

9-(2-Pyridylmethoxy)-1,10-phenanthroline-1-ium perchlorate methanol solvate

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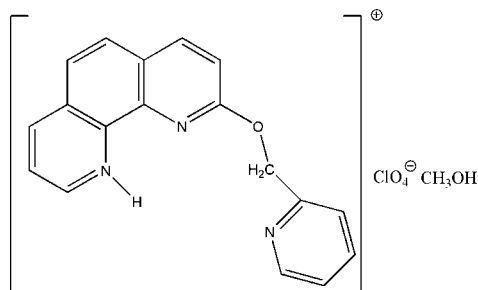
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.057; wR factor = 0.164; data-to-parameter ratio = 13.3.

In the title organic salt, $\text{C}_{18}\text{H}_{14}\text{N}_3\text{O}^+\cdot\text{ClO}_4^-\cdot\text{CH}_4\text{O}$, there is a π - π stacking interaction between neighbouring 1,10-phenanthroline rings and the relevant distances are 3.5453 (18) Å for the centroid-centroid distance and 3.354 Å for the perpendicular distance. There is also a relatively close contact between a C-H bond and a symmetry-related pyridine ring. There are classical N-H...O and O-H...N hydrogen bonds and non-classical C-H...O hydrogen bonds involving the cation, methanol solvent molecule and perchlorate anion.

Related literature

For a related structure, see: Liu *et al.* (2008).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{14}\text{N}_3\text{O}^+\cdot\text{ClO}_4^-\cdot\text{CH}_4\text{O}$
 $M_r = 419.81$
 Triclinic, $P\bar{1}$
 $a = 7.0765$ (15) Å
 $b = 10.597$ (2) Å
 $c = 14.164$ (3) Å
 $\alpha = 110.003$ (3)°
 $\beta = 94.999$ (3)°

$\gamma = 105.304$ (3)°
 $V = 944.1$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.25$ mm⁻¹
 $T = 298$ (2) K
 $0.38 \times 0.31 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.912$, $T_{\max} = 0.957$

5027 measured reflections
 3504 independent reflections
 2695 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.164$
 $S = 1.05$
 3504 reflections

263 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.41$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1-H4...O6	0.81	1.85	2.648 (3)	167
O6-H5...N3	0.89	1.85	2.738 (4)	175
C3-H3...O2	0.93	2.32	3.238 (5)	170
C13-H13B...O6	0.97	2.58	3.405 (4)	143
C8-H8...Cg3 ⁱ	0.93	2.81	3.650 (2)	151

Symmetry code: (i) $-x + 1, -y, -z + 1$. Cg3 is the centroid of the pyridine ring

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2085).

References

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supplementary materials

Acta Cryst. (2008). E64, o1450 [doi:10.1107/S1600536808020606]

9-(2-Pyridylmethoxy)-1,10-phenanthroline-1-ium perchlorate methanol solvate

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Comment

Derivatives of 1,10-phenanthroline play an important role in modern coordination chemistry (Liu *et al.*, 2008) and we have tried to prepare a complex containing Manganese(II) and iron(III) metallic ions and 2-((pyridin-2-yl)methoxy)-1,10-phenanthroline ligand, but we obtained the title organic salt.

Fig. 1 shows the structure, revealing that one of N atoms from phenanthroline ring was protonated and it was turned into a cation. There is a π - π stacking interaction involving symmetry-related 1,10-phenanthroline rings, the relevant distances being $Cg1 \cdots Cg2^i = 3.5453$ (18) Å and $Cg1 \cdots Cg2^i_{\text{perp}} = 3.354$ Å and $\alpha = 1.09^\circ$; there also exists interaction between C8-H8 bond and pyridine ring and the relevant distance is $H8 \cdots Cg3^{ii} = 2.81$ Å for H8 atom to the centroid of the pyridine ring and $H8 \cdots Cg3^{ii}_{\text{perp}} = 2.803$ Å for the perpendicular distance from H8 atom to the pyridine ring plane [symmetry code: (i) $-X, -Y, 1-Z$; (ii) $1-X, -Y, 1-Z$; $Cg1, Cg2$ and $Cg3$ are the centroids of the N2/C6C7C10-C12 ring, C4-C9 ring and N3/C14-C18 rings, respectively; $Cg1 \cdots Cg2^i_{\text{perp}}$ is the perpendicular distance from ring $Cg1$ to ring $Cg2^i$; α is the dihedral angle between ring plane $Cg1$ and ring plane $Cg2^i$;]. There exist N-H \cdots O and O-H \cdots N classic hydrogen bonds and C-H \cdots O non-classic hydrogen bonds (Fig. 1 and Table 1) in the asymmetric unit.

