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(2,5-Dichloro-4-hydroxyphenyl)(phenyl)-methanone

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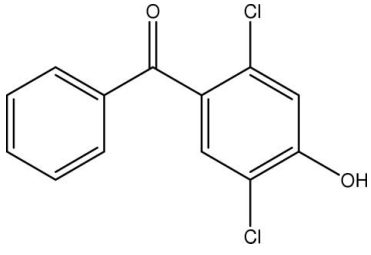
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.134; data-to-parameter ratio = 44.7.

The title compound, $C_{13}H_8Cl_2O_2$, crystallizes with two independent molecules in the asymmetric unit. Each of the two unique molecules is twisted about the C—C single bonds, making dihedral angles of 24.29 (5) and 73.01 (5)° between the two rings. In the crystal structure, the molecules are interlinked into columns along the b axis by intermolecular O—H···O and C—H···O interactions and short Cl···Cl and O···Cl contacts. In addition, the crystal packing is further stabilized by weak C—H···π interactions.

Related literature

For related literature on hydrogen-bond motifs, see: Bernstein *et al.* (1995). For related literature on values of bond lengths, see: Allen *et al.* (1987). For related structures, see: Harrison *et al.* (2005); Kutzke *et al.* (2000); Patai & Rappoport (1988); Thomson (1997); Zhang *et al.* (2000).



Experimental

Crystal data

$C_{13}H_8Cl_2O_2$
M_r = 267.09
Triclinic, $P\overline{1}$
a = 7.8450 (2) Å
b = 12.1815 (3) Å
c = 12.9442 (3) Å
α = 73.087 (1)°
β = 80.468 (1)°
γ = 77.869 (1)°
V = 1149.83 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 100.0 (1) K
0.69 × 0.14 × 0.13 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.851, T_{max} = 0.932
45186 measured reflections
14083 independent reflections
10281 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.134
S = 1.03
14083 reflections
315 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C8*A*–C13*A* and C8*B*–C13*B* rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1*A*—H1*A*···Cl2*A*	0.82 (2)	2.57 (2)	3.0208 (9)	116 (2)
O1*A*—H1*A*···O2*B*	0.82 (2)	1.97 (2)	2.7241 (12)	153 (2)
C9*A*—H9*A*···O1*B*	0.93	2.58	3.3070 (15)	135
O1*B*—H1*B*···O2*A*^{i}	0.91 (3)	1.80 (3)	2.6936 (13)	166 (2)
C5*B*—H5*B*···O2*B*^{ii}	0.93	2.42	3.3336 (13)	167
C9*B*—H9*B*···O1*A*^{i}	0.93	2.55	3.3268 (15)	142
C10*A*—H10*A*···O2*A*^{i}	0.93	2.60	3.5115 (16)	168
C13*A*—H13*A*···*Cg*1^{iii}	0.93	3.34	3.6615 (12)	103
C2*A*—H2*A*···*Cg*2^{ii}	0.93	2.65	3.5687 (11)	170

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y, -z$; (iii) $-x+2, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2171).

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supplementary materials

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(2,5-Dichloro-4-hydroxyphenyl)(phenyl)methanone

H.-K. Fun, S.-L. Ng, Z. Li and J.-H. Xu

Comment

The photochemistry of quinone compounds is of continuing research interest (Patai & Rappoport, 1988; Thomson, 1997). In continuation of our recent work on photoinduced reactions of quinones with alkynes (Zhang *et al.*, 2000), the title compound, (I), was obtained by the reaction of photoexcited 2,5-dichlorobenzoquinone with trimethylsilyphenylethyne. A crystallographic analysis of (I) was carried out to elucidate its structure.

The asymmetric unit of (I) contains two unique molecules, labelled A and B (Fig. 1). Bond lengths and angles in the two molecules are similar, display normal values (Allen *et al.*, 1987) and are comparable to those observed in related structures (Kutzke *et al.*, 2000; Harrison *et al.*, 2005). Each of the two unique molecules is twisted about C6—C7 and C7—C8 bonds with dihedral angle between the phenyl (C8—C13) and benzene (C1—C6) rings of 24.29 (5)° in molecule A and 73.01 (5)° in molecule B.

