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(1*R*,2*R*,5*R*,6*S*,9*R*,10*S*,13*S*,14*S*,18*R*)-1,6,7,8,9,14,15,16,17,17,18-Undecachloropentacyclo[12.2.1.1^{6,9}.0^{2,13}.0^{5,10}]octadeca-7,15-diene

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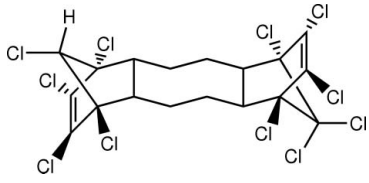
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.051; wR factor = 0.119; data-to-parameter ratio = 19.6.

The title compound, $C_{18}H_{13}Cl_{11}$, is an undecachlorinated commercial flame retardant. The asymmetric unit contains two independent half-molecules. The complete molecules are generated by crystallographic inversion symmetry, causing the terminal H atoms and one of the Cl atoms to be disordered equally over two sites in each molecule. The central eight-membered rings are in chair-type conformations. In the crystal structure, there is a single weak intermolecular C—H···Cl hydrogen bond.

Related literature

For related literature, see: Riddell *et al.* (2008).



Experimental

Crystal data

$C_{18}H_{13}Cl_{11}$
M_r = 619.23
Monoclinic, $P2_1/c$
a = 13.3129 (5) Å
b = 12.1263 (6) Å
c = 14.7229 (7) Å
β = 99.505 (3)°
V = 2344.18 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.31 mm^{-1}
T = 150 (1) K
0.26 × 0.20 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.715, T_{max} = 0.825
15654 measured reflections
5338 independent reflections
3481 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.118
S = 1.05
5338 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1B—H1B···Cl4A^{i}	1.00	2.70	3.656 (4)	160

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); 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: PK2101).

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Riddell, N., McCrindle, R., Arsenault, G. & Lough, A. J. (2008). *Acta Cryst.* E**64**, o1249.
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supporting information

Acta Cryst. (2008). E**64**, o1250 [doi:10.1107/S160053680801622X]

(1*R*,2*R*,5*R*,6*S*,9*R*,10*S*,13*S*,14*S*,18*R*)-1,6,7,8,9,14,15,16,17,17,18-Undecachloropentacyclo[12.2.1.1^{6,9}.0^{2,13}.0^{5,10}]octadeca-7,15-diene

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S1. Comment

For background information and related references see the previous paper (Riddell *et al.*, 2008). Dechlorane Plus (DP) is a commercial chlorinated flame retardant used in styrenic plastics (http://www.inchem.org/documents/ehc/ehc/ehc192.htm) to protect human life and property against fires. We have synthesized the dechlorinated compound (1R,2R,5R,6S,9R,10S,13S,14S,18R)-1,6,7,8,9,14,15,16,17,17,18- undecachloropentacyclo[12.2.1.1^{6,9}.0^{2,13}.0^{5,10}]-octadeca-7,15-diene. GC/MS and ^{1}H NMR spectroscopy have confirmed the basic structure of as having the DP-like structure with only 11 chlorine atoms. An NOE NMR experiment also strongly indicated that the proton on the bridging carbon atom was facing towards the cyclooctadiene ring since a positive through space interaction was observed. However, an X-ray structure determination was required to positively confirm the stereochemistry.

The asymmetric unit contains two independent half molecules. The symmetry complete molecules are generated by crystallographic inversion symmetry, causing atoms Cl6A and Cl6B, as well as the H atoms bonded to C9A and C9B to be disordered over two sites with equal occupancies. In both independent molecules the geometric parameters are the same within experimental error. The asymmetric unit is shown in Fig. 2. In the crystal structure there is a single weak intermolecular C—H···Cl interaction (Table 1).

S2. Experimental

The synthesis of the title compound was carried out at Wellington Laboratories using proprietary methods. The compound was isolated and purified using chromatographic techniques. For single-crystal *x*-ray crystallography, colourless crystals were grown from a solution in toluene.

S3. Refinement

All hydrogen atoms were placed in calculated positions with C—H distances of 0.99 and 1.00 Å and they were included in the refinement in a riding-model approximation with $U_{iso} = 1.2U_{eq}$(C).

