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1,3,5-Trichloro-2,4,6-tris(dichloromethyl)benzene

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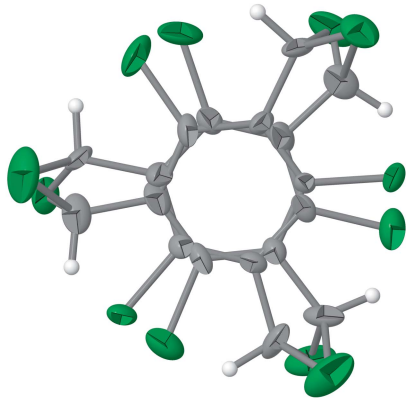
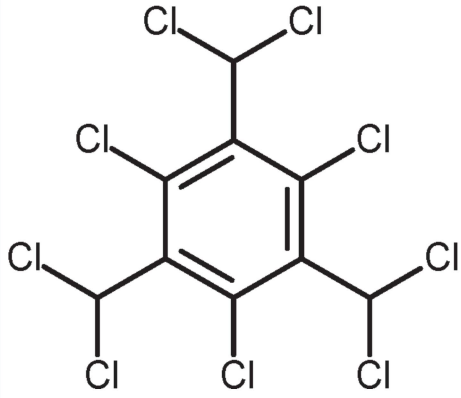
The asymmetric unit of the title compound, $C_9H_3Cl_9$, contains one molecule. Two slightly different conformations with nearly C_{3h} symmetry are mutually disordered in a 1:1 ratio. This disorder enhances the overall structural symmetry to D_{3h}.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1) is a central intermediate for star-shaped conjugated oligomers (Demenev *et al.*, 2010; Detert *et al.*, 2010). A bromo derivative has been reported by Holst *et al.* (2011). This compound combines our interest in perchloro hydrocarbons (Detert *et al.*, 2009; Schollmeyer & Detert, 2017) and star-shaped discotic liquid crystals (Rieth *et al.*, 2014; Glang *et al.*, 2014).

The asymmetric unit contains one molecule of the title compound and two very similar conformations with nearly C_{3h} symmetry occur in a 1:1 ratio (Fig. 2). This disorder enhances the symmetry of the overall structure to D_{3h}. Assuming the D_{3h} symmetry for one nondisordered molecule, the space group will rise from $P4_3$ to $P4_32_12$. However, then the refinement is not stable and the molecular symmetry is in contradiction to the chemistry. Distances between H atoms and ring-bound Cl atoms are 2.262 Å for H7···Cl3 and also for H8···Cl6, but the spacing between H9 and Cl9 is 2.43 Å. Similarly, two C—H bonds are nearly coplanar with the ring (H8—C8—C3—C4 = −3° and H9—C9—C5—C6 = 3°), whereas H7—C7—C1—C2 is twisted by −9°.

Synthesis and crystallization

The title compound was prepared according to Veciana *et al.* (1993) and Taerum *et al.* (2009) with the modification that a steel bomb (2.2 × 25 cm) was used as reaction vessel. This allows scale-up to 3.0 g (16.5 mmol, 1.0 equivalent) 1,3,5-trichlorbenzene in 30 ml absolute chloroform with 2.7 g (19.8 mmol, 1.2 equivalents) $AlCl_3$, and frequent pressure reduction was not necessary. The temperature was regulated with ISOHEAT

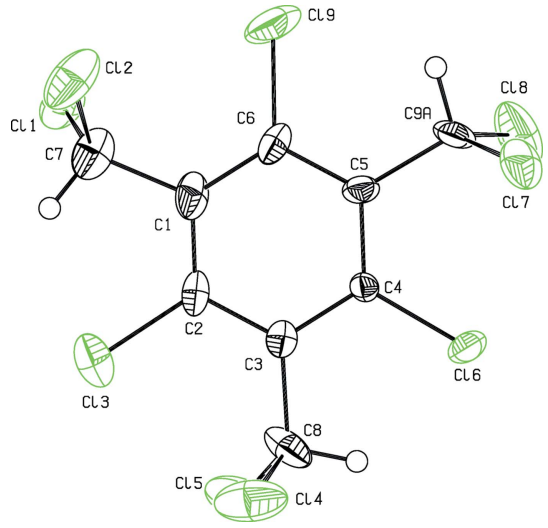


Figure 1
The crystal structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

(typ: MIL-HT–H, P = 175 W) by a heat panel (JUMBO iTRON 16). The reaction mixture was heated slowly (over 3 h) to 383 K and held at 383 K for 67 h with magnetic stirring. After cooling to room temperature, the pressure was reduced through a swagelok valve (SS-41GS2). Purification was carried out according to Taerum *et al.* (2009). The title compound was obtained after column chromatography (SiO_2, petroleum ether) in 31.6% yield (2.2 g, 5.2 mmol) as colourless crystals (m.p. 453–457 K). Crystallization from acetonitrile and chloroform resulted in single crystals.