Intramolecular O1A—H1A···O2B and O9A—H9A···O1B interactions are observed in the molecular structure and another intramolecular O1A—H1A···Cl2A interaction generates a S(5) ring motif (Bernstein *et al.*, 1995) (Table 1 and Fig. 1). In the crystal structure, the molecules are linked into columns along the *b* axis by intermolecular O1B—H1B···O2A, C5B—H5B···O2B, C9B—H9B···O1A, C10A—H10A···O2A interactions (Table 1) and short Cl1A···Cl2B contact (2 − *x*, 1 − *y*, −*z*) of 3.3109 (4)Å and short O2B···Cl2A (*x*, *y*, *z*) contact of 3.2387 (9) Å. In addition, the crystal structure is further stabilized by C—H···π interactions involving the C8A—C13A ring (centroid *Cg*1) and C8B—C13B ring (centroid *Cg*2; Table 1).

Experimental

The title compound, (I), was synthesized by photo-induced reaction between 2,5-dichlorobenzoquinone (0.05*M*) and an excess amount of 1-phenyl-2-trimethyl-silylacetylene (0.1*M*) in a benzene solution. The title compound was isolated using silica gel column chromatography. Single crystal suitable for X-ray Diffraction analysis were obtained by slow evaporation of the solvent from a petroleum ether-acetone solution (v:v = 2:1).

Refinement

O-bound H atoms were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

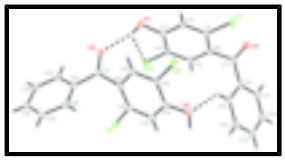

Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed lines indicate intramolecular hydrogen bonds.

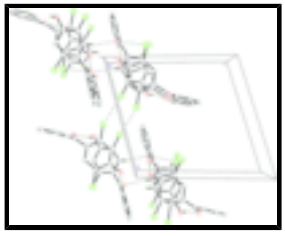

Fig. 2. The crystal packing of (I), viewed down the *a* axis. The intermolecular O—H···O, C—H···O interactions and short Cl···Cl and O···Cl contacts are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

(2,5-Dichloro-4-hydroxyphenyl)(phenyl)methanone

Crystal data

$C_{13}H_8Cl_2O_2$	$Z = 4$
$M_r = 267.09$	$F_{000} = 544$
Triclinic, $P\overline{1}$	$D_x = 1.543$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.8450$ (2) Å	Cell parameters from 9206 reflections
$b = 12.1815$ (3) Å	$\theta = 1.7$–40.0º
$c = 12.9442$ (3) Å	$\mu = 0.55$ mm^{-1}
$\alpha = 73.087$ (1)º	$T = 100.0$ (1) K
$\beta = 80.468$ (1)º	Needle, yellow
$\gamma = 77.869$ (1)º	0.69 × 0.14 × 0.13 mm
$V = 1149.83$ (5) Å^3	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	14083 independent reflections
Radiation source: fine-focus sealed tube	10281 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 40.0$º
$T = 100.0(1)$ K	$\theta_{min} = 1.7$º
ω scans	$h = -14 \rightarrow 13$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -22 \rightarrow 22$
$T_{min} = 0.851$, $T_{max} = 0.932$	$l = -23 \rightarrow 23$
45186 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.134$	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.1204P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = <0.001$
14083 reflections	$\Delta\rho_{max} = 0.71$ e Å^{-3}
315 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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}
Cl1A	1.21145 (4)	0.42758 (2)	0.14684 (2)	0.02036 (6)
Cl2A	1.11196 (4)	−0.08855 (2)	0.34500 (2)	0.02122 (6)
O1A	1.20212 (11)	0.02950 (7)	0.10794 (7)	0.01715 (14)
O2A	1.29008 (11)	0.33763 (7)	0.40468 (7)	0.01849 (14)
C1A	1.19193 (14)	0.28251 (8)	0.20409 (8)	0.01425 (15)
C2A	1.20829 (14)	0.21146 (9)	0.13519 (8)	0.01515 (16)
H2A	1.2358	0.2406	0.0608	0.018*
C3A	1.18331 (14)	0.09584 (9)	0.17802 (8)	0.01402 (15)
C4A	1.14106 (15)	0.05442 (9)	0.29037 (8)	0.01506 (16)
C5A	1.12360 (15)	0.12666 (9)	0.35824 (8)	0.01615 (17)
H5A	1.0928	0.0984	0.4324	0.019*
C6A	1.15179 (14)	0.24117 (8)	0.31614 (8)	0.01425 (15)
C7A	1.15246 (14)	0.30976 (9)	0.39545 (8)	0.01504 (16)
C8A	0.98836 (14)	0.33652 (9)	0.46450 (8)	0.01536 (16)
C9A	0.82712 (15)	0.33859 (10)	0.43122 (9)	0.01840 (18)
H9A	0.8233	0.3208	0.3665	0.022*

