

1-Chloro-4-(3,4-dichlorophenyl)-3,4-dihydronaphthalene-2-carbaldehyde

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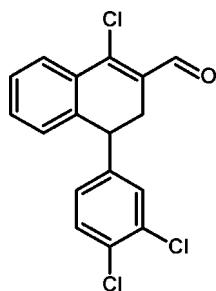
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.050; wR factor = 0.149; data-to-parameter ratio = 12.8.

The title compound, $\text{C}_{17}\text{H}_{11}\text{Cl}_3\text{O}$, was synthesized *via* the Vilsmeier–Haack reaction. The dihydronaphthalene ring system is non-planar, the dihedral angle between the two fused rings being 10.87 (13)°; it forms a dihedral angle of 81.45 (10)° with the dichlorophenyl ring. The crystal structure features intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For general background to 4-(3,4-dichlorophenyl)-3,4-dihydronaphthalen-1(2*H*)-one, see: Zhengxu *et al.* (2007); Jerussi *et al.* (2004); Taber *et al.* (2004); Ray *et al.* (2003); Meth-Cohn & Stanforth (1991); Hurd & Webb (1941); Mallegol *et al.* (2005). For the synthesis, see Vilsmeier *et al.* (1937). For a related structure, see: Gowda *et al.* (2008).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{11}\text{Cl}_3\text{O}$
 $M_r = 337.61$
 Monoclinic, $P2_1/c$
 $a = 10.2969$ (5) Å
 $b = 10.8849$ (5) Å
 $c = 13.6144$ (7) Å
 $\beta = 91.436$ (5)°

$V = 1525.43$ (13) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.60$ mm⁻¹
 $T = 293$ K
 $0.22 \times 0.15 \times 0.12$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2010)
 $T_{\min} = 0.546$, $T_{\max} = 1.000$

15902 measured reflections
 3006 independent reflections
 2143 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.149$
 $S = 1.09$
 3006 reflections
 234 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.52$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C18}-\text{H18}\cdots\text{O4}^i$	0.90 (3)	2.58 (3)	3.201 (3)	128 (2)

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Professor T. N. Guru Row and Mr Venkatesha R. Hathwar, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, for their help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2168).

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supplementary materials

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1-Chloro-4-(3,4-dichlorophenyl)-3,4-dihydronaphthalene-2-carbaldehyde

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Comment

Recently drug candidates for blocking the monoamine reuptake trasporters have considerable interest in the pharmaceutical industry for treatment of central nervous system disorders (Zhengxu *et al.*, 2007). 1,2,3,4-tetrahydronaphthalene derivatives are for the treatment of central nervous system disorders (Jerussi *et al.*, 2004; Taber *et al.*, 2004). Tetrahydronaphthalene derivatives are also used in liquid crystal display elements (Ray *et al.*, 2003). Potent pharmaceutically active 1-chloro-4-(3,4-dichlorophenyl)-3, 4-dihydronaphthalene-2-carbaldehyde was prepared by the Vilsmeier- Haack reaction (Vilsmeier *et al.*, 1937; Meth-Cohn *et al.* , 1991; Hurd *et al.*, 1941; Mallegol *et al.*, 2005) of 4-(3,4-dichlorophenyl)-3,4-dihydronaphthalen-1(2*H*)-one.

The asymmetric unit of the 1-chloro-4-(3,4-dichlorophenyl)-3,4- dihydronaphthalene-2-carbaldehyde contains one molecule (Fig. 1). The dihydronaphthalene ring system is non-planar; the dihedral angle between the two ring system of the naphthalene ring is 10.87 (13)° and also the dihedral angle between the dihydronaphthalene ring system and the dichlorophenyl ring is 81.45 (10)°. The crystal structure shows intramolecular C5—H5···Cl1, C9—H9···Cl1, C15—H15B···O4 and C18—H18···O4 intermolecular hydrogen bonds. Bond distances within the aromatic rings are in agreement with those observed related structures (Gowda *et al.*, 2008). The packing of the molecules shows when viewed along the *a* axis (Fig.2).