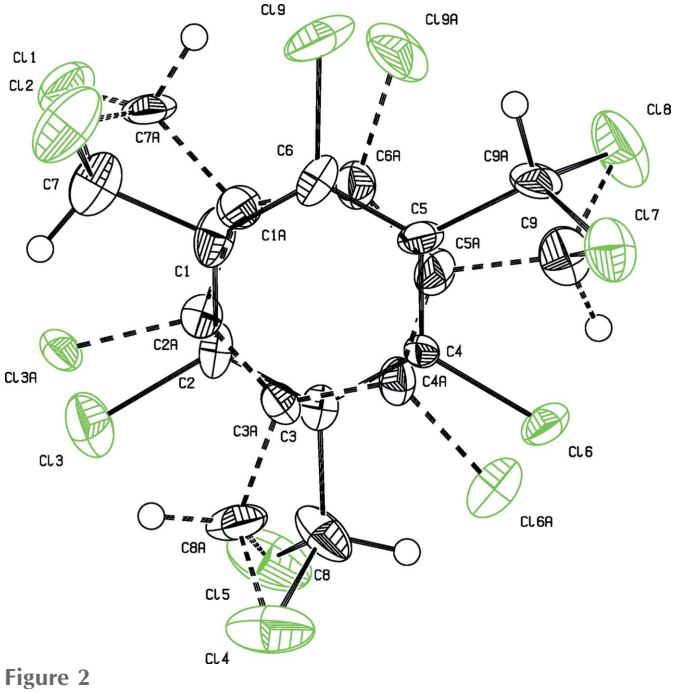


Figure 2
Perspective view of the two superposed orientations of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_9H_3Cl_9$
M_r	430.16
Crystal system, space group	Tetragonal, $P4_3$
Temperature (K)	120
a, c (Å)	9.5435 (2), 15.9424 (4)
V (Å^3)	1452.01 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.71
Crystal size (mm)	0.43 × 0.33 × 0.13
Data collection	
Diffractometer	Stoe IPDS 2T
Absorption correction	Integration (*X-RED*; Stoe & Cie, 1999)
T_{min}, T_{max}	0.496, 0.813
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34268, 3561, 3429
R_{int}	0.018
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.135, 1.11
No. of reflections	3561
No. of parameters	248
No. of restraints	73
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.11, −0.67
Absolute structure	Flack x determined using 1575 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.04 (3)

Computer programs: *X-AREA* (Stoe & Cie, 1999), *X-RED* (Stoe & Cie, 1999), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The site-occupancy factors [0.501 (6)/0.499 (6)] for the disordered atoms were refined using one common parameter. Disordered phenyl rings were refined assuming a regular six-membered ring with C—C = 1.39 Å. Their displacement parameters were refined using a RIGU restraint.

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full crystallographic data

IUCrData (2017). **2**, x170227 [https://doi.org/10.1107/S2414314617002279]

