Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(7,10-dichloro-2-methoxybenzo[*b*]-[1,5]naphthyridinium) chloride perchlorate

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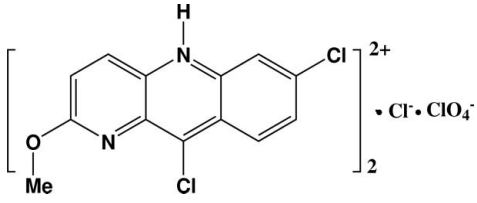
Received 15 June 2007; accepted 6 July 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.052; wR factor = 0.125; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, $2C_{13}H_9Cl_2N_2O^+\cdot Cl^-\cdot ClO_4^-$, contains two cations, one chloride ion and one perchlorate ion. Intermolecular N—H···Cl hydrogen bonds link the cations and anions to form clusters of two cations and a chloride anion. In the crystal packing, the ClO_4^- anions bridge neighboring clusters to form a three-dimensional network structure. The relatively short distances $Cg1\cdots Cg1^{i}$ of 3.664 (3) Å [where $Cg1$ is the centroid of the central six-membered ring of the organic cation and (i) is $1-x$, $1-y$, $1-z$] are indicative of weak $\pi\cdots\pi$ interactions contributing to the stabilization of the crystal packing.

Related literature

For a large number of derivatives belonging to the general class of anilinoacridines, see: Anderson *et al.* (2006); Ferlin *et al.* (2000) and Gamage *et al.* (1994).



Experimental

Crystal data

$2C_{13}H_9Cl_2N_2O^+\cdot Cl^-\cdot ClO_4^-$
M_r = 695.14
Monoclinic, $P2_1/n$
a = 7.944 (1) Å
b = 33.972 (5) Å
c = 11.292 (2) Å
β = 107.511 (2)°
V = 2905.9 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.83, T_{max} = 0.86
15872 measured reflections
5707 independent reflections
4631 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.125
S = 1.09
5707 reflections
387 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl6	0.86 (4)	2.13 (4)	2.978 (3)	169 (3)
N4—H4A···Cl6	0.86 (4)	2.21 (4)	3.055 (3)	169 (3)
C9—H9···O6^{i}	0.93	2.53	3.295 (4)	140
C9—H9···O7^{i}	0.93	2.66	3.453 (4)	143
C22—H22···O8^{ii}	0.93	2.39	3.124 (4)	136
C15—H15···O8	0.93	2.48	3.341 (4)	155
C16—H16···O7	0.93	2.64	3.327 (5)	132

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The author is grateful to the Starter Fund of Southeast University for financial support towards the purchase of the CCD X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2024).

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  doi:10.1107/S1600536807033193

supplementary materials

Acta Cryst. (2007). E**63**, o3430 [**doi:10.1107/S1600536807033193**]

Bis(7,10-dichloro-2-methoxybenzo[*b*][1,5]naphthyridinium) chloride perchlorate

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Comment

During the last 20–30 years a large number of derivatives belonging to the general class of anilinoacridines have been prepared and evaluated extensively as antimalarial, antileishmanial, antitrypanosomal and anticancer agents (Anderson, *et al.*, 2006; Ferlin, *et al.*, 2000; Gamage, *et al.*, 1994). Herein we report the crystal structure of the title compound (I) which is the main precursor used to synthesize anilinoacridine derivatives.

The crystal data show that in the title compound, $(C_{13}H_9Cl_2N_2O)_2(Cl)(ClO_4)$, the asymmetric unit of (I) contains two identical cations as well as one Cl^- and one ClO_4^- anion as counter anions. Intermolecular hydrogen bonds [N2—H2A···Cl6; N4—H4A···Cl6] link them to form a dimer (Fig. 1). In the crystal packing the ClO_4^- anion plays an important role linking neighboring dimers to form a three-dimensional network structure (Fig.2). Relatively short $Cg1\cdots Cg1^{i}$ distances of 3.664 (3) Å [*Cg*1 is the centroid of ring A (N2/C4/C5/C10/C11/C12)] are indicative of weak π···π interactions contributing to the stabilization of the crystal packing [symmetry codes: (i) $1-x,1-y,1-z$].