Experimental

To the Vilsmeier-Haack complex prepared from DMF and POCl₃ (0.03 mol) at 0°C, the compound 4-(3,4-dichlorophenyl)-3,4-dihydronaphthalen-1(2*H*)-one (0.01 mol) was added and the reaction mixture was stirred at 65°C for 4 h. The reaction completion was monitored by TLC. The contents were cooled, poured in to ice-cold water and neutralized using Na₂CO₃ solution. The product that separated was filtered and dried. X-ray quality crystals were obtained from an ethyl acetate solution.

Refinement

Hydrogen atoms were located in a difference Fourier map and were allowed to refine isotropically.

Figures

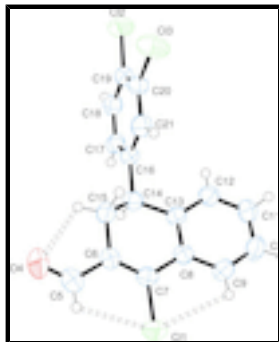


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds

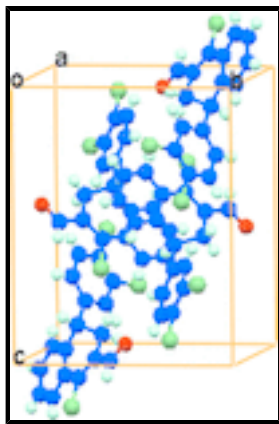


Fig. 2. A view of the structure down the axis *a*.

1-Chloro-4-(3,4-dichlorophenyl)-3,4-dihydronaphthalene-2-carbaldehyde

Crystal data

$C_{17}H_{11}Cl_3O$

$M_r = 337.61$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.2969 (5) \text{ \AA}$

$b = 10.8849 (5) \text{ \AA}$

$c = 13.6144 (7) \text{ \AA}$

$\beta = 91.436 (5)^\circ$

$V = 1525.43 (13) \text{ \AA}^3$

$Z = 4$

$F(000) = 688$

$D_x = 1.470 \text{ Mg m}^{-3}$

Melting point: 383 K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3006 reflections

$\theta = 2.4\text{--}26.0^\circ$

$\mu = 0.60 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Plate, colourless

$0.22 \times 0.15 \times 0.12 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur diffractometer

Radiation source: Enhance (Mo) X-ray Source graphite

Detector resolution: $16.0839 \text{ pixels mm}^{-1}$

3006 independent reflections

2143 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$

ω scans $h = -12 \rightarrow 12$
 Absorption correction: multi-scan $k = -13 \rightarrow 13$
 (*CrysAlis PRO RED*; Oxford Diffraction, 2010)
 $T_{\min} = 0.546$, $T_{\max} = 1.000$ $l = -16 \rightarrow 16$
 15902 measured reflections

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.050$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.149$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2]$
3006 reflections	where $P = (F_o^2 + 2F_c^2)/3$
234 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 0.52 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.33.55 (release 05-01-2010 CrysAlis171. NET) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

^1H NMR (CDCl_3 , 400 MHz): δ , 10.33 (s, 1H, -CHO), 6.92-8.00 (m, 7H, Ar-H), 4.13 (t, 1H, -CH proton of fused cyclohexane ring, $J=10.0$ Hz), 2.86-3.01 (m, 2H, -CH₂ proton of fused cyclohexane ring)

IR (KBr, cm^{-1}): 3443.28 (-CHO), 1662.34 (C=O of aldehyde), 1595.81 (C=C, aromatic), 838.883 (C-Cl), 1255.43 (C-H stretch).