Experimental

10 ml methanol solution of 2-((pyridin-2-yl)methoxy)-1,10-phenanthroline (0.1200 g, 0.418 mmol) was added into 20 ml methanol solution containing $FeCl_3 \cdot 6H_2O$ (0.0565 g, 0.209 mmol) and $Mn(ClO_4)_2 \cdot 6H_2O$ (0.0757 g, 0.209 mmol), and the mixed solution was stirred for half a hour. Yellow single crystals were obtained after the solution had been allowed to stand at room temperature for three days.

Refinement

Nitrogen-bound H atom and Oxygen-bound H atom were located in a difference Fourier map, then placed in calculated positions with N—H = 0.81 Å and O—H = 0.89 Å and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H atoms were placed in calculated positions with with C—H = 0.97 Å for methyl, C—H = 0.96 Å for methylene and C—H = 0.93 Å for other H atoms, and refined as riding with $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for methyl H and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for other H atoms.

Figures

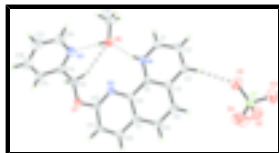


Fig. 1. Structure of title organic salt with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The classic hydrogen bonds are shown as dashed lines and non-classic hydrogen bonds as double dashed lines.

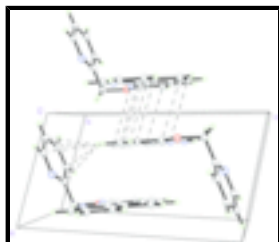


Fig. 2. The packing and π - π stacking interaction (dashed lines) and C—H \cdots π interaction (dashed lines), the methanol molecule and perchlorate anion have been omitted for clarity.

9-(2-Pyridylmethoxy)-1,10-phenanthroline perchlorate methanol solvate

Crystal data

$C_{18}H_{14}N_3O^+ \cdot ClO_4^- \cdot CH_4O$

$M_r = 419.81$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.0765$ (15) Å

$b = 10.597$ (2) Å

$c = 14.164$ (3) Å

$\alpha = 110.003$ (3)°

$\beta = 94.999$ (3)°

$\gamma = 105.304$ (3)°

$V = 944.1$ (3) Å³

$Z = 2$

$F_{000} = 436$

$D_x = 1.477$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 1588 reflections

$\theta = 3.0$ – 25.9 °

$\mu = 0.25$ mm⁻¹

$T = 298$ (2) K

Block, yellow

$0.38 \times 0.31 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.912$, $T_{\max} = 0.957$

5027 measured reflections

3504 independent reflections

2695 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 25.7$ °

$\theta_{\min} = 1.6$ °

$h = -7 \rightarrow 8$

$k = -12 \rightarrow 12$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.164$	$w = 1/[\sigma^2(F_o^2) + (0.0858P)^2 + 0.2952P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3504 reflections	$(\Delta/\sigma)_{\max} = 0.002$
263 parameters	$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2377 (5)	0.4244 (3)	0.6774 (2)	0.0530 (7)
H1	0.2292	0.4775	0.7435	0.064*
C2	0.2448 (5)	0.4829 (3)	0.6041 (3)	0.0613 (8)
H2	0.2393	0.5744	0.6204	0.074*
C3	0.2598 (5)	0.4057 (3)	0.5080 (2)	0.0546 (7)
H3	0.2663	0.4450	0.4584	0.066*
C4	0.2655 (4)	0.2661 (3)	0.4831 (2)	0.0430 (6)
C5	0.2549 (4)	0.2104 (3)	0.55982 (18)	0.0374 (6)
C6	0.2521 (3)	0.0678 (3)	0.53855 (18)	0.0349 (5)
C7	0.2587 (4)	-0.0143 (3)	0.43867 (19)	0.0402 (6)
C8	0.2705 (4)	0.0441 (3)	0.3616 (2)	0.0471 (7)
H8	0.2750	-0.0120	0.2955	0.057*
C9	0.2753 (4)	0.1789 (3)	0.3827 (2)	0.0485 (7)
H9	0.2851	0.2153	0.3315	0.058*
C10	0.2529 (4)	-0.1564 (3)	0.4190 (2)	0.0443 (6)
H10	0.2592	-0.2151	0.3541	0.053*
C11	0.2382 (4)	-0.2049 (3)	0.4948 (2)	0.0455 (6)
H11	0.2333	-0.2976	0.4831	0.055*