Experimental

2,4-dichlorobenzoic acid (1 mmol) and 6-methoxypyridin-3-amine (1 mmol, 0.124 g) in 40 ml 2-propanol were refluxed at 140°C for 3 h affording a pale yellow precipitate. By filtering the solution we obtained the intermediate ready for the next step (Anderson *et al.*, 2006). The intermediate was then reacted with PCl_3 at 80°C for additional 3 h. Then the solution was poured into ice water affording a yellow precipitate. After being cooled down to room temperature, the solution was filtered. The yellow solids were washed with water and finally recrystallized from acetone yielding block shaped colorless crystals of compound I.

Refinement

H atoms bonded to N atoms were located in a difference map and refined with distance restraints of N—H = 0.86 (4) Å, and with $U_{iso}(H) = 1.2U_{eq}(N)$. Other H atoms were positioned geometrically and refined using a riding model (including free rotation about the methanol C—C bond), with C—H = 0.93—0.96 Å and with $U_{iso}(H) = 1.2$(1.5 for methyl groups) times $U_{eq}(C)$.

Figures

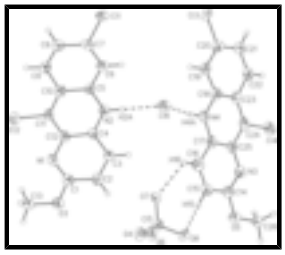


Fig. 1. The structure of the asymmetric unit, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. All the H atoms except H9, H15, H16 and H22 have been omitted for clarity.

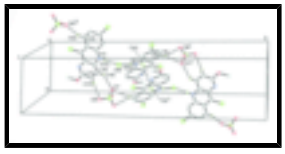


Fig. 2. View of the intermolecular hydrogen bonds and weak π···π interactions down *c* axis [symmetry codes: (i) 1 − *x*,1 − *y*,1 − *z*; (ii) −3/2 + *x*,1/2 − *y*,-1/2 + *x*].

Bis(7,10-dichloro-2-methoxybenzo[*b*][1,5]naphthyridinium) chloride perchlorate

Crystal data

$2C_{13}H_9Cl_2N_2O^+\cdot Cl^-\cdot ClO_4^-$	F_{000} = 1408
M_r = 695.14	D_x = 1.589 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2483 reflections
a = 7.944 (1) Å	θ = 2.6–20.8º
b = 33.972 (5) Å	μ = 0.64 mm^{-1}
c = 11.292 (2) Å	*T* = 291 (2) K
β = 107.511 (2)º	Block, colourless
V = 2905.9 (7) Å^3	0.30 × 0.26 × 0.24 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5707 independent reflections
Radiation source: sealed tube	4631 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −9→9
T_{min} = 0.83, T_{max} = 0.86	*k* = −33→41
15872 measured reflections	*l* = −13→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.125$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.99P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
5707 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
387 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
C1	0.6140 (5)	0.43021 (10)	0.7364 (3)	0.0539 (8)
C2	0.5768 (5)	0.40037 (10)	0.6408 (3)	0.0554 (8)
H2	0.6354	0.3763	0.6543	0.067*
C3	0.4540 (4)	0.40846 (10)	0.5306 (3)	0.0540 (8)
H3	0.4294	0.3903	0.4660	0.065*
C4	0.3638 (4)	0.44505 (9)	0.5156 (3)	0.0462 (7)
C5	0.1587 (4)	0.48925 (9)	0.3868 (3)	0.0471 (7)
C6	0.0365 (4)	0.49704 (10)	0.2711 (3)	0.0531 (8)
H6	0.0114	0.4782	0.2083	0.064*
C7	−0.0445 (4)	0.53268 (11)	0.2525 (3)	0.0564 (9)
C8	−0.0108 (4)	0.56188 (10)	0.3500 (3)	0.0527 (8)
H8	−0.0716	0.5857	0.3352	0.063*
C9	0.1064 (4)	0.55524 (9)	0.4609 (3)	0.0497 (7)
H9	0.1270	0.5744	0.5226	0.060*
C10	0.2016 (4)	0.51805 (9)	0.4853 (3)	0.0466 (7)
C11	0.3271 (4)	0.50868 (9)	0.5972 (3)	0.0492 (7)
C12	0.4115 (4)	0.47234 (9)	0.6160 (3)	0.0437 (7)
C13	0.7692 (5)	0.44844 (12)	0.9444 (3)	0.0644 (10)
H13A	0.6603	0.4546	0.9606	0.097*
H13B	0.8189	0.4720	0.9221	0.097*
H13C	0.8503	0.4372	1.0175	0.097*

