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2,4-Dichloro-7,8-dimethylquinoline

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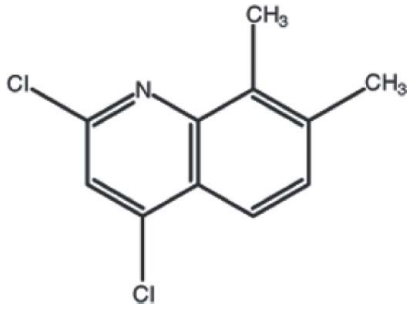
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.049; wR factor = 0.119; data-to-parameter ratio = 15.6.

There are two independent molecules in the asymmetric unit of the title compound, $C_{11}H_9Cl_2N$, both of which are essentially planar [maximum deviations of 0.072 (5) and 0.072 (7) Å]. In the crystal structure, weak π–π stacking interactions [centroid-centroid distances = 3.791 (3) Å and 3.855 (3) Å] link pairs of molecules.

Related literature

For the properties and applications of related compounds, see: Biavatti *et al.* (2002); Fournet *et al.* (1981); McCormick *et al.* (1996); Towers *et al.* (1981); Ziegler & Gelfert (1959). For similar crystal structures, see: Subashini *et al.* (2009); Somvanshi *et al.* (2008).



Experimental

Crystal data

$C_{11}H_9Cl_2N$
M_r = 226.09
Orthorhombic, $Pca2_1$
a = 20.3054 (9) Å
b = 3.9992 (2) Å
c = 25.5743 (11) Å
V = 2076.77 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 295 K
0.30 × 0.24 × 0.15 mm

Data collection

Oxford Xcalibur Eos (Nova) CCD detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2009)
T_{min} = 0.845, T_{max} = 0.918
19807 measured reflections
4009 independent reflections
2599 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.119
S = 0.94
4009 reflections
257 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1943 Friedel pairs
Flack parameter: 0.15 (10)

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2029).

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supplementary materials

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2,4-Dichloro-7,8-dimethylquinoline

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Comment

A wide range of medicinal properties have already been identified for compounds containing the quinoline ring system including antiprotozoal (Fournet *et al.*, 1981), antibacterial (Towers *et al.*, 1981), antifungal (Biavatti *et al.*, 2002) and antiviral activities (McCormick *et al.*, 1996). Reaction of aniline with malonic acid in an excess of phosphorus oxychloride at reflux to give 2,4-dichloroquinoline was first reported by Ziegler & Gelfert (1959). A similar derivative of quinoline was synthesized from the mixture of *p*-toluidine and malonic acid in a one-pot reaction from an aryl amine, malonic acid and phosphorous oxychloride and its cytotoxicity has been reported (Somvanshi *et al.*, 2008). Another derivative of quinoline prepared from *p*-anisidine and phosphorous oxychloride has been reported (Subashini *et al.*, 2009). In continuous of our work, the crystal structure of another derivative is reported in this paper.

The molecules A (Cl1/Cl2/N1/C1–C11) and B (Cl3/Cl4/N2/C12–C22) in the asymmetric unit of the title compound (I) are shown in Fig. 1. In both molecules A and B, the bond lengths and angles are comparable with those of similar structures (Somvanshi *et al.*, 2008; Subashini *et al.*, 2009). The molecules A and B are essentially planar, except the H atoms of their methyl groups, with maximum deviations of 0.072 (5)Å for C10 and 0.072 (7)Å for C21, respectively. Fitting of the non-H atoms of molecules A and B results in an r.m.s. fit of 0.063 Å). The least-squares plane through molecule A makes a dihedral angle of 56.72 (14)° with that of molecule B.