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Crystal data

$C_9H_3Cl_9$
M_r = 430.16
Tetragonal, $P4_3$
a = 9.5435 (2) Å
c = 15.9424 (4) Å
V = 1452.01 (7) Å^3
Z = 4
$F(000)$ = 840
D_x = 1.968 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 56414 reflections
θ = 2.5–28.2°
μ = 1.71 mm^{-1}
T = 120 K
Block, colourless
0.43 × 0.33 × 0.13 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED; Stoe & Cie, 1999)
T_{min} = 0.496, T_{max} = 0.813
34268 measured reflections
3561 independent reflections
3429 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.3°, θ_{min} = 2.5°
h = −12→12
k = −12→12
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.135
S = 1.11
3561 reflections
248 parameters
73 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 3.8476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}
Absolute structure: Flack x determined using 1575 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.04 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.5937 (17)	0.1944 (16)	−0.0704 (8)	0.034 (4)	0.501 (6)
C2	0.5029 (16)	0.0821 (18)	−0.0594 (9)	0.027 (3)	0.501 (6)
C3	0.5150 (15)	−0.0029 (15)	0.0110 (10)	0.024 (3)	0.501 (6)
C4	0.6180 (16)	0.0245 (14)	0.0704 (8)	0.018 (3)	0.501 (6)
C5	0.7089 (14)	0.1368 (15)	0.0594 (8)	0.026 (3)	0.501 (6)
C6	0.6967 (15)	0.2218 (13)	−0.0110 (9)	0.030 (4)	0.501 (6)
C1A	0.6360 (16)	0.2079 (15)	−0.0608 (9)	0.030 (3)	0.499 (6)
C2A	0.5235 (16)	0.1174 (18)	−0.0722 (9)	0.023 (3)	0.499 (6)
C3A	0.4956 (15)	0.0141 (15)	−0.0130 (10)	0.024 (3)	0.499 (6)
C4A	0.5803 (17)	0.0014 (14)	0.0576 (9)	0.026 (3)	0.499 (6)
C5A	0.6928 (15)	0.0919 (17)	0.0689 (8)	0.031 (4)	0.499 (6)
C6A	0.7206 (13)	0.1952 (15)	0.0097 (10)	0.029 (3)	0.499 (6)
C7	0.5684 (19)	0.2814 (16)	−0.1497 (10)	0.042 (4)	0.501 (6)
H7	0.4779	0.2467	−0.1736	0.050*	0.501 (6)
C7A	0.6720 (15)	0.3144 (14)	−0.1321 (9)	0.033 (3)	0.499 (6)
H7A	0.7628	0.3585	−0.1153	0.040*	0.499 (6)
Cl1	0.7014 (2)	0.2405 (2)	−0.22796 (11)	0.0453 (4)	
Cl2	0.5463 (3)	0.4547 (2)	−0.13480 (17)	0.0650 (7)	
Cl3	0.3692 (5)	0.0489 (5)	−0.1302 (3)	0.0491 (13)	0.501 (6)
Cl3A	0.4128 (3)	0.1317 (4)	−0.15464 (19)	0.0310 (9)	0.499 (6)
C8	0.4159 (15)	−0.1286 (16)	0.0251 (12)	0.042 (4)	0.501 (6)
H8	0.4500	−0.1737	0.0779	0.050*	0.501 (6)
C8A	0.3712 (15)	−0.0836 (15)	−0.0272 (12)	0.041 (4)	0.499 (6)
H8A	0.3261	−0.0495	−0.0800	0.049*	0.499 (6)
Cl4	0.2420 (2)	−0.0756 (2)	0.0476 (2)	0.0665 (8)	
Cl5	0.4243 (2)	−0.2580 (2)	−0.0493 (2)	0.0662 (8)	
Cl6	0.6317 (4)	−0.0872 (3)	0.15285 (19)	0.0312 (9)	0.501 (6)
Cl6A	0.5491 (5)	−0.1308 (5)	0.1285 (3)	0.0486 (13)	0.499 (6)
C9A	0.8142 (14)	0.1718 (15)	0.1307 (9)	0.034 (3)	0.501 (6)
H9A	0.8586	0.2626	0.1141	0.041*	0.501 (6)
C9	0.7810 (16)	0.0677 (19)	0.1479 (10)	0.041 (3)	0.499 (6)
H9	0.7469	−0.0227	0.1722	0.050*	0.499 (6)
Cl7	0.7406 (2)	0.2015 (2)	0.22621 (11)	0.0454 (4)	
Cl8	0.9548 (2)	0.0463 (3)	0.13319 (16)	0.0649 (7)	
Cl9	0.8193 (6)	0.3484 (5)	−0.0272 (4)	0.0571 (14)	0.501 (6)
Cl9A	0.8484 (5)	0.3195 (6)	0.0255 (4)	0.0561 (14)	0.499 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.054 (10)	0.032 (7)	0.016 (6)	0.006 (6)	−0.003 (6)	−0.006 (5)
C2	0.036 (8)	0.028 (9)	0.017 (6)	0.012 (5)	−0.004 (6)	0.000 (5)
C3	0.027 (7)	0.024 (6)	0.021 (8)	0.004 (5)	−0.001 (5)	0.000 (5)
C4	0.014 (7)	0.025 (6)	0.017 (5)	−0.002 (4)	0.001 (4)	0.001 (4)
C5	0.028 (6)	0.029 (8)	0.022 (7)	−0.012 (5)	0.005 (5)	0.001 (5)