C14	0.4137 (5)	0.22930 (10)	0.3372 (3)	0.0539 (8)
C15	0.4782 (5)	0.26862 (11)	0.3520 (3)	0.0571 (8)
H15	0.5966	0.2737	0.3927	0.068*
C16	0.3658 (5)	0.29848 (12)	0.3065 (3)	0.0612 (9)
H16	0.4029	0.3246	0.3140	0.073*
C17	0.1844 (4)	0.28774 (10)	0.2453 (3)	0.0495 (7)
C18	−0.1062 (4)	0.30885 (10)	0.1355 (3)	0.0512 (8)
C19	−0.2228 (5)	0.34054 (10)	0.0994 (3)	0.0546 (8)
H19	−0.1847	0.3665	0.1143	0.066*
C20	−0.3982 (5)	0.33131 (11)	0.0402 (4)	0.0609 (9)
C21	−0.4638 (5)	0.29252 (11)	0.0251 (3)	0.0569 (8)
H21	−0.5826	0.2878	−0.0149	0.068*
C22	−0.3486 (5)	0.26132 (11)	0.0709 (4)	0.0621 (9)
H22	−0.3908	0.2356	0.0633	0.075*
C23	−0.1634 (5)	0.26903 (10)	0.1302 (3)	0.0513 (8)
C24	−0.0407 (5)	0.23928 (10)	0.1797 (3)	0.0579 (9)
C25	0.1374 (5)	0.24841 (10)	0.2374 (3)	0.0499 (7)
C26	0.4847 (5)	0.16054 (10)	0.3696 (3)	0.0571 (8)
H26A	0.3919	0.1557	0.4060	0.086*
H26B	0.5838	0.1440	0.4086	0.086*
H26C	0.4431	0.1548	0.2824	0.086*
Cl1	−0.19461 (12)	0.54375 (3)	0.11131 (9)	0.0644 (3)
Cl2	0.38505 (13)	0.54239 (3)	0.71456 (9)	0.0647 (3)
Cl3	−0.54565 (12)	0.36936 (3)	−0.01420 (9)	0.0651 (3)
Cl4	−0.10915 (12)	0.19125 (3)	0.16924 (9)	0.0628 (2)
Cl5	0.88340 (11)	0.34019 (2)	0.45436 (8)	0.0549 (2)
Cl6	0.17575 (11)	0.40244 (3)	0.18450 (8)	0.0579 (2)
N1	0.5355 (4)	0.46412 (8)	0.7254 (2)	0.0480 (6)
N2	0.2435 (4)	0.45403 (8)	0.4072 (3)	0.0478 (6)
H2A	0.219 (5)	0.4369 (11)	0.348 (3)	0.057*
N3	0.2544 (4)	0.21900 (8)	0.2831 (3)	0.0550 (7)
N4	0.0660 (4)	0.31670 (9)	0.1966 (3)	0.0519 (7)
H4A	0.101 (5)	0.3408 (11)	0.205 (3)	0.062*
O3	0.7353 (3)	0.41992 (7)	0.8414 (2)	0.0629 (6)
O4	0.9062 (4)	0.33980 (8)	0.5734 (2)	0.0685 (7)
O5	0.5383 (3)	0.20162 (8)	0.3877 (2)	0.0626 (6)
O6	1.0101 (4)	0.36333 (7)	0.4258 (2)	0.0676 (7)
O7	0.7177 (3)	0.35640 (8)	0.4075 (2)	0.0712 (8)
O8	0.8922 (3)	0.30120 (7)	0.4116 (2)	0.0567 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.055 (2)	0.056 (2)	0.0471 (18)	−0.0052 (16)	0.0096 (15)	0.0004 (15)
C2	0.064 (2)	0.0474 (18)	0.0551 (19)	−0.0029 (15)	0.0187 (16)	−0.0069 (15)
C3	0.0476 (18)	0.0488 (18)	0.059 (2)	0.0046 (14)	0.0056 (15)	−0.0055 (15)
C4	0.0393 (16)	0.0394 (16)	0.0562 (18)	−0.0064 (12)	0.0085 (14)	−0.0083 (14)
C5	0.0395 (16)	0.0426 (17)	0.0602 (19)	0.0011 (13)	0.0167 (14)	−0.0054 (14)