C10A	0.67211 (16)	0.36722 (11)	0.49482 (10)	0.02078 (19)
H10A	0.5645	0.3705	0.4719	0.025*
C11A	0.67853 (16)	0.39093 (11)	0.59253 (10)	0.0214 (2)
H11A	0.5749	0.4090	0.6355	0.026*
C12A	0.83915 (16)	0.38791 (10)	0.62660 (9)	0.02002 (19)
H12A	0.8424	0.4030	0.6926	0.024*
C13A	0.99431 (15)	0.36248 (9)	0.56253 (9)	0.01752 (17)
H13A	1.1014	0.3626	0.5843	0.021*
Cl1B	0.60271 (4)	−0.12704 (2)	0.38336 (2)	0.02222 (6)
Cl2B	0.78417 (4)	0.32958 (2)	0.05205 (2)	0.02021 (6)
O1B	0.57634 (12)	0.31234 (7)	0.26102 (7)	0.01826 (14)
O2B	0.99729 (10)	−0.13362 (7)	0.13368 (7)	0.01718 (14)
C1B	0.64770 (14)	−0.00127 (9)	0.28591 (8)	0.01513 (16)
C2B	0.58807 (14)	0.10414 (9)	0.31248 (8)	0.01622 (17)
H2B	0.5217	0.1056	0.3788	0.019*
C3B	0.62768 (14)	0.20750 (9)	0.23996 (9)	0.01485 (16)
C4B	0.73060 (14)	0.20223 (9)	0.14140 (8)	0.01504 (16)
C5B	0.79192 (14)	0.09678 (9)	0.11646 (8)	0.01471 (16)
H5B	0.8614	0.0951	0.0512	0.018*
C6B	0.75091 (13)	−0.00739 (8)	0.18803 (8)	0.01396 (15)
C7B	0.83740 (14)	−0.11867 (9)	0.15979 (8)	0.01430 (15)
C8B	0.73470 (14)	−0.20686 (9)	0.15805 (8)	0.01449 (15)
C9B	0.55771 (15)	−0.17591 (10)	0.14169 (9)	0.01820 (18)
H9B	0.4995	−0.1003	0.1382	0.022*
C10B	0.46854 (16)	−0.25846 (11)	0.13056 (10)	0.0214 (2)
H10B	0.3512	−0.2376	0.1180	0.026*
C11B	0.55468 (17)	−0.37246 (11)	0.13812 (10)	0.0219 (2)
H11B	0.4946	−0.4275	0.1308	0.026*
C12B	0.73054 (17)	−0.40425 (10)	0.15661 (10)	0.01992 (19)
H12B	0.7871	−0.4808	0.1633	0.024*
C13B	0.82109 (15)	−0.32137 (9)	0.16503 (9)	0.01722 (17)
H13B	0.9393	−0.3419	0.1753	0.021*
H1A	1.152 (3)	−0.026 (2)	0.1361 (19)	0.041 (6)*
H1B	0.483 (4)	0.308 (2)	0.313 (2)	0.067 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.02938 (14)	0.01235 (10)	0.01944 (11)	−0.00720 (9)	−0.00470 (9)	−0.00072 (8)
Cl2A	0.03286 (15)	0.01249 (10)	0.01933 (11)	−0.00818 (9)	−0.00370 (10)	−0.00230 (8)
O1A	0.0191 (3)	0.0172 (3)	0.0182 (3)	−0.0055 (3)	0.0006 (3)	−0.0091 (3)
O2A	0.0171 (3)	0.0186 (3)	0.0228 (4)	−0.0044 (3)	−0.0011 (3)	−0.0098 (3)
C1A	0.0165 (4)	0.0117 (3)	0.0150 (4)	−0.0046 (3)	−0.0017 (3)	−0.0028 (3)
C2A	0.0183 (4)	0.0141 (4)	0.0137 (4)	−0.0051 (3)	−0.0017 (3)	−0.0032 (3)
C3A	0.0144 (4)	0.0136 (4)	0.0152 (4)	−0.0028 (3)	−0.0018 (3)	−0.0051 (3)
C4A	0.0193 (4)	0.0114 (3)	0.0149 (4)	−0.0048 (3)	−0.0018 (3)	−0.0027 (3)
C5A	0.0215 (5)	0.0137 (4)	0.0138 (4)	−0.0051 (3)	−0.0009 (3)	−0.0038 (3)
C6A	0.0166 (4)	0.0122 (3)	0.0144 (4)	−0.0036 (3)	−0.0009 (3)	−0.0039 (3)