C6	0.043 (8)	0.026 (6)	0.020 (7)	0.004 (6)	0.003 (5)	0.006 (5)
C1A	0.036 (8)	0.030 (6)	0.024 (7)	−0.009 (5)	−0.002 (5)	−0.002 (5)
C2A	0.028 (6)	0.018 (7)	0.023 (6)	0.002 (5)	0.000 (5)	−0.003 (4)
C3A	0.019 (5)	0.030 (7)	0.023 (8)	0.000 (5)	−0.003 (5)	−0.004 (5)
C4A	0.024 (8)	0.032 (7)	0.022 (7)	0.008 (5)	−0.002 (5)	0.002 (6)
C5A	0.029 (7)	0.047 (10)	0.017 (6)	0.001 (6)	0.005 (5)	0.004 (6)
C6A	0.028 (6)	0.037 (8)	0.022 (7)	0.002 (6)	−0.002 (5)	0.000 (5)
C7	0.059 (10)	0.035 (7)	0.030 (7)	0.012 (7)	0.007 (6)	−0.001 (5)
C7A	0.037 (7)	0.032 (6)	0.031 (7)	−0.022 (5)	0.007 (5)	0.001 (5)
Cl1	0.0480 (10)	0.0552 (11)	0.0328 (9)	−0.0015 (8)	0.0136 (8)	0.0089 (7)
Cl2	0.103 (2)	0.0362 (10)	0.0560 (14)	0.0163 (10)	0.0161 (13)	0.0138 (9)
Cl3	0.045 (2)	0.064 (3)	0.038 (2)	0.002 (2)	−0.0137 (17)	−0.0075 (19)
Cl3A	0.0238 (14)	0.0446 (19)	0.0247 (14)	−0.0102 (13)	−0.0052 (11)	−0.0027 (13)
C8	0.032 (7)	0.032 (7)	0.062 (11)	−0.002 (5)	−0.018 (7)	−0.014 (7)
C8A	0.029 (6)	0.031 (7)	0.062 (11)	−0.003 (5)	0.012 (7)	0.020 (7)
Cl4	0.0398 (10)	0.0459 (11)	0.114 (2)	−0.0037 (8)	0.0262 (12)	0.0030 (12)
Cl5	0.0459 (11)	0.0401 (10)	0.113 (2)	−0.0039 (8)	−0.0033 (12)	−0.0263 (12)
Cl6	0.045 (2)	0.0239 (14)	0.0249 (14)	−0.0102 (13)	0.0030 (13)	0.0046 (11)
Cl6A	0.064 (3)	0.045 (2)	0.037 (2)	0.002 (2)	0.0071 (19)	0.0139 (17)
C9A	0.033 (6)	0.039 (7)	0.030 (7)	−0.022 (5)	−0.001 (5)	−0.007 (5)
C9	0.036 (7)	0.057 (10)	0.031 (7)	0.008 (7)	0.004 (6)	−0.007 (6)
Cl7	0.0553 (11)	0.0479 (10)	0.0328 (9)	−0.0013 (8)	−0.0093 (7)	−0.0136 (8)
Cl8	0.0360 (10)	0.102 (2)	0.0565 (14)	0.0165 (10)	−0.0139 (9)	−0.0162 (13)
Cl9	0.072 (3)	0.047 (2)	0.051 (3)	−0.022 (2)	0.020 (3)	0.0154 (19)
Cl9A	0.047 (2)	0.071 (3)	0.051 (3)	−0.021 (2)	−0.0149 (19)	−0.020 (3)

Geometric parameters (Å, º)