FAB MASS: $m/z = 337$, mol. formulae: $\text{C}_{17}\text{H}_{11}\text{Cl}_3\text{O}$.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.40177 (8)	0.17987 (7)	0.18417 (6)	0.0642 (3)
Cl2	1.03593 (8)	0.22018 (9)	-0.40674 (6)	0.0809 (3)
Cl3	1.07383 (9)	0.35613 (9)	-0.20272 (7)	0.0853 (3)

supplementary materials

O4	0.3558 (2)	0.4375 (2)	-0.04817 (19)	0.0873 (8)
C5	0.3745 (3)	0.3618 (3)	0.0142 (3)	0.0654 (8)
C6	0.4835 (3)	0.2751 (2)	0.01503 (19)	0.0461 (6)
C7	0.5053 (2)	0.1922 (2)	0.08561 (18)	0.0410 (6)
C8	0.6168 (2)	0.1084 (2)	0.08586 (17)	0.0389 (6)
C9	0.6561 (3)	0.0405 (2)	0.16846 (19)	0.0474 (6)
C10	0.7619 (3)	-0.0361 (3)	0.1655 (2)	0.0604 (8)
C11	0.8291 (3)	-0.0479 (3)	0.0801 (2)	0.0595 (8)
C12	0.7912 (3)	0.0171 (2)	-0.0023 (2)	0.0520 (7)
C13	0.6860 (2)	0.0965 (2)	-0.00149 (17)	0.0409 (6)
C14	0.6365 (3)	0.1633 (2)	-0.09391 (19)	0.0462 (6)
C15	0.5787 (3)	0.2861 (3)	-0.0664 (2)	0.0539 (7)
C16	0.7379 (2)	0.1794 (2)	-0.17227 (19)	0.0433 (6)
C17	0.7223 (3)	0.1248 (2)	-0.26254 (19)	0.0447 (6)
C18	0.8128 (3)	0.1384 (2)	-0.3336 (2)	0.0475 (6)
C19	0.9213 (3)	0.2083 (2)	-0.31643 (19)	0.0451 (6)
C20	0.9393 (3)	0.2661 (2)	-0.2272 (2)	0.0476 (6)
C21	0.8493 (3)	0.2513 (2)	-0.1548 (2)	0.0503 (7)
H5	0.327 (3)	0.359 (3)	0.067 (2)	0.080 (11)*
H9	0.616 (3)	0.050 (2)	0.224 (2)	0.061 (8)*
H10	0.792 (3)	-0.082 (3)	0.218 (2)	0.088 (11)*
H11	0.904 (3)	-0.096 (2)	0.0799 (18)	0.050 (7)*
H12	0.836 (3)	0.009 (2)	-0.054 (2)	0.057 (8)*
H14	0.561 (2)	0.111 (2)	-0.1275 (17)	0.040 (6)*
H17	0.653 (3)	0.068 (2)	-0.2739 (18)	0.049 (7)*
H18	0.807 (3)	0.103 (2)	-0.393 (2)	0.055 (8)*
H15A	0.668 (4)	0.339 (3)	-0.040 (3)	0.101 (12)*
H15B	0.536 (3)	0.324 (2)	-0.121 (2)	0.057 (8)*
H21	0.867 (3)	0.291 (3)	-0.090 (2)	0.061 (8)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0575 (5)	0.0748 (5)	0.0613 (5)	0.0080 (3)	0.0232 (4)	0.0094 (4)
C12	0.0618 (5)	0.1218 (8)	0.0600 (5)	0.0032 (5)	0.0216 (4)	0.0190 (5)
C13	0.0590 (5)	0.0868 (6)	0.1103 (8)	-0.0339 (4)	0.0057 (5)	-0.0100 (5)
O4	0.0824 (17)	0.0849 (16)	0.0945 (18)	0.0370 (13)	-0.0004 (14)	0.0272 (14)
C5	0.0517 (19)	0.073 (2)	0.072 (2)	0.0171 (15)	0.0058 (17)	0.0092 (18)
C6	0.0425 (14)	0.0474 (14)	0.0484 (15)	0.0052 (11)	-0.0004 (12)	0.0029 (11)
C7	0.0372 (13)	0.0438 (13)	0.0421 (13)	-0.0044 (11)	0.0042 (11)	-0.0034 (11)
C8	0.0386 (13)	0.0339 (12)	0.0442 (13)	-0.0052 (10)	0.0001 (11)	-0.0009 (10)
C9	0.0547 (17)	0.0480 (14)	0.0396 (14)	0.0000 (12)	0.0037 (13)	0.0049 (12)
C10	0.071 (2)	0.0574 (17)	0.0522 (17)	0.0116 (15)	-0.0045 (16)	0.0149 (14)
C11	0.0551 (18)	0.0571 (17)	0.0664 (19)	0.0192 (14)	0.0034 (15)	0.0116 (14)
C12	0.0526 (17)	0.0517 (15)	0.0521 (17)	0.0102 (13)	0.0116 (14)	0.0049 (13)
C13	0.0409 (13)	0.0389 (13)	0.0430 (13)	-0.0027 (10)	0.0021 (11)	0.0042 (10)
C14	0.0415 (14)	0.0513 (15)	0.0458 (14)	-0.0039 (12)	0.0028 (12)	0.0036 (12)
C15	0.0569 (18)	0.0555 (16)	0.0496 (16)	0.0149 (14)	0.0075 (14)	0.0144 (13)