C7A	0.0176 (4)	0.0119 (3)	0.0157 (4)	−0.0028 (3)	−0.0016 (3)	−0.0038 (3)
C8A	0.0169 (4)	0.0130 (4)	0.0165 (4)	−0.0027 (3)	−0.0016 (3)	−0.0046 (3)
C9A	0.0188 (4)	0.0185 (4)	0.0190 (4)	−0.0029 (3)	−0.0027 (3)	−0.0066 (3)
C10A	0.0166 (4)	0.0225 (5)	0.0232 (5)	−0.0015 (4)	−0.0025 (4)	−0.0071 (4)
C11A	0.0204 (5)	0.0209 (5)	0.0205 (5)	0.0003 (4)	0.0002 (4)	−0.0058 (4)
C12A	0.0241 (5)	0.0187 (4)	0.0165 (4)	−0.0007 (4)	−0.0015 (4)	−0.0060 (3)
C13A	0.0202 (5)	0.0167 (4)	0.0170 (4)	−0.0025 (3)	−0.0034 (3)	−0.0062 (3)
Cl1B	0.03089 (14)	0.01500 (10)	0.01745 (11)	−0.00506 (9)	0.00498 (9)	−0.00264 (8)
Cl2B	0.02614 (13)	0.01347 (10)	0.01999 (11)	−0.00595 (8)	−0.00007 (9)	−0.00241 (8)
O1B	0.0192 (4)	0.0139 (3)	0.0231 (4)	−0.0017 (3)	−0.0004 (3)	−0.0090 (3)
O2B	0.0138 (3)	0.0177 (3)	0.0221 (3)	−0.0033 (2)	0.0003 (3)	−0.0093 (3)
C1B	0.0165 (4)	0.0130 (4)	0.0149 (4)	−0.0027 (3)	0.0007 (3)	−0.0034 (3)
C2B	0.0173 (4)	0.0153 (4)	0.0158 (4)	−0.0021 (3)	0.0005 (3)	−0.0055 (3)
C3B	0.0143 (4)	0.0137 (4)	0.0176 (4)	−0.0013 (3)	−0.0021 (3)	−0.0063 (3)
C4B	0.0169 (4)	0.0120 (3)	0.0162 (4)	−0.0030 (3)	−0.0014 (3)	−0.0035 (3)
C5B	0.0155 (4)	0.0136 (4)	0.0148 (4)	−0.0028 (3)	0.0002 (3)	−0.0044 (3)
C6B	0.0149 (4)	0.0122 (3)	0.0147 (4)	−0.0022 (3)	−0.0003 (3)	−0.0042 (3)
C7B	0.0153 (4)	0.0137 (4)	0.0143 (4)	−0.0025 (3)	−0.0007 (3)	−0.0049 (3)
C8B	0.0154 (4)	0.0130 (4)	0.0159 (4)	−0.0034 (3)	−0.0012 (3)	−0.0047 (3)
C9B	0.0157 (4)	0.0175 (4)	0.0221 (4)	−0.0026 (3)	−0.0013 (3)	−0.0069 (3)
C10B	0.0176 (5)	0.0231 (5)	0.0264 (5)	−0.0069 (4)	−0.0019 (4)	−0.0087 (4)
C11B	0.0247 (5)	0.0219 (5)	0.0231 (5)	−0.0109 (4)	−0.0005 (4)	−0.0083 (4)
C12B	0.0250 (5)	0.0147 (4)	0.0215 (4)	−0.0049 (4)	−0.0029 (4)	−0.0059 (3)
C13B	0.0190 (4)	0.0137 (4)	0.0194 (4)	−0.0018 (3)	−0.0032 (3)	−0.0052 (3)

Geometric parameters (Å, °)