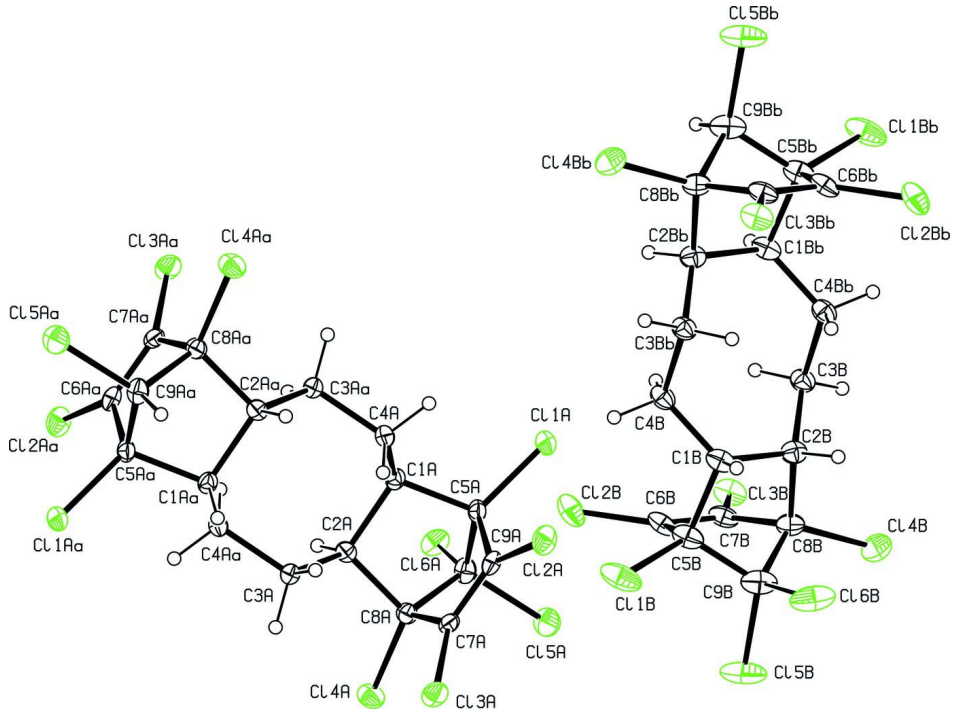

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. The disorder is not shown and the atoms labeled with lower case suffixes a and b are related by the symmetry operators (-x, -y+1, -z+1) and (-x+1, - y+1, -z) respectively.

(1R,2R,5R,6S,9R,10S,13S,14S,18R)-1,6,7,8,9,14,15,16,17,17,18-Undecachloropentacyclo[12.2.1.1^{6,9}.0^{2,13}.0^{5,10}]octadeca-7,15-diene

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β = 99.505 (3)°
V = 2344.18 (18) Å^3
Z = 4
$F(000)$ = 1232
D_x = 1.755 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 15654 reflections
θ = 2.8–27.5°
μ = 1.31 mm^{-1}
T = 150 K
Block, colourless
0.26 × 0.20 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
φ scans and ω scans with κ offsets
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.715, T_{max} = 0.825
15654 measured reflections
5338 independent reflections
3481 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 27.5°, θ_{min} = 2.8°
h = −17→17
k = −14→15
l = −16→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.118$
$S = 1.05$
5338 reflections
272 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
$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 4.5718P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0011 (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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1A	0.12630 (8)	0.59357 (8)	0.23239 (6)	0.0351 (3)	
Cl2A	−0.04105 (8)	0.77914 (9)	0.28215 (7)	0.0390 (3)	
Cl3A	0.03958 (8)	0.87394 (8)	0.49922 (7)	0.0371 (3)	
Cl4A	0.25958 (7)	0.75232 (9)	0.58340 (7)	0.0375 (3)	
Cl5A	0.28655 (8)	0.77926 (10)	0.35627 (7)	0.0449 (3)	
Cl6A	0.32477 (14)	0.57426 (16)	0.42481 (15)	0.0351 (5)	0.50
C1A	0.0896 (3)	0.5390 (3)	0.4083 (2)	0.0235 (8)	
H1A	0.1293	0.4710	0.3993	0.028*	
C2A	0.1294 (3)	0.5849 (3)	0.5085 (2)	0.0229 (8)	
H2A	0.1854	0.5355	0.5384	0.027*	
C3A	0.0525 (3)	0.5978 (3)	0.5746 (2)	0.0246 (8)	
H3A1	−0.0099	0.6331	0.5412	0.030*	
H3A2	0.0817	0.6477	0.6254	0.030*	
C4A	−0.0227 (3)	0.5119 (3)	0.3837 (2)	0.0268 (8)	
H4A1	−0.0412	0.5080	0.3158	0.032*	
H4A2	−0.0626	0.5724	0.4054	0.032*	
C5A	0.1236 (3)	0.6328 (3)	0.3464 (2)	0.0255 (8)	
C6A	0.0612 (3)	0.7346 (3)	0.3593 (3)	0.0263 (8)	
C7A	0.0923 (3)	0.7720 (3)	0.4438 (3)	0.0243 (8)	
C8A	0.1776 (3)	0.6973 (3)	0.4878 (2)	0.0245 (8)	
C9A	0.2268 (3)	0.6680 (3)	0.4039 (3)	0.0289 (9)	
H9C	0.2739	0.6037	0.4170	0.035*	0.50
Cl1B	0.50434 (8)	0.70192 (12)	0.26767 (8)	0.0573 (4)	