C16	0.0392 (14)	0.0436 (13)	0.0472 (15)	0.0002 (11)	0.0037 (11)	0.0098 (11)
C17	0.0467 (15)	0.0380 (13)	0.0493 (15)	-0.0048 (11)	-0.0035 (12)	0.0064 (11)
C18	0.0510 (16)	0.0484 (14)	0.0430 (15)	0.0036 (12)	-0.0020 (12)	0.0014 (12)
C19	0.0425 (14)	0.0483 (14)	0.0446 (14)	0.0042 (11)	0.0053 (12)	0.0112 (12)
C20	0.0395 (14)	0.0460 (14)	0.0570 (17)	-0.0077 (11)	-0.0005 (12)	0.0046 (12)
C21	0.0529 (16)	0.0534 (15)	0.0444 (15)	-0.0016 (12)	-0.0017 (13)	-0.0031 (13)

Geometric parameters (Å, °)

C11—C7	1.740 (2)	C12—C13	1.386 (3)
C12—C19	1.731 (2)	C12—H12	0.86 (3)
C13—C20	1.722 (3)	C13—C14	1.530 (3)
O4—C5	1.195 (4)	C14—C15	1.514 (4)
C5—C6	1.466 (4)	C14—C16	1.521 (3)
C5—H5	0.88 (3)	C14—H14	1.06 (2)
C6—C7	1.333 (3)	C15—H15A	1.14 (4)
C6—C15	1.503 (3)	C15—H15B	0.94 (3)
C7—C8	1.465 (3)	C16—C17	1.371 (4)
C8—C9	1.398 (3)	C16—C21	1.404 (4)
C8—C13	1.408 (3)	C17—C18	1.368 (4)
C9—C10	1.373 (4)	C17—H17	0.95 (3)
C9—H9	0.88 (3)	C18—C19	1.367 (4)
C10—C11	1.374 (4)	C18—H18	0.89 (3)
C10—H10	0.92 (3)	C19—C20	1.377 (4)
C11—C12	1.375 (4)	C20—C21	1.379 (4)
C11—H11	0.93 (3)	C21—H21	0.99 (3)
O4—C5—C6	123.9 (3)	C16—C14—C13	114.3 (2)
O4—C5—H5	121 (2)	C15—C14—H14	106.9 (12)
C6—C5—H5	115 (2)	C16—C14—H14	105.6 (12)
C7—C6—C5	123.8 (2)	C13—C14—H14	109.1 (12)
C7—C6—C15	119.0 (2)	C6—C15—C14	112.3 (2)
C5—C6—C15	117.1 (2)	C6—C15—H15A	110.4 (19)
C6—C7—C8	122.7 (2)	C14—C15—H15A	101.8 (18)
C6—C7—C11	120.84 (19)	C6—C15—H15B	108.2 (16)
C8—C7—C11	116.44 (17)	C14—C15—H15B	111.5 (16)
C9—C8—C13	119.2 (2)	H15A—C15—H15B	113 (2)
C9—C8—C7	122.8 (2)	C17—C16—C21	118.1 (2)
C13—C8—C7	117.9 (2)	C17—C16—C14	120.8 (2)
C10—C9—C8	120.8 (2)	C21—C16—C14	121.2 (2)
C10—C9—H9	119.4 (19)	C18—C17—C16	121.4 (3)
C8—C9—H9	119.7 (19)	C18—C17—H17	118.4 (15)
C9—C10—C11	119.9 (3)	C16—C17—H17	119.8 (15)
C9—C10—H10	124 (2)	C19—C18—C17	120.5 (3)
C11—C10—H10	116 (2)	C19—C18—H18	115.4 (18)
C10—C11—C12	120.2 (3)	C17—C18—H18	124.1 (18)
C10—C11—H11	119.2 (16)	C18—C19—C20	119.8 (2)
C12—C11—H11	120.4 (16)	C18—C19—C12	119.3 (2)
C11—C12—C13	121.3 (3)	C20—C19—C12	120.9 (2)
C11—C12—H12	117.9 (19)	C19—C20—C21	119.9 (2)