C1—C2	1.3900	C5A—C6A	1.3900
C1—C6	1.3900	C5A—C9	1.532 (19)
C1—C7	1.531 (18)	C6A—Cl9A	1.719 (9)
C2—C3	1.3900	C7—Cl2	1.684 (15)
C2—Cl3	1.732 (9)	C7—Cl1	1.822 (16)
C3—C4	1.3900	C7—H7	1.0000
C3—C8	1.544 (17)	C7A—Cl1	1.706 (14)
C4—C5	1.3900	C7A—Cl2	1.799 (16)
C4—Cl6	1.697 (9)	C7A—H7A	1.0000
C5—C6	1.3900	C8—Cl5	1.714 (16)
C5—C9A	1.553 (16)	C8—Cl4	1.772 (15)
C6—Cl9	1.701 (10)	C8—H8	1.0000
C1A—C2A	1.3900	C8A—Cl4	1.718 (15)
C1A—C6A	1.3900	C8A—Cl5	1.775 (15)
C1A—C7A	1.563 (16)	C8A—H8A	1.0000
C2A—C3A	1.3900	C9A—Cl7	1.701 (14)
C2A—Cl3A	1.692 (9)	C9A—Cl8	1.799 (16)
C3A—C4A	1.3900	C9A—H9A	1.0000
C3A—C8A	1.527 (17)	C9—Cl8	1.688 (15)
C4A—C5A	1.3900	C9—Cl7	1.827 (16)

C4A—Cl6A	1.720 (9)	C9—H9	1.0000
C2—C1—C6	120.0	C1—C7—Cl2	115.8 (12)
C2—C1—C7	115.1 (12)	C1—C7—Cl1	109.8 (11)
C6—C1—C7	124.9 (12)	Cl2—C7—Cl1	113.2 (10)
C3—C2—C1	120.0	C1—C7—H7	105.7
C3—C2—Cl3	118.7 (9)	Cl2—C7—H7	105.7
C1—C2—Cl3	121.2 (9)	Cl1—C7—H7	105.7
C2—C3—C4	120.0	C1A—C7A—Cl1	114.8 (10)
C2—C3—C8	121.3 (11)	C1A—C7A—Cl2	110.8 (11)
C4—C3—C8	118.7 (11)	Cl1—C7A—Cl2	113.3 (8)
C5—C4—C3	120.0	C1A—C7A—H7A	105.7
C5—C4—Cl6	122.3 (8)	Cl1—C7A—H7A	105.7
C3—C4—Cl6	117.7 (8)	Cl2—C7A—H7A	105.7
C6—C5—C4	120.0	C3—C8—Cl5	115.5 (13)
C6—C5—C9A	121.3 (10)	C3—C8—Cl4	112.4 (11)
C4—C5—C9A	118.5 (10)	Cl5—C8—Cl4	112.9 (7)
C5—C6—C1	120.0	C3—C8—H8	104.9
C5—C6—Cl9	118.7 (9)	Cl5—C8—H8	104.9
C1—C6—Cl9	121.1 (9)	Cl4—C8—H8	104.9
C2A—C1A—C6A	120.0	C3A—C8A—Cl4	115.3 (13)
C2A—C1A—C7A	118.6 (10)	C3A—C8A—Cl5	112.3 (11)
C6A—C1A—C7A	121.1 (10)	Cl4—C8A—Cl5	112.6 (7)
C3A—C2A—C1A	120.0	C3A—C8A—H8A	105.1
C3A—C2A—Cl3A	117.7 (8)	Cl4—C8A—H8A	105.1
C1A—C2A—Cl3A	122.2 (8)	Cl5—C8A—H8A	105.1
C4A—C3A—C2A	120.0	C5—C9A—Cl7	115.0 (10)
C4A—C3A—C8A	121.3 (11)	C5—C9A—Cl8	110.9 (10)
C2A—C3A—C8A	118.7 (11)	Cl7—C9A—Cl8	113.5 (8)
C3A—C4A—C5A	120.0	C5—C9A—H9A	105.5
C3A—C4A—Cl6A	119.7 (9)	Cl7—C9A—H9A	105.5
C5A—C4A—Cl6A	120.3 (9)	Cl8—C9A—H9A	105.5
C6A—C5A—C4A	120.0	C5A—C9—Cl8	116.3 (11)
C6A—C5A—C9	124.0 (12)	C5A—C9—Cl7	109.9 (11)
C4A—C5A—C9	116.0 (12)	Cl8—C9—Cl7	112.8 (9)
C5A—C6A—C1A	120.0	C5A—C9—H9	105.6
C5A—C6A—Cl9A	121.7 (9)	Cl8—C9—H9	105.6
C1A—C6A—Cl9A	118.0 (9)	Cl7—C9—H9	105.6
C6—C1—C2—C3	0.0	C3A—C4A—C5A—C6A	0.0
C7—C1—C2—C3	−179.1 (14)	Cl6A—C4A—C5A—C6A	177.6 (12)
C6—C1—C2—Cl3	177.6 (14)	C3A—C4A—C5A—C9	−179.1 (14)
C7—C1—C2—Cl3	−1.6 (12)	Cl6A—C4A—C5A—C9	−1.5 (12)
C1—C2—C3—C4	0.0	C4A—C5A—C6A—C1A	0.0
Cl3—C2—C3—C4	−177.6 (13)	C9—C5A—C6A—C1A	179.0 (15)
C1—C2—C3—C8	−179.9 (15)	C4A—C5A—C6A—Cl9A	174.0 (12)
Cl3—C2—C3—C8	2.5 (13)	C9—C5A—C6A—Cl9A	−7.0 (14)
C2—C3—C4—C5	0.0	C2A—C1A—C6A—C5A	0.0