Cl2B	0.68792 (8)	0.51251 (11)	0.29107 (7)	0.0488 (3)	
Cl3B	0.83732 (7)	0.55922 (9)	0.12642 (7)	0.0400 (3)	
Cl4B	0.74566 (9)	0.77648 (10)	0.00260 (9)	0.0501 (3)	
Cl5B	0.70173 (9)	0.85653 (11)	0.21603 (10)	0.0647 (4)	
Cl6B	0.52623 (17)	0.8699 (2)	0.0840 (2)	0.0609 (8)	0.50
C1B	0.5100 (3)	0.6208 (3)	0.0915 (3)	0.0312 (9)	
H1B	0.4460	0.6647	0.0747	0.037*	
C2B	0.5781 (3)	0.6426 (3)	0.0152 (3)	0.0306 (9)	
H2B	0.5410	0.6952	−0.0308	0.037*	
C3B	0.6089 (3)	0.5433 (3)	−0.0368 (3)	0.0310 (9)	
H3B1	0.6333	0.4843	0.0079	0.037*	
H3B2	0.6663	0.5644	−0.0683	0.037*	
C4B	0.4792 (3)	0.5024 (3)	0.1091 (3)	0.0304 (9)	
H4B1	0.4586	0.4988	0.1706	0.037*	
H4B2	0.5394	0.4542	0.1104	0.037*	
C5B	0.5738 (3)	0.6757 (4)	0.1780 (3)	0.0362 (10)	
C6B	0.6701 (3)	0.6059 (4)	0.2039 (3)	0.0344 (10)	
C7B	0.7274 (3)	0.6241 (3)	0.1398 (3)	0.0324 (9)	
C8B	0.6712 (3)	0.7049 (3)	0.0715 (3)	0.0343 (9)	
C9B	0.6180 (3)	0.7760 (4)	0.1363 (3)	0.0444 (11)	
H9D	0.5630	0.8225	0.1008	0.053*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0514 (6)	0.0324 (5)	0.0245 (5)	−0.0025 (5)	0.0149 (4)	−0.0003 (4)
Cl2A	0.0392 (6)	0.0357 (6)	0.0398 (6)	0.0080 (5)	−0.0005 (4)	0.0127 (5)
Cl3A	0.0473 (6)	0.0243 (5)	0.0446 (6)	0.0049 (5)	0.0217 (5)	−0.0033 (4)
Cl4A	0.0297 (5)	0.0500 (7)	0.0331 (5)	−0.0137 (5)	0.0057 (4)	−0.0082 (5)
Cl5A	0.0406 (6)	0.0562 (7)	0.0428 (6)	−0.0200 (5)	0.0212 (5)	−0.0039 (5)
Cl6A	0.0289 (10)	0.0275 (10)	0.0519 (13)	0.0056 (8)	0.0154 (9)	0.0000 (9)
C1A	0.0272 (18)	0.0192 (19)	0.025 (2)	0.0036 (16)	0.0068 (15)	0.0029 (15)
C2A	0.0234 (18)	0.0228 (19)	0.0222 (19)	0.0048 (16)	0.0031 (15)	−0.0005 (15)
C3A	0.0278 (19)	0.024 (2)	0.0225 (19)	−0.0043 (16)	0.0055 (15)	0.0007 (16)
C4A	0.034 (2)	0.026 (2)	0.0194 (19)	−0.0004 (17)	0.0010 (16)	0.0025 (16)
C5A	0.033 (2)	0.024 (2)	0.0217 (19)	0.0011 (17)	0.0105 (16)	0.0037 (16)
C6A	0.0250 (19)	0.024 (2)	0.031 (2)	−0.0031 (16)	0.0074 (16)	0.0079 (16)
C7A	0.0302 (19)	0.0164 (18)	0.029 (2)	−0.0018 (16)	0.0139 (16)	−0.0012 (15)
C8A	0.0234 (18)	0.028 (2)	0.0231 (19)	−0.0042 (16)	0.0059 (15)	−0.0017 (16)
C9A	0.0264 (19)	0.031 (2)	0.031 (2)	0.0052 (17)	0.0111 (16)	0.0046 (17)
Cl1B	0.0337 (6)	0.0861 (10)	0.0536 (8)	0.0007 (6)	0.0119 (5)	−0.0381 (7)
Cl2B	0.0441 (6)	0.0722 (9)	0.0271 (6)	0.0022 (6)	−0.0024 (5)	0.0005 (5)
Cl3B	0.0233 (5)	0.0504 (7)	0.0458 (6)	0.0043 (5)	0.0042 (4)	−0.0118 (5)
Cl4B	0.0484 (7)	0.0451 (7)	0.0570 (8)	−0.0176 (6)	0.0088 (5)	−0.0010 (6)
Cl5B	0.0413 (6)	0.0622 (8)	0.0884 (10)	−0.0096 (6)	0.0042 (6)	−0.0458 (8)
Cl6B	0.0358 (12)	0.0373 (13)	0.100 (2)	0.0108 (10)	−0.0158 (12)	−0.0205 (13)
C1B	0.0195 (18)	0.040 (2)	0.032 (2)	0.0056 (18)	−0.0011 (16)	−0.0101 (19)
C2B	0.0257 (19)	0.030 (2)	0.034 (2)	0.0015 (17)	−0.0028 (17)	−0.0019 (17)