supplementary materials

C13—C12—H12	120.7 (19)	C19—C20—C13	121.4 (2)
C12—C13—C8	118.5 (2)	C21—C20—C13	118.7 (2)
C12—C13—C14	122.3 (2)	C20—C21—C16	120.3 (3)
C8—C13—C14	119.1 (2)	C20—C21—H21	118.3 (17)
C15—C14—C16	110.7 (2)	C16—C21—H21	121.3 (17)
C15—C14—C13	110.0 (2)		
O4—C5—C6—C7	178.8 (3)	C12—C13—C14—C16	-24.0 (3)
O4—C5—C6—C15	2.0 (5)	C8—C13—C14—C16	160.9 (2)
C5—C6—C7—C8	-178.5 (3)	C7—C6—C15—C14	34.9 (4)
C15—C6—C7—C8	-1.7 (4)	C5—C6—C15—C14	-148.1 (3)
C5—C6—C7—C11	0.6 (4)	C16—C14—C15—C6	-176.7 (2)
C15—C6—C7—C11	177.4 (2)	C13—C14—C15—C6	-49.5 (3)
C6—C7—C8—C9	165.8 (3)	C15—C14—C16—C17	-118.7 (3)
C11—C7—C8—C9	-13.4 (3)	C13—C14—C16—C17	116.5 (3)
C6—C7—C8—C13	-14.4 (4)	C15—C14—C16—C21	60.7 (3)
C11—C7—C8—C13	166.37 (17)	C13—C14—C16—C21	-64.1 (3)
C13—C8—C9—C10	0.8 (4)	C21—C16—C17—C18	0.7 (4)
C7—C8—C9—C10	-179.4 (2)	C14—C16—C17—C18	-179.9 (2)
C8—C9—C10—C11	-1.0 (5)	C16—C17—C18—C19	-0.6 (4)
C9—C10—C11—C12	0.2 (5)	C17—C18—C19—C20	-0.4 (4)
C10—C11—C12—C13	0.6 (5)	C17—C18—C19—C12	178.27 (19)
C11—C12—C13—C8	-0.8 (4)	C18—C19—C20—C21	1.3 (4)
C11—C12—C13—C14	-175.9 (3)	C12—C19—C20—C21	-177.3 (2)
C9—C8—C13—C12	0.1 (4)	C18—C19—C20—C13	-179.4 (2)
C7—C8—C13—C12	-179.7 (2)	C12—C19—C20—C13	1.9 (3)
C9—C8—C13—C14	175.4 (2)	C19—C20—C21—C16	-1.3 (4)
C7—C8—C13—C14	-4.4 (3)	C13—C20—C21—C16	179.5 (2)
C12—C13—C14—C15	-149.2 (3)	C17—C16—C21—C20	0.3 (4)
C8—C13—C14—C15	35.7 (3)	C14—C16—C21—C20	-179.2 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C5—H5...C11	0.88 (3)	2.62 (3)	3.053 (4)	111 (2)
C9—H9...C11	0.88 (3)	2.66 (3)	3.039 (3)	107 (2)
C15—H15B...O4	0.94 (3)	2.46 (3)	2.841 (4)	103.8 (19)
C18—H18...O4 ⁱ	0.90 (3)	2.58 (3)	3.201 (3)	128 (2)