C8—C3—C4—C5	179.9 (15)	C7A—C1A—C6A—C5A	−174.7 (15)
C2—C3—C4—Cl6	−177.5 (12)	C2A—C1A—C6A—Cl9A	−174.2 (11)
C8—C3—C4—Cl6	2.4 (13)	C7A—C1A—C6A—Cl9A	11.0 (14)
C3—C4—C5—C6	0.0	C2—C1—C7—Cl2	125.8 (11)
Cl6—C4—C5—C6	177.4 (12)	C6—C1—C7—Cl2	−53.3 (18)
C3—C4—C5—C9A	174.9 (14)	C2—C1—C7—Cl1	−104.4 (11)
Cl6—C4—C5—C9A	−7.8 (13)	C6—C1—C7—Cl1	76.5 (14)
C4—C5—C6—C1	0.0	C2A—C1A—C7A—Cl1	−55.8 (14)
C9A—C5—C6—C1	−174.7 (14)	C6A—C1A—C7A—Cl1	119.0 (11)
C4—C5—C6—Cl9	−174.2 (11)	C2A—C1A—C7A—Cl2	74.1 (12)
C9A—C5—C6—Cl9	11.1 (13)	C6A—C1A—C7A—Cl2	−111.2 (11)
C2—C1—C6—C5	0.0	C2—C3—C8—Cl5	62.3 (14)
C7—C1—C6—C5	179.0 (15)	C4—C3—C8—Cl5	−117.6 (12)
C2—C1—C6—Cl9	174.0 (12)	C2—C3—C8—Cl4	−69.3 (15)
C7—C1—C6—Cl9	−6.9 (15)	C4—C3—C8—Cl4	110.8 (11)
C6A—C1A—C2A—C3A	0.0	C4A—C3A—C8A—Cl4	62.0 (15)
C7A—C1A—C2A—C3A	174.8 (15)	C2A—C3A—C8A—Cl4	−117.9 (11)
C6A—C1A—C2A—Cl3A	177.5 (14)	C4A—C3A—C8A—Cl5	−68.9 (15)
C7A—C1A—C2A—Cl3A	−7.7 (13)	C2A—C3A—C8A—Cl5	111.2 (11)
C1A—C2A—C3A—C4A	0.0	C6—C5—C9A—Cl7	118.7 (10)
Cl3A—C2A—C3A—C4A	−177.6 (13)	C4—C5—C9A—Cl7	−56.1 (14)
C1A—C2A—C3A—C8A	179.9 (15)	C6—C5—C9A—Cl8	−110.8 (10)
Cl3A—C2A—C3A—C8A	2.3 (13)	C4—C5—C9A—Cl8	74.4 (11)
C2A—C3A—C4A—C5A	0.0	C6A—C5A—C9—Cl8	−53.2 (17)
C8A—C3A—C4A—C5A	−179.9 (15)	C4A—C5A—C9—Cl8	125.8 (11)
C2A—C3A—C4A—Cl6A	−177.6 (12)	C6A—C5A—C9—Cl7	76.5 (13)
C8A—C3A—C4A—Cl6A	2.5 (14)	C4A—C5A—C9—Cl7	−104.5 (11)