C6	0.0460 (18)	0.0544 (19)	0.0561 (19)	0.0122 (14)	0.0112 (15)	0.0081 (15)
C7	0.0414 (18)	0.062 (2)	0.059 (2)	0.0038 (15)	0.0043 (15)	0.0140 (17)
C8	0.0513 (19)	0.0474 (18)	0.061 (2)	−0.0017 (14)	0.0188 (16)	0.0103 (15)
C9	0.0568 (19)	0.0342 (15)	0.0593 (19)	−0.0016 (13)	0.0193 (16)	0.0084 (14)
C10	0.0489 (18)	0.0340 (15)	0.0600 (19)	−0.0065 (13)	0.0212 (15)	−0.0028 (13)
C11	0.0505 (18)	0.0419 (17)	0.0517 (18)	−0.0069 (14)	0.0101 (14)	−0.0054 (14)
C12	0.0446 (17)	0.0432 (16)	0.0465 (17)	−0.0086 (13)	0.0184 (13)	−0.0057 (13)
C13	0.055 (2)	0.065 (2)	0.063 (2)	0.0072 (17)	0.0019 (17)	−0.0048 (18)
C14	0.0507 (19)	0.057 (2)	0.0524 (19)	0.0038 (15)	0.0128 (15)	0.0017 (15)
C15	0.0501 (19)	0.062 (2)	0.054 (2)	−0.0067 (16)	0.0079 (15)	−0.0010 (16)
C16	0.060 (2)	0.064 (2)	0.059 (2)	−0.0079 (18)	0.0166 (17)	−0.0032 (17)
C17	0.0500 (18)	0.0475 (18)	0.0536 (19)	−0.0093 (14)	0.0194 (15)	−0.0120 (14)
C18	0.0525 (19)	0.0485 (18)	0.0573 (19)	−0.0027 (14)	0.0237 (16)	−0.0104 (15)
C19	0.058 (2)	0.0535 (19)	0.057 (2)	−0.0020 (16)	0.0251 (16)	−0.0129 (16)
C20	0.054 (2)	0.059 (2)	0.071 (2)	0.0121 (16)	0.0199 (18)	−0.0052 (18)
C21	0.053 (2)	0.062 (2)	0.0509 (19)	0.0007 (16)	0.0082 (15)	−0.0106 (16)
C22	0.055 (2)	0.055 (2)	0.071 (2)	−0.0099 (16)	0.0108 (17)	−0.0195 (18)
C23	0.057 (2)	0.0504 (19)	0.0482 (18)	−0.0100 (15)	0.0176 (15)	−0.0142 (14)
C24	0.066 (2)	0.0466 (19)	0.060 (2)	−0.0155 (16)	0.0166 (17)	−0.0145 (15)
C25	0.058 (2)	0.0487 (18)	0.0430 (17)	−0.0003 (15)	0.0148 (14)	−0.0057 (14)
C26	0.055 (2)	0.053 (2)	0.060 (2)	0.0063 (15)	0.0106 (16)	−0.0039 (16)
Cl1	0.0581 (5)	0.0611 (5)	0.0603 (5)	0.0229 (4)	−0.0031 (4)	0.0164 (4)
Cl2	0.0639 (6)	0.0605 (5)	0.0655 (5)	−0.0015 (4)	0.0132 (4)	−0.0174 (4)
Cl3	0.0613 (5)	0.0599 (5)	0.0729 (6)	0.0212 (4)	0.0183 (4)	−0.0141 (4)
Cl4	0.0583 (5)	0.0550 (5)	0.0700 (6)	−0.0195 (4)	0.0115 (4)	−0.0077 (4)
Cl5	0.0589 (5)	0.0539 (5)	0.0546 (5)	0.0103 (4)	0.0213 (4)	−0.0095 (4)
Cl6	0.0565 (5)	0.0559 (5)	0.0556 (5)	0.0088 (4)	0.0082 (4)	0.0090 (4)
N1	0.0489 (15)	0.0534 (16)	0.0408 (14)	−0.0068 (12)	0.0119 (12)	−0.0074 (11)
N2	0.0470 (15)	0.0439 (15)	0.0495 (15)	0.0007 (11)	0.0100 (12)	−0.0003 (12)
N3	0.0542 (17)	0.0493 (16)	0.0591 (17)	0.0002 (13)	0.0133 (13)	−0.0021 (13)
N4	0.0541 (17)	0.0540 (17)	0.0455 (15)	−0.0056 (13)	0.0119 (12)	−0.0108 (13)
O3	0.0684 (16)	0.0528 (14)	0.0554 (14)	0.0090 (12)	0.0001 (12)	0.0033 (11)
O4	0.0756 (18)	0.0705 (17)	0.0610 (16)	0.0110 (13)	0.0229 (13)	−0.0152 (13)
O5	0.0537 (14)	0.0634 (15)	0.0628 (15)	0.0107 (12)	0.0056 (11)	0.0031 (12)
O6	0.0681 (16)	0.0607 (16)	0.0749 (17)	−0.0193 (13)	0.0228 (13)	−0.0239 (13)
O7	0.0613 (15)	0.0619 (15)	0.0660 (16)	0.0168 (12)	−0.0176 (12)	−0.0235 (12)
O8	0.0597 (14)	0.0455 (12)	0.0626 (14)	0.0144 (10)	0.0148 (11)	−0.0057 (11)