Weak intramolecular C—H···Cl and C—H···N interactions contribute to the stabilization of the molecular conformation of (I) (Table 1). In the crystal structure, weak π-π stacking interactions [*Cg*1···*Cg*2(*x*, 1 + *y*, *z*) = 3.791 (3) Å and *Cg*4···*Cg*5 (*x*, 1 + *y*, *z*) = 3.855 (3) Å; where *Cg*1, *Cg*2, *Cg*4 and *Cg*5 are centroids of the N1/C1–C4/C9, C4–C9, N2/C12–C15/C20 and C15–C20 rings, respectively] link pairs of molecules. In the structure, no classical hydrogen bonds are observed. Fig. 2 shows the crystal packing down the *b* axis.

Experimental

2,3-Dimethylaniline (10 mmol) and malonic acid (10 mmol) were heated under reflux in phosphorus oxychloride (30 ml), with stirring, for 5 h. The mixture was cooled, poured into crushed ice with vigorous stirring and then made alkaline with 5 *M* sodium hydroxide. Filtration gave the crude product as a brown solid. Column chromatography (95:5 hexane–EtOAc) yielded the pure 2,4-dichloro-7,8-dimethylquinoline. White needles of the synthesized compound have been grown from DMSO.

Refinement

H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å, for aromatic and methyl H and refined as a riding method, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

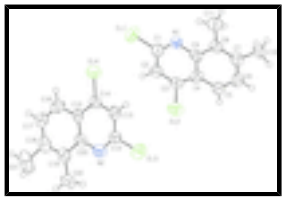

Fig. 1. View of the two molecules in the same asymmetric unit of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

Fig. 2. The molecular packing of (I) showing π-π stacking interactions (dashed lines) between the adjacent molecules down *b* axis. H atoms are omitted for clarity.

2,4-Dichloro-7,8-dimethylquinoline

Crystal data

$C_{11}H_9Cl_2N$	$F(000) = 928$
$M_r = 226.09$	$D_x = 1.446$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2ac	Cell parameters from 895 reflections
$a = 20.3054$ (9) Å	$\theta = 1.8–24.7°$
$b = 3.9992$ (2) Å	$\mu = 0.58$ mm^{-1}
$c = 25.5743$ (11) Å	$T = 295$ K
$V = 2076.77$ (17) Å^3	Needle, colourless
$Z = 8$	0.30 × 0.24 × 0.15 mm

Data collection

Oxford Xcalibur Eos (Nova) CCD detector diffractometer	4009 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2599 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.048$
ω scans	$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2009)	$h = -25\rightarrow25$
$T_{min} = 0.845$, $T_{max} = 0.918$	$k = -4\rightarrow4$
19807 measured reflections	$l = -31\rightarrow31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained

$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} < 0.001$
4009 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
257 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 1943 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.15 (10)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
Cl1	0.68230 (6)	0.6442 (5)	0.97181 (6)	0.0916 (6)
Cl2	0.50757 (6)	0.7463 (3)	0.81738 (5)	0.0709 (4)
N1	0.56446 (17)	0.4177 (12)	0.97981 (17)	0.0530 (12)
C1	0.6040 (3)	0.5681 (15)	0.9491 (2)	0.0630 (19)
C2	0.5891 (2)	0.6763 (11)	0.89752 (18)	0.0550 (16)
C3	0.5272 (2)	0.6141 (12)	0.88079 (17)	0.0490 (14)
C4	0.4813 (3)	0.4506 (11)	0.9111 (3)	0.0510 (19)
C5	0.4158 (2)	0.3859 (13)	0.8958 (2)	0.0593 (17)
C6	0.3744 (2)	0.2192 (11)	0.9295 (2)	0.0647 (17)
C7	0.3943 (2)	0.1131 (13)	0.9795 (2)	0.0623 (19)
C8	0.4577 (2)	0.1780 (10)	0.99705 (18)	0.0553 (17)
C9	0.50171 (19)	0.3483 (10)	0.96177 (17)	0.0477 (14)
C10	0.3437 (3)	−0.0425 (13)	1.0129 (2)	0.0640 (19)
C11	0.4804 (3)	0.0815 (14)	1.0504 (2)	0.074 (2)
Cl3	0.56576 (6)	1.1324 (5)	0.69164 (6)	0.0964 (6)
Cl4	0.73974 (6)	1.2634 (3)	0.84687 (5)	0.0694 (4)
N2	0.6857 (2)	0.9027 (12)	0.68457 (18)	0.0627 (17)
C12	0.6456 (3)	1.0586 (13)	0.7160 (2)	0.0540 (17)
C13	0.6582 (2)	1.1805 (11)	0.76636 (19)	0.0553 (16)
C14	0.7208 (2)	1.1269 (12)	0.78476 (17)	0.0500 (16)
C15	0.7689 (2)	0.9656 (10)	0.7534 (3)	0.0420 (18)
C16	0.8335 (3)	0.8998 (14)	0.7678 (2)	0.0620 (17)
C17	0.8766 (2)	0.7485 (11)	0.73560 (19)	0.0590 (17)
C18	0.8568 (2)	0.6444 (12)	0.6858 (2)	0.0610 (19)

