C3	1.730 (4)	Cl4—C23	1.744 (4)
Cl2—C7	1.737 (4)	Cl5—C27	1.735 (3)
Cl3—C15	1.758 (4)	Cl6—C35	1.764 (3)
O1—C14	1.203 (4)	O2—C34	1.207 (4)
C1—C2	1.371 (5)	C21—C22	1.385 (5)
C1—C11	1.395 (5)	C21—C31	1.388 (5)
C1—H1	0.9300	C21—H21	0.9300
C2—C3	1.382 (4)	C22—C23	1.375 (5)
C2—H2	0.9300	C22—H22	0.9300
C3—C4	1.383 (5)	C23—C24	1.369 (5)
C4—C10	1.372 (5)	C24—C30	1.375 (5)
C4—H4	0.9300	C24—H24	0.9300
C5—C12	1.491 (5)	C25—C30	1.494 (5)
C5—C10	1.503 (5)	C25—C32	1.504 (5)
C5—H5A	0.9700	C25—H25A	0.9700
C5—H5B	0.9700	C25—H25B	0.9700
C6—C7	1.361 (5)	C26—C27	1.374 (5)
C6—C12	1.382 (5)	C26—C32	1.375 (5)
C6—H6	0.9300	C26—H26	0.9300
C7—C8	1.384 (5)	C27—C28	1.379 (5)
C8—C9	1.403 (5)	C28—C29	1.391 (4)
C8—H8	0.9300	C28—H28	0.9300
C9—C13	1.397 (4)	C29—C33	1.401 (4)
C9—C14	1.486 (5)	C29—C34	1.491 (4)
C10—C11	1.396 (4)	C30—C31	1.409 (4)
C11—C13	1.468 (5)	C31—C33	1.475 (5)
C12—C13	1.412 (4)	C32—C33	1.398 (5)
C14—C15	1.512 (5)	C34—C35	1.505 (5)
C15—H15A	0.9700	C35—H35A	0.9700
C15—H15B	0.9700	C35—H35B	0.9700
C2—C1—C11	118.9 (3)	C22—C21—C31	119.6 (3)
C2—C1—H1	120.5	C22—C21—H21	120.2
C11—C1—H1	120.5	C31—C21—H21	120.2
C1—C2—C3	121.0 (3)	C23—C22—C21	119.5 (4)
C1—C2—H2	119.5	C23—C22—H22	120.3
C3—C2—H2	119.5	C21—C22—H22	120.3
C2—C3—C4	120.8 (3)	C24—C23—C22	122.7 (3)
C2—C3—Cl1	118.7 (3)	C24—C23—Cl4	118.3 (3)
C4—C3—Cl1	120.5 (3)	C22—C23—Cl4	119.1 (3)
C10—C4—C3	118.4 (3)	C23—C24—C30	117.9 (3)
C10—C4—H4	120.8	C23—C24—H24	121.0
C3—C4—H4	120.8	C30—C24—H24	121.0
C12—C5—C10	103.2 (3)	C30—C25—C32	102.9 (3)
C12—C5—H5A	111.1	C30—C25—H25A	111.2
C10—C5—H5A	111.1	C32—C25—H25A	111.2

C12—C5—H5B	111.1	C30—C25—H25B	111.2
C10—C5—H5B	111.1	C32—C25—H25B	111.2
H5A—C5—H5B	109.1	H25A—C25—H25B	109.1
C7—C6—C12	118.6 (3)	C27—C26—C32	118.3 (3)
C7—C6—H6	120.7	C27—C26—H26	120.9
C12—C6—H6	120.7	C32—C26—H26	120.9
C6—C7—C8	122.3 (3)	C26—C27—C28	121.3 (3)
C6—C7—Cl2	119.3 (3)	C26—C27—Cl5	118.8 (3)
C8—C7—Cl2	118.4 (3)	C28—C27—Cl5	119.9 (3)
C7—C8—C9	119.9 (3)	C27—C28—C29	120.6 (3)
C7—C8—H8	120.0	C27—C28—H28	119.7
C9—C8—H8	120.0	C29—C28—H28	119.7
C13—C9—C8	118.6 (3)	C28—C29—C33	118.9 (3)
C13—C9—C14	122.6 (3)	C28—C29—C34	117.0 (3)
C8—C9—C14	118.6 (3)	C33—C29—C34	124.0 (3)
C4—C10—C11	121.4 (3)	C24—C30—C31	121.3 (3)
C4—C10—C5	128.6 (3)	C24—C30—C25	128.1 (3)
C11—C10—C5	110.0 (3)	C31—C30—C25	110.6 (3)
C1—C11—C10	119.3 (3)	C21—C31—C30	118.9 (3)
C1—C11—C13	131.7 (3)	C21—C31—C33	133.4 (3)
C10—C11—C13	108.9 (3)	C30—C31—C33	107.7 (3)
C6—C12—C13	121.1 (3)	C26—C32—C33	122.2 (3)
C6—C12—C5	128.5 (3)	C26—C32—C25	127.4 (3)
C13—C12—C5	110.4 (3)	C33—C32—C25	110.4 (3)
C9—C13—C12	119.4 (3)	C32—C33—C29	118.6 (3)
C9—C13—C11	133.0 (3)	C32—C33—C31	108.4 (3)
C12—C13—C11	107.5 (3)	C29—C33—C31	133.0 (3)
O1—C14—C9	122.1 (3)	O2—C34—C29	122.0 (3)
O1—C14—C15	122.0 (3)	O2—C34—C35	121.9 (3)
C9—C14—C15	115.9 (3)	C29—C34—C35	116.1 (3)
C14—C15—Cl3	113.4 (2)	C34—C35—Cl6	113.8 (2)
C14—C15—H15A	108.9	C34—C35—H35A	108.8
Cl3—C15—H15A	108.9	Cl6—C35—H35A	108.8
C14—C15—H15B	108.9	C34—C35—H35B	108.8
Cl3—C15—H15B	108.9	Cl6—C35—H35B	108.8
H15A—C15—H15B	107.7	H35A—C35—H35B	107.7