Geometric parameters (Å, °)

C1—N1	1.298 (4)	C15—H15	0.9300
C1—O3	1.330 (4)	C16—C17	1.445 (5)
C1—C2	1.445 (5)	C16—H16	0.9300
C2—C3	1.358 (5)	C17—N4	1.358 (4)
C2—H2	0.9300	C17—C25	1.383 (4)
C3—C4	1.419 (4)	C18—N4	1.360 (4)
C3—H3	0.9300	C18—C19	1.398 (5)
C4—N2	1.342 (4)	C18—C23	1.422 (5)
C4—C12	1.424 (4)	C19—C20	1.388 (5)

C5—N2	1.358 (4)	C19—H19	0.9300
C5—C6	1.399 (5)	C20—C21	1.408 (5)
C5—C10	1.442 (4)	C20—Cl3	1.728 (4)
C6—C7	1.358 (5)	C21—C22	1.394 (5)
C6—H6	0.9300	C21—H21	0.9300
C7—C8	1.445 (5)	C22—C23	1.445 (5)
C7—Cl1	1.721 (3)	C22—H22	0.9300
C8—C9	1.336 (5)	C23—C24	1.399 (5)
C8—H8	0.9300	C24—C25	1.402 (5)
C9—C10	1.456 (4)	C24—Cl4	1.713 (3)
C9—H9	0.9300	C25—N3	1.356 (4)
C10—C11	1.391 (5)	C26—O5	1.455 (4)
C11—C12	1.390 (4)	C26—H26A	0.9600
C11—Cl2	1.707 (3)	C26—H26B	0.9600
C12—N1	1.357 (4)	C26—H26C	0.9600
C13—O3	1.475 (4)	Cl5—O4	1.301 (3)
C13—H13A	0.9600	Cl5—O7	1.377 (2)
C13—H13B	0.9600	Cl5—O6	1.389 (3)
C13—H13C	0.9600	Cl5—O8	1.419 (2)
C14—N3	1.278 (4)	Cl6—N2	2.978 (3)
C14—O5	1.359 (4)	Cl6—N4	3.055 (3)
C14—C15	1.422 (5)	N2—H2A	0.86 (4)
C15—C16	1.347 (5)	N4—H4A	0.86 (4)
N1—C1—O3	121.1 (3)	C25—C17—C16	119.1 (3)
N1—C1—C2	124.5 (3)	N4—C18—C19	118.3 (3)
O3—C1—C2	114.3 (3)	N4—C18—C23	117.9 (3)
C3—C2—C1	118.1 (3)	C19—C18—C23	123.0 (3)
C3—C2—H2	120.9	C20—C19—C18	116.6 (3)
C1—C2—H2	120.9	C20—C19—H19	121.7
C2—C3—C4	119.0 (3)	C18—C19—H19	121.7
C2—C3—H3	120.5	C19—C20—C21	123.4 (3)
C4—C3—H3	120.5	C19—C20—Cl3	118.5 (3)
N2—C4—C3	120.2 (3)	C21—C20—Cl3	118.1 (3)
N2—C4—C12	121.6 (3)	C22—C21—C20	119.3 (3)
C3—C4—C12	118.1 (3)	C22—C21—H21	120.4
N2—C5—C6	119.6 (3)	C20—C21—H21	120.4
N2—C5—C10	118.5 (3)	C21—C22—C23	119.8 (3)
C6—C5—C10	121.9 (3)	C21—C22—H22	120.1
C7—C6—C5	118.5 (3)	C23—C22—H22	120.1
C7—C6—H6	120.8	C24—C23—C18	119.7 (3)
C5—C6—H6	120.8	C24—C23—C22	123.0 (3)
C6—C7—C8	121.6 (3)	C18—C23—C22	117.4 (3)
C6—C7—Cl1	120.1 (3)	C23—C24—C25	120.7 (3)
C8—C7—Cl1	118.3 (3)	C23—C24—Cl4	119.5 (3)
C9—C8—C7	121.0 (3)	C25—C24—Cl4	119.9 (3)
C9—C8—H8	119.5	N3—C25—C17	123.1 (3)
C7—C8—H8	119.5	N3—C25—C24	119.6 (3)
C8—C9—C10	120.0 (3)	C17—C25—C24	117.3 (3)
C8—C9—H9	120.0	O5—C26—H26A	109.5