C19	0.7928 (2)	0.6889 (10)	0.66826 (18)	0.0567 (17)
C20	0.74761 (19)	0.8565 (11)	0.70266 (17)	0.0507 (16)
C21	0.9046 (4)	0.4700 (17)	0.6447 (4)	0.112 (4)
C22	0.7674 (3)	0.5740 (13)	0.6163 (2)	0.0650 (19)
H2	0.62010	0.78320	0.87660	0.0660*
H5	0.40070	0.45540	0.86320	0.0710*
H6	0.33150	0.17480	0.91870	0.0780*
H10A	0.32250	0.12660	1.03360	0.0960*
H10B	0.36400	−0.20380	1.03550	0.0960*
H10C	0.31150	−0.15180	0.99130	0.0960*
H11A	0.46530	0.24420	1.07530	0.1120*
H11B	0.52760	0.07210	1.05100	0.1120*
H11C	0.46280	−0.13390	1.05930	0.1120*
H13	0.62630	1.29030	0.78600	0.0660*
H16	0.84760	0.96260	0.80100	0.0740*
H17	0.91970	0.71310	0.74650	0.0700*
H21A	0.90020	0.57790	0.61130	0.1670*
H21B	0.89310	0.23810	0.64140	0.1670*
H21C	0.94930	0.48880	0.65650	0.1670*
H22A	0.79460	0.66330	0.58900	0.0970*
H22B	0.72290	0.65090	0.61180	0.0970*
H22C	0.76820	0.33420	0.61490	0.0970*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0611 (8)	0.1339 (13)	0.0798 (10)	−0.0212 (8)	−0.0161 (7)	0.0013 (12)
Cl2	0.0827 (8)	0.0806 (7)	0.0495 (6)	0.0103 (6)	−0.0061 (6)	0.0020 (6)
N1	0.047 (2)	0.068 (2)	0.044 (2)	0.004 (2)	−0.0064 (19)	−0.008 (2)
C1	0.048 (3)	0.069 (3)	0.072 (4)	−0.003 (3)	−0.001 (3)	−0.013 (3)
C2	0.062 (3)	0.056 (3)	0.047 (2)	−0.002 (2)	0.005 (2)	−0.007 (2)
C3	0.060 (3)	0.048 (2)	0.039 (2)	0.006 (2)	0.000 (2)	−0.005 (2)
C4	0.052 (3)	0.041 (3)	0.060 (4)	0.009 (2)	−0.008 (3)	−0.020 (2)
C5	0.045 (3)	0.075 (3)	0.058 (3)	0.010 (3)	−0.003 (2)	−0.019 (3)
C6	0.046 (3)	0.067 (3)	0.081 (3)	0.007 (2)	−0.004 (2)	−0.016 (3)
C7	0.054 (3)	0.054 (3)	0.079 (4)	0.005 (3)	0.012 (3)	−0.016 (3)
C8	0.066 (3)	0.048 (3)	0.052 (3)	0.004 (2)	0.008 (2)	−0.012 (2)
C9	0.055 (2)	0.038 (2)	0.050 (3)	0.001 (2)	0.011 (2)	−0.012 (2)
C10	0.062 (4)	0.062 (3)	0.068 (3)	−0.004 (2)	0.018 (3)	−0.018 (3)
C11	0.088 (4)	0.067 (3)	0.068 (4)	0.002 (3)	−0.001 (3)	−0.004 (3)
Cl3	0.0610 (8)	0.1433 (13)	0.0848 (10)	0.0298 (9)	−0.0193 (7)	−0.0122 (13)
Cl4	0.0783 (7)	0.0777 (7)	0.0523 (6)	−0.0045 (6)	−0.0028 (6)	−0.0053 (6)
N2	0.067 (3)	0.067 (3)	0.054 (3)	0.006 (2)	−0.002 (2)	−0.002 (3)
C12	0.046 (3)	0.073 (3)	0.043 (3)	0.005 (2)	−0.002 (2)	−0.006 (3)
C13	0.042 (2)	0.061 (3)	0.063 (3)	0.008 (2)	0.005 (2)	0.002 (2)
C14	0.058 (3)	0.047 (3)	0.045 (2)	−0.003 (2)	0.006 (2)	0.002 (2)
C15	0.034 (3)	0.039 (2)	0.053 (4)	0.0013 (16)	0.004 (3)	0.0138 (19)
C16	0.070 (3)	0.057 (3)	0.059 (3)	−0.014 (3)	−0.009 (3)	0.004 (3)