supplementary materials

C12	0.2304 (4)	-0.1128 (3)	0.59278 (19)	0.0386 (6)
C13	0.2012 (4)	-0.0886 (3)	0.7665 (2)	0.0490 (7)
H13A	0.1173	-0.1480	0.7956	0.059*
H13B	0.1426	-0.0160	0.7652	0.059*
C14	0.4068 (4)	-0.0208 (3)	0.8319 (2)	0.0460 (7)
C15	0.5178 (5)	-0.1004 (3)	0.8526 (2)	0.0557 (8)
H15	0.4653	-0.1986	0.8265	0.067*
C16	0.7067 (5)	-0.0345 (4)	0.9121 (3)	0.0692 (9)
H16	0.7833	-0.0868	0.9270	0.083*
C17	0.7788 (6)	0.1094 (4)	0.9488 (3)	0.0753 (10)
H17	0.9061	0.1570	0.9890	0.090*
C18	0.6621 (6)	0.1827 (4)	0.9257 (3)	0.0720 (10)
H18	0.7132	0.2808	0.9511	0.086*
C19	0.2308 (7)	0.3748 (4)	0.9157 (3)	0.0887 (12)
H19A	0.2483	0.3543	0.9762	0.133*
H19B	0.1107	0.4000	0.9102	0.133*
H19C	0.3431	0.4521	0.9197	0.133*
C11	0.20777 (12)	0.45705 (7)	0.21213 (5)	0.0541 (3)
N1	0.2429 (3)	0.2941 (2)	0.65502 (16)	0.0419 (5)
H4	0.2362	0.2694	0.7032	0.050*
N2	0.2387 (3)	0.0189 (2)	0.61631 (15)	0.0377 (5)
N3	0.4780 (4)	0.1207 (3)	0.86832 (19)	0.0580 (7)
O1	0.2091 (3)	-0.17350 (18)	0.66282 (14)	0.0476 (5)
O2	0.2322 (8)	0.5077 (4)	0.3177 (2)	0.1432 (16)
O3	0.2709 (7)	0.5724 (3)	0.1857 (3)	0.1279 (13)
O4	0.3128 (7)	0.3648 (4)	0.1769 (3)	0.1583 (17)
O5	0.0081 (6)	0.3882 (4)	0.1659 (3)	0.1494 (16)
O6	0.2165 (4)	0.2545 (2)	0.82875 (15)	0.0664 (6)
H5	0.3072	0.2151	0.8417	0.100*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0681 (19)	0.0396 (14)	0.0503 (16)	0.0211 (14)	0.0085 (14)	0.0135 (12)
C2	0.080 (2)	0.0411 (15)	0.068 (2)	0.0208 (15)	0.0100 (17)	0.0261 (15)
C3	0.0631 (19)	0.0527 (17)	0.0588 (18)	0.0173 (15)	0.0088 (15)	0.0356 (15)
C4	0.0392 (14)	0.0474 (15)	0.0473 (15)	0.0123 (12)	0.0085 (12)	0.0248 (12)
C5	0.0343 (13)	0.0415 (13)	0.0373 (13)	0.0109 (11)	0.0062 (10)	0.0170 (11)
C6	0.0291 (12)	0.0387 (13)	0.0363 (13)	0.0085 (10)	0.0057 (10)	0.0156 (10)
C7	0.0315 (13)	0.0474 (14)	0.0397 (14)	0.0116 (11)	0.0057 (10)	0.0149 (11)
C8	0.0455 (15)	0.0615 (17)	0.0344 (13)	0.0174 (13)	0.0117 (11)	0.0169 (12)
C9	0.0496 (16)	0.0619 (18)	0.0435 (15)	0.0187 (14)	0.0125 (12)	0.0298 (13)
C10	0.0430 (15)	0.0437 (14)	0.0389 (14)	0.0149 (12)	0.0062 (11)	0.0064 (11)
C11	0.0461 (15)	0.0361 (13)	0.0488 (16)	0.0137 (12)	0.0051 (12)	0.0100 (12)
C12	0.0339 (13)	0.0379 (13)	0.0434 (14)	0.0105 (11)	0.0031 (11)	0.0162 (11)
C13	0.0567 (17)	0.0508 (16)	0.0479 (16)	0.0167 (14)	0.0156 (13)	0.0276 (13)
C14	0.0619 (18)	0.0460 (15)	0.0369 (14)	0.0193 (13)	0.0143 (12)	0.0211 (12)
C15	0.075 (2)	0.0495 (16)	0.0492 (17)	0.0266 (15)	0.0100 (15)	0.0215 (13)