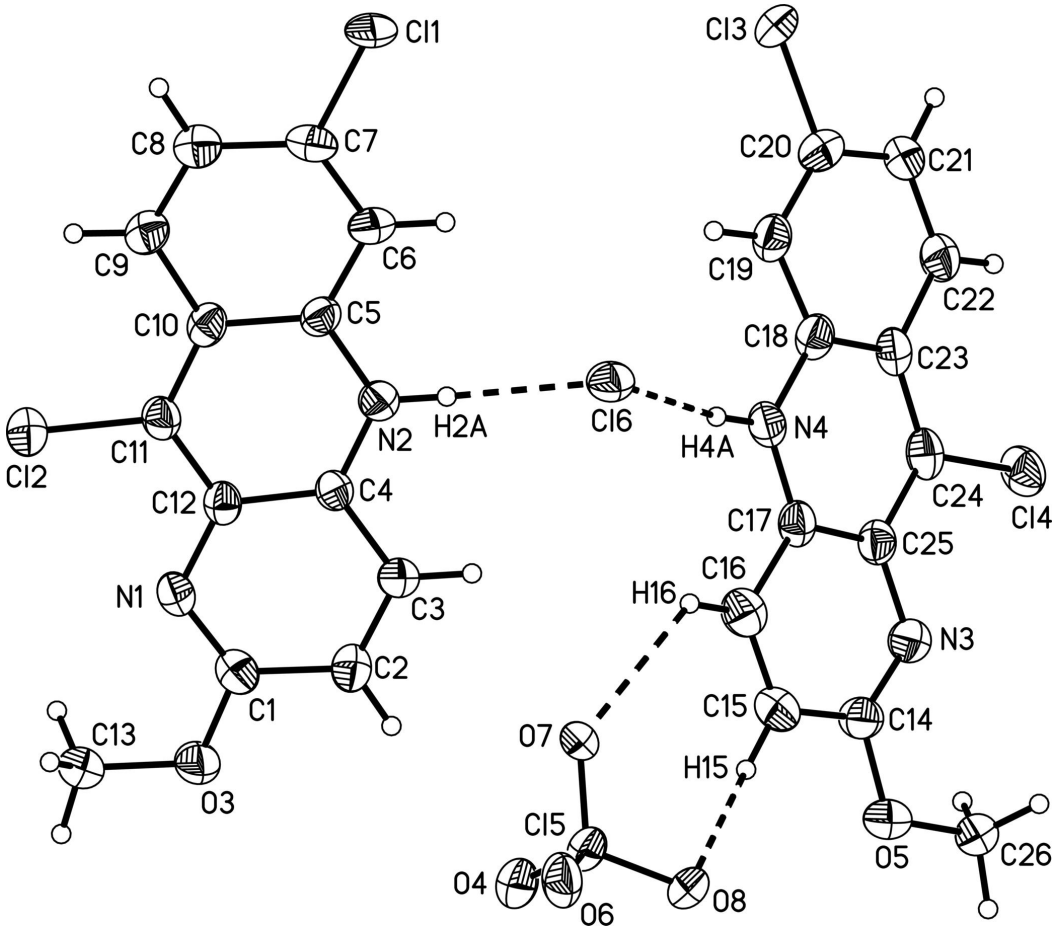
C10—C9—H9	120.0	O5—C26—H26B	109.5
C11—C10—C5	118.9 (3)	H26A—C26—H26B	109.5
C11—C10—C9	124.1 (3)	O5—C26—H26C	109.5
C5—C10—C9	117.0 (3)	H26A—C26—H26C	109.5
C12—C11—C10	121.5 (3)	H26B—C26—H26C	109.5
C12—C11—Cl2	118.2 (2)	O4—Cl5—O7	102.72 (17)
C10—C11—Cl2	120.3 (2)	O4—Cl5—O6	111.11 (18)
N1—C12—C11	120.4 (3)	O7—Cl5—O6	111.09 (19)
N1—C12—C4	122.5 (3)	O4—Cl5—O8	109.67 (16)
C11—C12—C4	117.1 (3)	O7—Cl5—O8	112.46 (15)
O3—C13—H13A	109.5	O6—Cl5—O8	109.63 (15)
O3—C13—H13B	109.5	N2—Cl6—N4	120.32 (8)
H13A—C13—H13B	109.5	C1—N1—C12	117.8 (3)
O3—C13—H13C	109.5	C4—N2—C5	122.4 (3)
H13A—C13—H13C	109.5	C4—N2—Cl6	122.3 (2)
H13B—C13—H13C	109.5	C5—N2—Cl6	114.9 (2)
N3—C14—O5	120.2 (3)	C4—N2—H2A	119 (2)