C17	0.050 (3)	0.060 (3)	0.067 (3)	−0.001 (2)	−0.004 (2)	0.006 (3)
C18	0.060 (3)	0.043 (3)	0.080 (4)	−0.001 (2)	0.016 (3)	0.018 (3)
C19	0.063 (3)	0.049 (3)	0.058 (3)	−0.008 (2)	0.007 (2)	0.011 (2)
C20	0.047 (2)	0.054 (3)	0.051 (3)	0.000 (2)	0.009 (2)	0.007 (2)
C21	0.084 (5)	0.086 (5)	0.166 (8)	0.018 (3)	0.056 (5)	0.007 (4)
C22	0.084 (4)	0.072 (3)	0.039 (3)	0.016 (3)	0.007 (3)	−0.002 (3)

Geometric parameters (Å, °)

Cl1—C1	1.720 (6)	C10—H10C	0.9600
Cl2—C3	1.752 (5)	C11—H11B	0.9600
Cl3—C12	1.762 (6)	C11—H11C	0.9600
Cl4—C14	1.723 (5)	C11—H11A	0.9600
N1—C9	1.383 (5)	C12—C13	1.401 (7)
N1—C1	1.274 (7)	C13—C14	1.372 (6)
N2—C20	1.352 (6)	C14—C15	1.419 (7)
N2—C12	1.303 (7)	C15—C16	1.388 (7)
C1—C2	1.421 (7)	C15—C20	1.436 (8)
C2—C3	1.351 (6)	C16—C17	1.345 (7)
C3—C4	1.377 (8)	C17—C18	1.399 (7)
C4—C5	1.410 (7)	C18—C19	1.386 (6)
C4—C9	1.421 (8)	C18—C21	1.592 (10)
C5—C6	1.376 (7)	C19—C20	1.437 (6)
C6—C7	1.407 (7)	C19—C22	1.498 (7)
C7—C10	1.474 (7)	C13—H13	0.9300
C7—C8	1.388 (6)	C16—H16	0.9300
C8—C11	1.491 (7)	C17—H17	0.9300
C8—C9	1.441 (6)	C21—H21A	0.9600
C2—H2	0.9300	C21—H21B	0.9600
C5—H5	0.9300	C21—H21C	0.9600
C6—H6	0.9300	C22—H22A	0.9600
C10—H10A	0.9600	C22—H22B	0.9600
C10—H10B	0.9600	C22—H22C	0.9600
Cl1···H22A^{i}	3.0300	H5···H16^{iii}	2.5500
Cl2···H5	2.7300	H6···H10C	2.3100
Cl2···H13^{ii}	3.1300	H6···Cl4^{iii}	3.1500
Cl2···H17^{iii}	3.1400	H10A···C22^{viii}	3.0400
Cl3···H21C^{iv}	2.9500	H10A···H22B^{viii}	2.3800
Cl4···H6^{v}	3.1500	H10B···C11	2.6500
Cl4···H16	2.7600	H10B···H11C	2.1200
N1···H11B	2.4100	H10C···H6	2.3100
N2···H22B	2.2500	H11A···H11C^{vi}	2.5200
C3···C4^{vi}	3.558 (7)	H11B···N1	2.4100
C4···C3^{ii}	3.558 (7)	H11C···H11A^{ii}	2.5200
C5···C6^{vi}	3.543 (7)	H11C···C10	2.7200
C6···C5^{ii}	3.543 (7)	H11C···H10B	2.1200
C8···C9^{ii}	3.553 (6)	H13···Cl2^{vi}	3.1300