Cl1A—C1A	1.7347 (10)	Cl1B—C1B	1.7373 (10)
Cl2A—C4A	1.7270 (10)	Cl2B—C4B	1.7291 (10)
O1A—C3A	1.3526 (12)	O1B—C3B	1.3481 (12)
O1A—H1A	0.82 (2)	O1B—H1B	0.91 (3)
O2A—C7A	1.2310 (14)	O2B—C7B	1.2329 (13)
C1A—C2A	1.3878 (14)	C1B—C2B	1.3919 (14)
C1A—C6A	1.3953 (14)	C1B—C6B	1.3986 (14)
C2A—C3A	1.3982 (14)	C2B—C3B	1.3940 (15)
C2A—H2A	0.9300	C2B—H2B	0.9300
C3A—C4A	1.4012 (14)	C3B—C4B	1.4030 (15)
C4A—C5A	1.3871 (14)	C4B—C5B	1.3842 (14)
C5A—C6A	1.3925 (14)	C5B—C6B	1.4003 (14)
C5A—H5A	0.9300	C5B—H5B	0.9300
C6A—C7A	1.5016 (14)	C6B—C7B	1.5004 (13)
C7A—C8A	1.4746 (15)	C7B—C8B	1.4790 (15)
C8A—C9A	1.3954 (16)	C8B—C9B	1.3949 (16)
C8A—C13A	1.4041 (15)	C8B—C13B	1.4010 (14)
C9A—C10A	1.3913 (16)	C9B—C10B	1.3909 (17)
C9A—H9A	0.9300	C9B—H9B	0.9300
C10A—C11A	1.3875 (17)	C10B—C11B	1.3940 (18)
C10A—H10A	0.9300	C10B—H10B	0.9300
C11A—C12A	1.3924 (18)	C11B—C12B	1.3934 (18)

C11A—H11A	0.9300	C11B—H11B	0.9300
C12A—C13A	1.3863 (16)	C12B—C13B	1.3881 (16)
C12A—H12A	0.9300	C12B—H12B	0.9300
C13A—H13A	0.9300	C13B—H13B	0.9300
C3A—O1A—H1A	109.4 (16)	C3B—O1B—H1B	108.4 (18)
C2A—C1A—C6A	121.50 (9)	C2B—C1B—C6B	121.63 (9)
C2A—C1A—Cl1A	118.25 (8)	C2B—C1B—Cl1B	117.40 (8)
C6A—C1A—Cl1A	120.17 (8)	C6B—C1B—Cl1B	120.81 (8)
C1A—C2A—C3A	119.78 (9)	C1B—C2B—C3B	120.14 (9)
C1A—C2A—H2A	120.1	C1B—C2B—H2B	119.9
C3A—C2A—H2A	120.1	C3B—C2B—H2B	119.9
O1A—C3A—C2A	117.74 (9)	O1B—C3B—C2B	123.29 (9)
O1A—C3A—C4A	123.40 (9)	O1B—C3B—C4B	118.08 (9)
C2A—C3A—C4A	118.87 (9)	C2B—C3B—C4B	118.60 (9)
C5A—C4A—C3A	120.77 (9)	C5B—C4B—C3B	120.86 (9)
C5A—C4A—Cl2A	119.66 (8)	C5B—C4B—Cl2B	120.14 (8)
C3A—C4A—Cl2A	119.56 (8)	C3B—C4B—Cl2B	118.98 (8)
C4A—C5A—C6A	120.52 (9)	C4B—C5B—C6B	121.01 (9)
C4A—C5A—H5A	119.7	C4B—C5B—H5B	119.5
C6A—C5A—H5A	119.7	C6B—C5B—H5B	119.5
C5A—C6A—C1A	118.54 (9)	C1B—C6B—C5B	117.73 (9)
C5A—C6A—C7A	117.61 (9)	C1B—C6B—C7B	124.50 (9)
C1A—C6A—C7A	123.63 (9)	C5B—C6B—C7B	117.40 (9)
O2A—C7A—C8A	121.80 (9)	O2B—C7B—C8B	120.02 (9)
O2A—C7A—C6A	119.70 (10)	O2B—C7B—C6B	118.30 (9)
C8A—C7A—C6A	118.42 (9)	C8B—C7B—C6B	121.62 (9)
C9A—C8A—C13A	120.05 (10)	C9B—C8B—C13B	119.89 (10)
C9A—C8A—C7A	119.99 (10)	C9B—C8B—C7B	121.09 (9)
C13A—C8A—C7A	119.95 (10)	C13B—C8B—C7B	118.85 (10)
C10A—C9A—C8A	119.97 (10)	C10B—C9B—C8B	119.81 (10)
C10A—C9A—H9A	120.0	C10B—C9B—H9B	120.1
C8A—C9A—H9A	120.0	C8B—C9B—H9B	120.1
C11A—C10A—C9A	119.83 (11)	C9B—C10B—C11B	120.12 (11)
C11A—C10A—H10A	120.1	C9B—C10B—H10B	119.9
C9A—C10A—H10A	120.1	C11B—C10B—H10B	119.9
C10A—C11A—C12A	120.41 (11)	C12B—C11B—C10B	120.21 (11)
C10A—C11A—H11A	119.8	C12B—C11B—H11B	119.9
C12A—C11A—H11A	119.8	C10B—C11B—H11B	119.9
C13A—C12A—C11A	120.27 (11)	C13B—C12B—C11B	119.79 (10)
C13A—C12A—H12A	119.9	C13B—C12B—H12B	120.1
C11A—C12A—H12A	119.9	C11B—C12B—H12B	120.1
C12A—C13A—C8A	119.44 (11)	C12B—C13B—C8B	120.14 (11)
C12A—C13A—H13A	120.3	C12B—C13B—H13B	119.9
C8A—C13A—H13A	120.3	C8B—C13B—H13B	119.9
C6A—C1A—C2A—C3A	0.36 (16)	C6B—C1B—C2B—C3B	1.34 (17)
Cl1A—C1A—C2A—C3A	−176.33 (8)	Cl1B—C1B—C2B—C3B	176.73 (9)
C1A—C2A—C3A—O1A	−179.41 (10)	C1B—C2B—C3B—O1B	−179.05 (10)
C1A—C2A—C3A—C4A	0.35 (16)	C1B—C2B—C3B—C4B	−1.06 (16)