N3—C14—C15	125.7 (3)	C5—N2—H2A	119 (2)
O5—C14—C15	114.2 (3)	C14—N3—C25	116.5 (3)
C16—C15—C14	119.3 (3)	C17—N4—C18	122.1 (3)
C16—C15—H15	120.4	C17—N4—Cl6	122.5 (2)
C14—C15—H15	120.4	C18—N4—Cl6	114.9 (2)
C15—C16—C17	116.3 (3)	C17—N4—H4A	119 (3)
C15—C16—H16	121.8	C18—N4—H4A	119 (3)
C17—C16—H16	121.8	C1—O3—C13	116.2 (3)
N4—C17—C25	122.2 (3)	C14—O5—C26	117.3 (3)
N4—C17—C16	118.7 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···Cl6	0.86 (4)	2.13 (4)	2.978 (3)	169 (3)
N4—H4A···Cl6	0.86 (4)	2.21 (4)	3.055 (3)	169 (3)
C9—H9···O6^{i}	0.93	2.53	3.295 (4)	140
C9—H9···O7^{i}	0.93	2.66	3.453 (4)	143
C22—H22···O8^{ii}	0.93	2.39	3.124 (4)	136
C15—H15···O8	0.93	2.48	3.341 (4)	155
C16—H16···O7	0.93	2.64	3.327 (5)	132