C9···C8^{vi}	3.553 (6)	H16···Cl4	2.7600
C14···C15^{vi}	3.584 (6)	H16···H5^{v}	2.5500
C15···C14^{ii}	3.584 (6)	H17···H21C	2.5400
C18···C21^{vi}	3.598 (9)	H17···Cl2^{v}	3.1400
C19···C20^{ii}	3.563 (6)	H21A···C22	2.7000
C20···C19^{vi}	3.563 (6)	H21A···H22A	2.2400
C21···C18^{ii}	3.598 (9)	H21B···C18^{ii}	2.7300
C10···H11C	2.7200	H21B···C19^{ii}	3.0700
C11···H10B	2.6500	H21B···C21^{ii}	3.0800
C18···H21B^{vi}	2.7300	H21B···C22	2.9500
C19···H21B^{vi}	3.0700	H21C···H17	2.5400
C19···H22C^{vi}	2.9600	H21C···Cl3^{ix}	2.9500
C20···H22C^{vi}	2.9800	H22A···C21	2.7600
C21···H21B^{vi}	3.0800	H22A···H21A	2.2400
C21···H22C	2.9200	H22A···Cl1^{x}	3.0300
C21···H22A	2.7600	H22B···N2	2.2500
C22···H22C^{vi}	3.0400	H22B···H10A^{vii}	2.3800
C22···H10A^{vii}	3.0400	H22C···C19^{ii}	2.9600
C22···H21B	2.9500	H22C···C20^{ii}	2.9800
C22···H21A	2.7000	H22C···C21	2.9200
H5···Cl2	2.7300	H22C···C22^{ii}	3.0400
C1—N1—C9	118.0 (4)	H11A—C11—H11B	110.00
C12—N2—C20	115.8 (5)	Cl3—C12—N2	115.9 (4)
Cl1—C1—N1	117.3 (4)	Cl3—C12—C13	115.8 (4)
N1—C1—C2	125.6 (5)	N2—C12—C13	128.3 (5)
Cl1—C1—C2	117.2 (4)	C12—C13—C14	115.5 (4)
C1—C2—C3	115.9 (4)	Cl4—C14—C13	118.3 (3)
Cl2—C3—C2	116.7 (3)	Cl4—C14—C15	120.8 (4)
C2—C3—C4	122.6 (5)	C13—C14—C15	121.0 (4)
Cl2—C3—C4	120.7 (4)	C14—C15—C16	125.9 (6)
C3—C4—C5	124.7 (6)	C14—C15—C20	116.2 (4)
C5—C4—C9	118.4 (5)	C16—C15—C20	117.8 (5)
C3—C4—C9	116.9 (5)	C15—C16—C17	122.5 (5)
C4—C5—C6	119.4 (5)	C16—C17—C18	120.3 (4)
C5—C6—C7	122.7 (4)	C17—C18—C19	121.7 (4)
C6—C7—C8	120.3 (4)	C17—C18—C21	123.8 (5)
C6—C7—C10	117.0 (4)	C19—C18—C21	114.5 (5)
C8—C7—C10	122.6 (5)	C18—C19—C20	117.4 (4)
C7—C8—C9	117.5 (4)	C18—C19—C22	124.8 (4)
C7—C8—C11	122.3 (4)	C20—C19—C22	117.8 (4)
C9—C8—C11	120.2 (4)	N2—C20—C15	123.2 (4)
N1—C9—C8	117.2 (4)	N2—C20—C19	116.6 (4)
C4—C9—C8	121.8 (4)	C15—C20—C19	120.2 (4)
N1—C9—C4	121.0 (4)	C12—C13—H13	122.00
C3—C2—H2	122.00	C14—C13—H13	122.00