C11—C1—C2—C3	0.3 (5)	C31—C21—C22—C23	0.9 (5)
C1—C2—C3—C4	1.3 (5)	C21—C22—C23—C24	−1.5 (6)
C1—C2—C3—Cl1	−178.6 (3)	C21—C22—C23—Cl4	177.8 (3)
C2—C3—C4—C10	−0.7 (5)	C22—C23—C24—C30	−0.3 (5)
Cl1—C3—C4—C10	179.1 (2)	Cl4—C23—C24—C30	−179.5 (3)
C12—C6—C7—C8	−1.4 (5)	C32—C26—C27—C28	0.5 (5)
C12—C6—C7—Cl2	179.1 (3)	C32—C26—C27—Cl5	−179.3 (3)
C6—C7—C8—C9	−0.9 (5)	C26—C27—C28—C29	−0.3 (5)
Cl2—C7—C8—C9	178.6 (3)	Cl5—C27—C28—C29	179.4 (3)
C7—C8—C9—C13	3.3 (5)	C27—C28—C29—C33	−1.0 (5)
C7—C8—C9—C14	−171.5 (3)	C27—C28—C29—C34	174.8 (3)

C3—C4—C10—C11	−1.5 (5)	C23—C24—C30—C31	2.5 (5)
C3—C4—C10—C5	177.6 (3)	C23—C24—C30—C25	−177.7 (3)
C12—C5—C10—C4	−179.6 (3)	C32—C25—C30—C24	−179.9 (3)
C12—C5—C10—C11	−0.4 (3)	C32—C25—C30—C31	−0.1 (4)
C2—C1—C11—C10	−2.5 (5)	C22—C21—C31—C30	1.2 (5)
C2—C1—C11—C13	−179.1 (3)	C22—C21—C31—C33	179.2 (3)
C4—C10—C11—C1	3.1 (5)	C24—C30—C31—C21	−3.0 (5)
C5—C10—C11—C1	−176.1 (3)	C25—C30—C31—C21	177.2 (3)
C4—C10—C11—C13	−179.6 (3)	C24—C30—C31—C33	178.5 (3)
C5—C10—C11—C13	1.2 (3)	C25—C30—C31—C33	−1.3 (4)
C7—C6—C12—C13	1.2 (5)	C27—C26—C32—C33	0.8 (5)
C7—C6—C12—C5	−179.0 (3)	C27—C26—C32—C25	−179.5 (3)
C10—C5—C12—C6	179.6 (3)	C30—C25—C32—C26	−178.2 (3)
C10—C5—C12—C13	−0.6 (3)	C30—C25—C32—C33	1.6 (4)
C8—C9—C13—C12	−3.4 (4)	C26—C32—C33—C29	−2.2 (5)
C14—C9—C13—C12	171.2 (3)	C25—C32—C33—C29	178.1 (3)
C8—C9—C13—C11	176.7 (3)	C26—C32—C33—C31	177.3 (3)
C14—C9—C13—C11	−8.8 (5)	C25—C32—C33—C31	−2.4 (4)
C6—C12—C13—C9	1.2 (5)	C28—C29—C33—C32	2.2 (5)
C5—C12—C13—C9	−178.6 (3)	C34—C29—C33—C32	−173.4 (3)
C6—C12—C13—C11	−178.9 (3)	C28—C29—C33—C31	−177.1 (3)
C5—C12—C13—C11	1.3 (3)	C34—C29—C33—C31	7.3 (6)
C1—C11—C13—C9	−4.8 (6)	C21—C31—C33—C32	−175.9 (4)
C10—C11—C13—C9	178.4 (3)	C30—C31—C33—C32	2.3 (4)
C1—C11—C13—C12	175.3 (3)	C21—C31—C33—C29	3.5 (6)
C10—C11—C13—C12	−1.6 (3)	C30—C31—C33—C29	−178.3 (3)
C13—C9—C14—O1	−40.8 (5)	C28—C29—C34—O2	−133.1 (4)
C8—C9—C14—O1	133.8 (4)	C33—C29—C34—O2	42.6 (5)
C13—C9—C14—C15	138.3 (3)	C28—C29—C34—C35	49.7 (4)
C8—C9—C14—C15	−47.1 (4)	C33—C29—C34—C35	−134.6 (3)
O1—C14—C15—Cl3	−8.4 (5)	O2—C34—C35—Cl6	31.8 (5)
C9—C14—C15—Cl3	172.5 (3)	C29—C34—C35—Cl6	−151.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1	0.93	2.37	2.998 (4)	124
C15—H15*B*···Cl6	0.97	2.80	3.678 (5)	151
C21—H21···O2	0.93	2.45	3.086 (5)	126
C35—H35*A*···O1^{i}	0.97	2.45	3.261 (5)	140

Symmetry code: (i) *x*−1, *y*, *z*.