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

Fig. 1

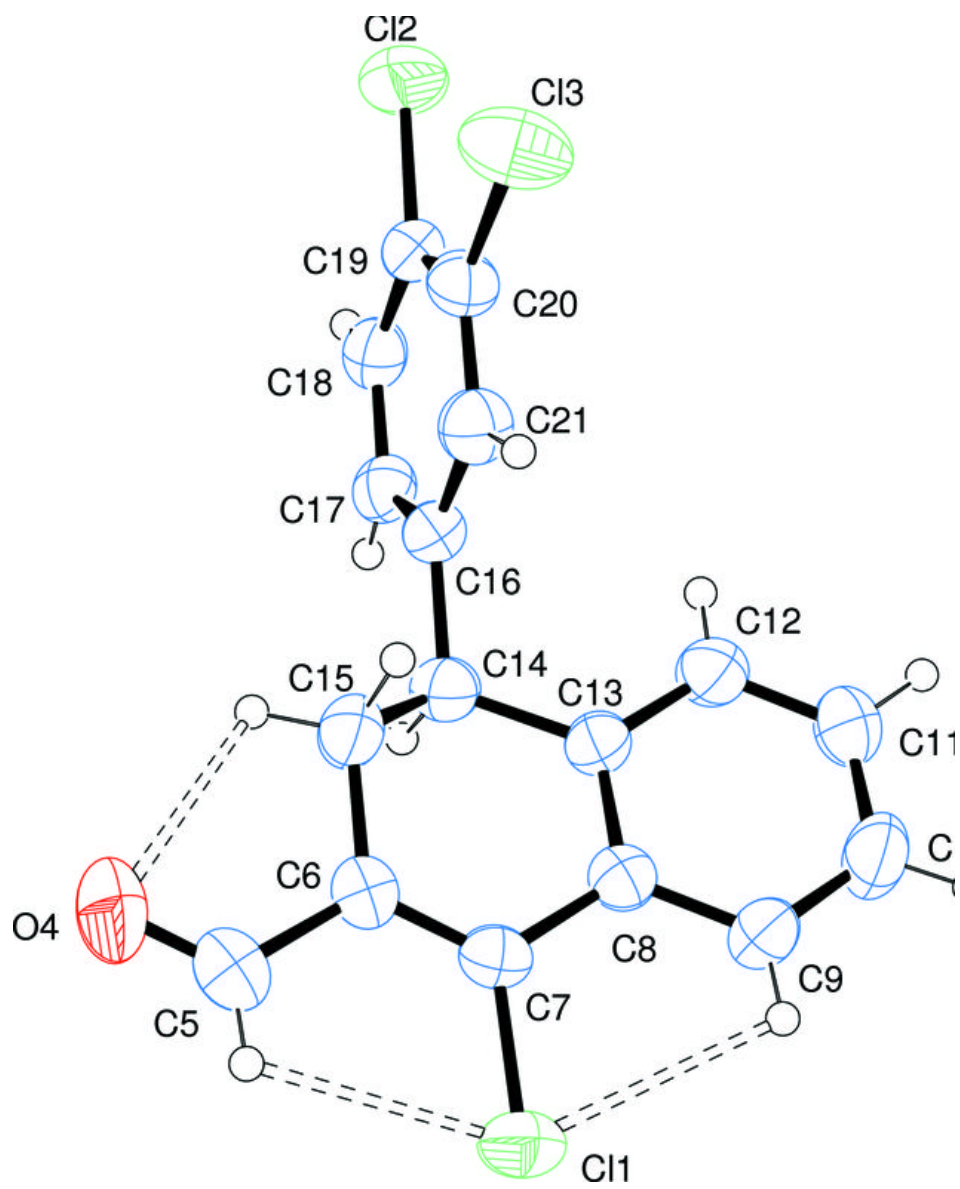


Fig. 2