C1—C2—H2	122.00	C15—C16—H16	119.00
C4—C5—H5	120.00	C17—C16—H16	119.00
C6—C5—H5	120.00	C16—C17—H17	120.00
C7—C6—H6	119.00	C18—C17—H17	120.00
C5—C6—H6	119.00	C18—C21—H21A	109.00
C7—C10—H10A	110.00	C18—C21—H21B	109.00
C7—C10—H10B	109.00	C18—C21—H21C	110.00
H10A—C10—H10B	110.00	H21A—C21—H21B	109.00
H10A—C10—H10C	109.00	H21A—C21—H21C	109.00
C7—C10—H10C	109.00	H21B—C21—H21C	109.00
H10B—C10—H10C	109.00	C19—C22—H22A	109.00
C8—C11—H11B	109.00	C19—C22—H22B	109.00
C8—C11—H11C	110.00	C19—C22—H22C	110.00
C8—C11—H11A	109.00	H22A—C22—H22B	110.00
H11A—C11—H11C	109.00	H22A—C22—H22C	110.00
H11B—C11—H11C	109.00	H22B—C22—H22C	109.00
C9—N1—C1—Cl1	−178.7 (4)	C7—C8—C9—C4	0.7 (6)
C9—N1—C1—C2	0.8 (8)	C11—C8—C9—N1	−0.4 (6)
C1—N1—C9—C4	−1.9 (7)	C11—C8—C9—C4	−178.6 (4)
C1—N1—C9—C8	180.0 (5)	C7—C8—C9—N1	178.9 (4)
C20—N2—C12—Cl3	177.8 (4)	Cl3—C12—C13—C14	−179.0 (4)
C20—N2—C12—C13	−0.9 (8)	N2—C12—C13—C14	−0.3 (8)
C12—N2—C20—C15	0.8 (7)	C12—C13—C14—Cl4	−178.9 (4)
C12—N2—C20—C19	−179.2 (4)	C12—C13—C14—C15	1.5 (7)
N1—C1—C2—C3	0.7 (8)	Cl4—C14—C15—C16	0.2 (7)
Cl1—C1—C2—C3	−179.8 (4)	Cl4—C14—C15—C20	178.9 (3)
C1—C2—C3—Cl2	179.8 (4)	C13—C14—C15—C16	179.7 (5)
C1—C2—C3—C4	−1.2 (7)	C13—C14—C15—C20	−1.6 (7)
Cl2—C3—C4—C5	−2.4 (7)	C14—C15—C16—C17	−179.3 (5)
Cl2—C3—C4—C9	179.2 (3)	C20—C15—C16—C17	2.0 (8)
C2—C3—C4—C9	0.2 (7)	C14—C15—C20—N2	0.3 (7)
C2—C3—C4—C5	178.7 (5)	C14—C15—C20—C19	−179.6 (4)
C3—C4—C5—C6	179.9 (5)	C16—C15—C20—N2	179.2 (5)
C9—C4—C5—C6	−1.7 (7)	C16—C15—C20—C19	−0.8 (7)
C5—C4—C9—C8	0.9 (7)	C15—C16—C17—C18	−1.3 (8)
C3—C4—C9—N1	1.4 (7)	C16—C17—C18—C19	−0.8 (7)
C3—C4—C9—C8	179.4 (4)	C16—C17—C18—C21	178.8 (5)
C5—C4—C9—N1	−177.2 (4)	C17—C18—C19—C20	1.9 (7)
C4—C5—C6—C7	1.0 (7)	C17—C18—C19—C22	−177.8 (4)
C5—C6—C7—C10	176.0 (5)	C21—C18—C19—C20	−177.7 (4)
C5—C6—C7—C8	0.7 (7)	C21—C18—C19—C22	2.6 (7)
C6—C7—C8—C9	−1.5 (7)	C18—C19—C20—N2	178.9 (4)
C6—C7—C8—C11	177.8 (4)	C18—C19—C20—C15	−1.1 (6)
C10—C7—C8—C9	−176.5 (4)	C22—C19—C20—N2	−1.3 (6)
C10—C7—C8—C11	2.8 (7)	C22—C19—C20—C15	178.7 (4)