C3B	0.0255 (19)	0.038 (2)	0.028 (2)	−0.0051 (18)	0.0023 (16)	−0.0041 (18)
C4B	0.0238 (19)	0.042 (2)	0.025 (2)	−0.0002 (18)	0.0016 (15)	−0.0035 (18)
C5B	0.0232 (19)	0.048 (3)	0.038 (2)	0.0026 (19)	0.0056 (17)	−0.016 (2)
C6B	0.027 (2)	0.050 (3)	0.024 (2)	0.0022 (19)	−0.0012 (16)	−0.0133 (19)
C7B	0.0218 (19)	0.041 (2)	0.033 (2)	0.0013 (18)	−0.0002 (16)	−0.0141 (19)
C8B	0.029 (2)	0.033 (2)	0.039 (2)	−0.0032 (18)	0.0017 (18)	−0.0076 (19)
C9B	0.031 (2)	0.041 (3)	0.058 (3)	0.006 (2)	−0.004 (2)	−0.017 (2)

Geometric parameters (Å, º)

Cl1A—C5A	1.751 (4)	Cl1B—C5B	1.761 (4)
Cl2A—C6A	1.710 (4)	Cl2B—C6B	1.698 (4)
Cl3A—C7A	1.696 (4)	Cl3B—C7B	1.701 (4)
Cl4A—C8A	1.763 (4)	Cl4B—C8B	1.760 (4)
Cl5A—C9A	1.769 (4)	Cl5B—C9B	1.772 (4)
Cl6A—C9A	1.720 (4)	Cl6B—C9B	1.752 (5)
C1A—C4A	1.515 (5)	C1B—C4B	1.527 (6)
C1A—C5A	1.570 (5)	C1B—C5B	1.559 (5)
C1A—C2A	1.584 (5)	C1B—C2B	1.579 (5)
C1A—H1A	1.0000	C1B—H1B	1.0000
C2A—C3A	1.533 (5)	C2B—C3B	1.518 (5)
C2A—C8A	1.558 (5)	C2B—C8B	1.567 (5)
C2A—H2A	1.0000	C2B—H2B	1.0000
C3A—C4A^{i}	1.544 (5)	C3B—C4B^{ii}	1.551 (5)
C3A—H3A1	0.9900	C3B—H3B1	0.9900
C3A—H3A2	0.9900	C3B—H3B2	0.9900
C4A—C3A^{i}	1.544 (5)	C4B—C3B^{ii}	1.551 (5)
C4A—H4A1	0.9900	C4B—H4B1	0.9900
C4A—H4A2	0.9900	C4B—H4B2	0.9900
C5A—C6A	1.518 (5)	C5B—C9B	1.524 (7)
C5A—C9A	1.548 (5)	C5B—C6B	1.531 (6)
C6A—C7A	1.324 (5)	C6B—C7B	1.328 (5)
C7A—C8A	1.512 (5)	C7B—C8B	1.511 (6)
C8A—C9A	1.533 (5)	C8B—C9B	1.542 (6)
C4A—C1A—C5A	112.7 (3)	C4B—C1B—C5B	112.8 (3)
C4A—C1A—C2A	117.6 (3)	C4B—C1B—C2B	118.7 (3)
C5A—C1A—C2A	101.6 (3)	C5B—C1B—C2B	102.2 (3)
C4A—C1A—H1A	108.1	C4B—C1B—H1B	107.5
C5A—C1A—H1A	108.1	C5B—C1B—H1B	107.5
C2A—C1A—H1A	108.1	C2B—C1B—H1B	107.5
C3A—C2A—C8A	112.0 (3)	C3B—C2B—C8B	113.2 (3)
C3A—C2A—C1A	118.2 (3)	C3B—C2B—C1B	117.4 (3)
C8A—C2A—C1A	102.2 (3)	C8B—C2B—C1B	101.6 (3)
C3A—C2A—H2A	108.0	C3B—C2B—H2B	108.1
C8A—C2A—H2A	108.0	C8B—C2B—H2B	108.1
C1A—C2A—H2A	108.0	C1B—C2B—H2B	108.1
C2A—C3A—C4A^{i}	114.1 (3)	C2B—C3B—C4B^{ii}	113.1 (3)