O1A—C3A—C4A—C5A	179.96 (10)	O1B—C3B—C4B—C5B	178.03 (10)
C2A—C3A—C4A—C5A	0.21 (16)	C2B—C3B—C4B—C5B	−0.07 (16)
O1A—C3A—C4A—Cl2A	0.43 (15)	O1B—C3B—C4B—Cl2B	−0.62 (14)
C2A—C3A—C4A—Cl2A	−179.32 (8)	C2B—C3B—C4B—Cl2B	−178.72 (8)
C3A—C4A—C5A—C6A	−1.49 (17)	C3B—C4B—C5B—C6B	0.97 (17)
Cl2A—C4A—C5A—C6A	178.04 (9)	Cl2B—C4B—C5B—C6B	179.60 (8)
C4A—C5A—C6A—C1A	2.16 (16)	C2B—C1B—C6B—C5B	−0.45 (16)
C4A—C5A—C6A—C7A	−172.64 (10)	Cl1B—C1B—C6B—C5B	−175.68 (8)
C2A—C1A—C6A—C5A	−1.61 (16)	C2B—C1B—C6B—C7B	172.36 (10)
Cl1A—C1A—C6A—C5A	175.02 (8)	Cl1B—C1B—C6B—C7B	−2.88 (16)
C2A—C1A—C6A—C7A	172.86 (10)	C4B—C5B—C6B—C1B	−0.70 (16)
Cl1A—C1A—C6A—C7A	−10.51 (15)	C4B—C5B—C6B—C7B	−174.02 (10)
C5A—C6A—C7A—O2A	111.68 (12)	C1B—C6B—C7B—O2B	−124.56 (12)
C1A—C6A—C7A—O2A	−62.84 (15)	C5B—C6B—C7B—O2B	48.27 (14)
C5A—C6A—C7A—C8A	−65.16 (13)	C1B—C6B—C7B—C8B	58.16 (15)
C1A—C6A—C7A—C8A	120.32 (11)	C5B—C6B—C7B—C8B	−129.01 (11)
O2A—C7A—C8A—C9A	159.50 (11)	O2B—C7B—C8B—C9B	−152.78 (11)
C6A—C7A—C8A—C9A	−23.73 (14)	C6B—C7B—C8B—C9B	24.46 (15)
O2A—C7A—C8A—C13A	−19.07 (16)	O2B—C7B—C8B—C13B	22.49 (15)
C6A—C7A—C8A—C13A	157.70 (10)	C6B—C7B—C8B—C13B	−160.27 (10)
C13A—C8A—C9A—C10A	0.47 (17)	C13B—C8B—C9B—C10B	−1.07 (17)
C7A—C8A—C9A—C10A	−178.10 (10)	C7B—C8B—C9B—C10B	174.15 (10)
C8A—C9A—C10A—C11A	−1.54 (18)	C8B—C9B—C10B—C11B	1.42 (18)
C9A—C10A—C11A—C12A	0.94 (18)	C9B—C10B—C11B—C12B	−0.15 (19)
C10A—C11A—C12A—C13A	0.75 (18)	C10B—C11B—C12B—C13B	−1.46 (18)
C11A—C12A—C13A—C8A	−1.81 (17)	C11B—C12B—C13B—C8B	1.81 (17)
C9A—C8A—C13A—C12A	1.21 (16)	C9B—C8B—C13B—C12B	−0.54 (16)
C7A—C8A—C13A—C12A	179.77 (10)	C7B—C8B—C13B—C12B	−175.87 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1A—H1A···Cl2A	0.82 (2)	2.57 (2)	3.0208 (9)	116 (2)
O1A—H1A···O2B	0.82 (2)	1.97 (2)	2.7241 (12)	153 (2)
C9A—H9A···O1B	0.93	2.58	3.3070 (15)	135
O1B—H1B···O2A^{i}	0.91 (3)	1.80 (3)	2.6936 (13)	166 (2)
C5B—H5B···O2B^{ii}	0.93	2.42	3.3336 (13)	167
C9B—H9B···O1A^{i}	0.93	2.55	3.3268 (15)	142
C10A—H10A···O2A^{i}	0.93	2.60	3.5115 (16)	168
C13A—H13A···Cg1^{iii}	0.93	3.34	3.6615 (12)	103
C2A—H2A···Cg2^{ii}	0.93	2.65	3.5687 (11)	170