Symmetry codes: (i) −*x*+3/2, *y*, *z*+1/2; (ii) *x*, *y*−1, *z*; (iii) *x*−1/2, −*y*+1, *z*; (iv) *x*−1/2, −*y*+2, *z*; (v) *x*+1/2, −*y*+1, *z*; (vi) *x*, *y*+1, *z*; (vii) −*x*+1, −*y*+1, *z*−1/2; (viii) −*x*+1, −*y*+1, *z*+1/2; (ix) *x*+1/2, −*y*+2, *z*; (x) −*x*+3/2, *y*, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Cl2	0.93	2.73	3.094 (5)	104
C11—H11B···N1	0.96	2.41	2.825 (7)	106
C16—H16···Cl4	0.93	2.76	3.135 (6)	105
C22—H22B···N2	0.96	2.25	2.744 (7)	111

Fig. 1

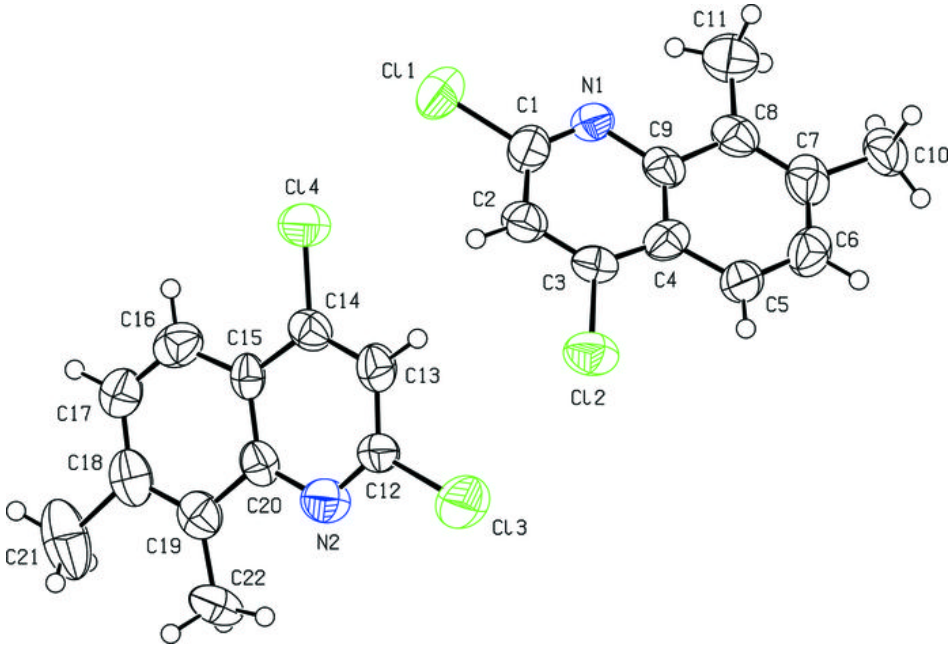
C11
Cl1
N1
C1
C9
C8
C7
C10
C2
C6
C3
C4
C5
Cl2
Cl4
C14
C16
C15
C13
C17
C18
C20
C12
Cl3
N2
C21
C19
C22

Fig. 2