C2A—C3A—H3A1	108.7	C2B—C3B—H3B1	109.0
C4A^{i}—C3A—H3A1	108.7	C4B^{ii}—C3B—H3B1	109.0
C2A—C3A—H3A2	108.7	C2B—C3B—H3B2	109.0
C4A^{i}—C3A—H3A2	108.7	C4B^{ii}—C3B—H3B2	109.0
H3A1—C3A—H3A2	107.6	H3B1—C3B—H3B2	107.8
C1A—C4A—C3A^{i}	113.6 (3)	C1B—C4B—C3B^{ii}	114.4 (3)
C1A—C4A—H4A1	108.8	C1B—C4B—H4B1	108.7
C3A^{i}—C4A—H4A1	108.8	C3B^{ii}—C4B—H4B1	108.7
C1A—C4A—H4A2	108.8	C1B—C4B—H4B2	108.7
C3A^{i}—C4A—H4A2	108.8	C3B^{ii}—C4B—H4B2	108.7
H4A1—C4A—H4A2	107.7	H4B1—C4B—H4B2	107.6
C6A—C5A—C9A	99.3 (3)	C9B—C5B—C6B	100.3 (3)
C6A—C5A—C1A	107.5 (3)	C9B—C5B—C1B	101.9 (3)
C9A—C5A—C1A	101.4 (3)	C6B—C5B—C1B	106.8 (3)
C6A—C5A—Cl1A	116.0 (3)	C9B—C5B—Cl1B	116.3 (3)
C9A—C5A—Cl1A	116.2 (2)	C6B—C5B—Cl1B	115.8 (3)
C1A—C5A—Cl1A	114.4 (3)	C1B—C5B—Cl1B	114.0 (3)
C7A—C6A—C5A	107.6 (3)	C7B—C6B—C5B	106.7 (4)
C7A—C6A—Cl2A	127.4 (3)	C7B—C6B—Cl2B	128.5 (3)
C5A—C6A—Cl2A	124.5 (3)	C5B—C6B—Cl2B	124.3 (3)
C6A—C7A—C8A	107.1 (3)	C6B—C7B—C8B	107.5 (3)
C6A—C7A—Cl3A	127.7 (3)	C6B—C7B—Cl3B	127.8 (4)
C8A—C7A—Cl3A	124.8 (3)	C8B—C7B—Cl3B	124.4 (3)
C7A—C8A—C9A	100.6 (3)	C7B—C8B—C9B	100.3 (3)
C7A—C8A—C2A	107.6 (3)	C7B—C8B—C2B	107.5 (3)
C9A—C8A—C2A	101.5 (3)	C9B—C8B—C2B	101.2 (3)
C7A—C8A—Cl4A	116.0 (3)	C7B—C8B—Cl4B	116.0 (3)
C9A—C8A—Cl4A	116.2 (3)	C9B—C8B—Cl4B	116.2 (3)
C2A—C8A—Cl4A	113.3 (3)	C2B—C8B—Cl4B	113.8 (3)
C8A—C9A—C5A	92.6 (3)	C5B—C9B—C8B	92.9 (3)
C8A—C9A—Cl6A	114.9 (3)	C5B—C9B—Cl6B	114.1 (3)
C5A—C9A—Cl6A	119.6 (3)	C8B—C9B—Cl6B	116.7 (3)
C8A—C9A—Cl5A	115.0 (3)	C5B—C9B—Cl5B	114.6 (3)
C5A—C9A—Cl5A	114.2 (3)	C8B—C9B—Cl5B	114.5 (3)
Cl6A—C9A—Cl5A	101.4 (2)	Cl6B—C9B—Cl5B	104.5 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1*B*—H1*B*···Cl4*A*^{iii}	1.00	2.70	3.656 (4)	160

Symmetry code: (iii) *x*, −*y*+3/2, *z*−1/2.