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+2, −*y*, −*z*; (iii) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

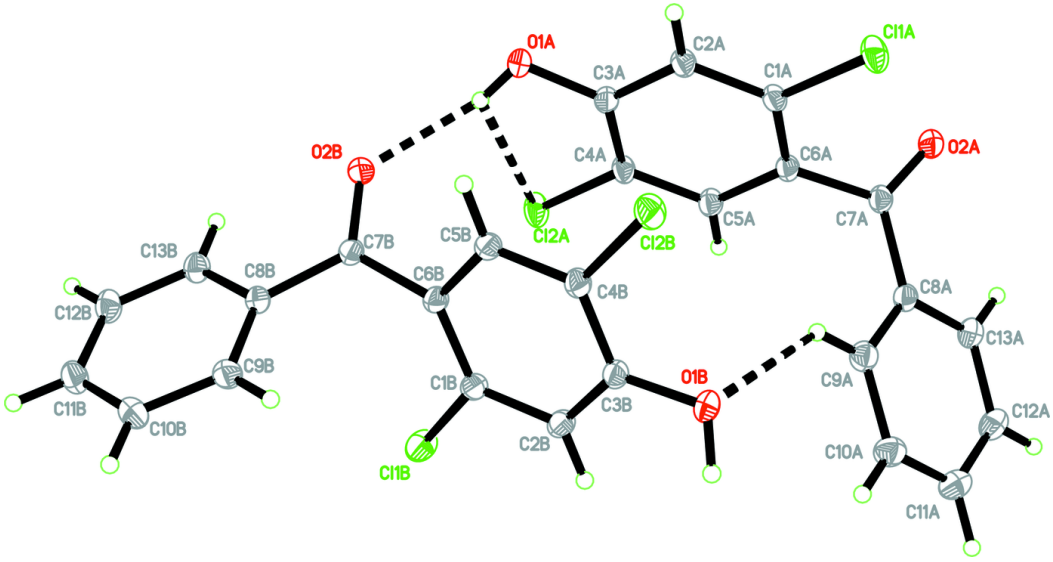
O1A
C2A
Cl1A
C3A
C1A
O2B
C4A
C6A
O2A
Cl2A
Cl2B
C5A
C7A
C13B
C8B
C7B
C5B
C6B
C4B
C8A
C12B
C13A
C9B
C1B
O1B
C9A
C11B
C10B
C3B
C12A
Cl1B
C2B
C10A
C11A

Fig. 2