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−3/2, −*y*+1/2, *z*−1/2.

Fig. 1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C8
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C9
C6
C10
C5
C11
N2
H2A
Cl2
C12
C4
N1
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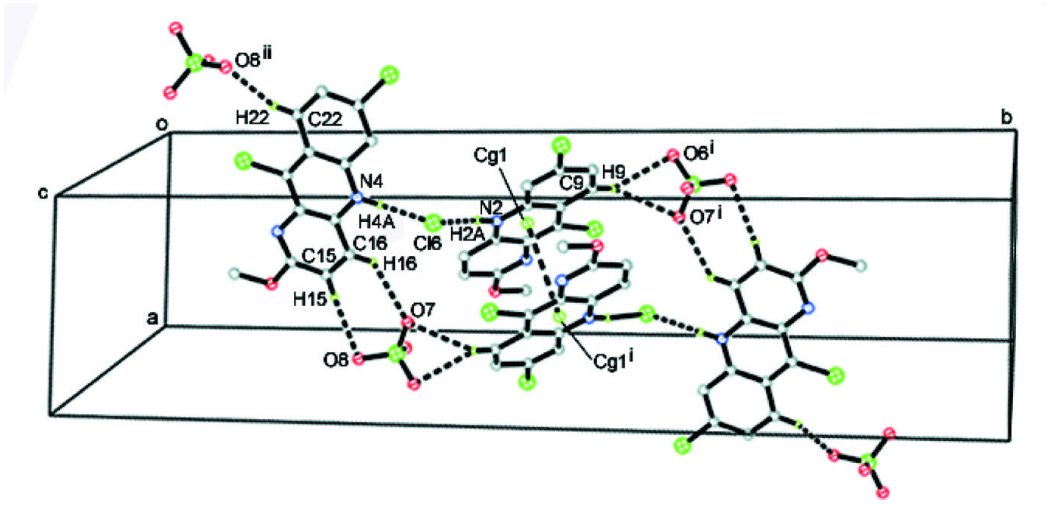
C1
C13
O3
Cl6
H4A
Cl3
C20
C21
C19
C22
C18
C23
N4
C24
Cl4
C17
C25
C16
H16
N3
C15
C14
O7
H15
Cl5
O5
C26
O4
O6
O8

Fig. 2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C22
c
b
a
Cg1
C9
H9
O6i
N4
N2
H4A
H2A
Cl6
C16
C15
H16
H15
O7
O8
O7i
Cg1i