C16	0.078 (2)	0.080 (2)	0.060 (2)	0.039 (2)	0.0054 (17)	0.0305 (18)
C17	0.072 (2)	0.082 (3)	0.061 (2)	0.019 (2)	-0.0055 (17)	0.0218 (19)
C18	0.085 (3)	0.0527 (18)	0.065 (2)	0.0110 (18)	-0.0040 (18)	0.0188 (16)
C19	0.124 (4)	0.088 (3)	0.057 (2)	0.051 (3)	0.022 (2)	0.0168 (19)
C11	0.0777 (6)	0.0433 (4)	0.0435 (4)	0.0249 (4)	0.0107 (3)	0.0149 (3)
N1	0.0504 (13)	0.0393 (11)	0.0388 (12)	0.0157 (10)	0.0074 (10)	0.0173 (9)
N2	0.0398 (12)	0.0377 (11)	0.0367 (11)	0.0126 (9)	0.0070 (9)	0.0152 (9)
N3	0.0745 (18)	0.0465 (14)	0.0524 (15)	0.0183 (13)	0.0056 (13)	0.0201 (11)
O1	0.0615 (12)	0.0371 (9)	0.0455 (11)	0.0141 (9)	0.0073 (9)	0.0189 (8)
O2	0.287 (5)	0.119 (3)	0.0502 (16)	0.101 (3)	0.037 (2)	0.0340 (17)
O3	0.204 (4)	0.087 (2)	0.108 (2)	0.035 (2)	0.043 (2)	0.0598 (19)
O4	0.217 (4)	0.144 (3)	0.135 (3)	0.143 (3)	0.026 (3)	0.015 (2)
O5	0.096 (3)	0.119 (3)	0.166 (4)	-0.003 (2)	-0.004 (2)	0.010 (3)
O6	0.0970 (17)	0.0684 (14)	0.0451 (12)	0.0420 (13)	0.0156 (11)	0.0226 (10)

Geometric parameters (Å, °)

C1—N1	1.318 (3)	C13—O1	1.451 (3)
C1—C2	1.377 (4)	C13—C14	1.500 (4)
C1—H1	0.9300	C13—H13A	0.9700
C2—C3	1.357 (4)	C13—H13B	0.9700
C2—H2	0.9300	C14—N3	1.340 (4)
C3—C4	1.411 (4)	C14—C15	1.377 (4)
C3—H3	0.9300	C15—C16	1.375 (5)
C4—C5	1.402 (4)	C15—H15	0.9300
C4—C9	1.426 (4)	C16—C17	1.362 (5)
C5—N1	1.361 (3)	C16—H16	0.9300
C5—C6	1.431 (3)	C17—C18	1.363 (5)
C6—N2	1.368 (3)	C17—H17	0.9300
C6—C7	1.397 (3)	C18—N3	1.337 (4)
C7—C10	1.423 (4)	C18—H18	0.9300
C7—C8	1.425 (4)	C19—O6	1.410 (4)
C8—C9	1.346 (4)	C19—H19A	0.9600
C8—H8	0.9300	C19—H19B	0.9600
C9—H9	0.9300	C19—H19C	0.9600
C10—C11	1.340 (4)	C11—O4	1.368 (3)
C10—H10	0.9300	C11—O3	1.375 (3)
C11—C12	1.413 (4)	C11—O2	1.383 (3)
C11—H11	0.9300	C11—O5	1.388 (4)
C12—N2	1.303 (3)	N1—H4	0.8111
C12—O1	1.354 (3)	O6—H5	0.8900
N1—C1—C2	120.9 (3)	C14—C13—H13A	109.5
N1—C1—H1	119.6	O1—C13—H13B	109.5
C2—C1—H1	119.6	C14—C13—H13B	109.5
C3—C2—C1	119.4 (3)	H13A—C13—H13B	108.1
C3—C2—H2	120.3	N3—C14—C15	121.6 (3)
C1—C2—H2	120.3	N3—C14—C13	116.9 (3)
C2—C3—C4	120.3 (3)	C15—C14—C13	121.5 (3)
C2—C3—H3	119.9	C16—C15—C14	119.8 (3)

supplementary materials

C4—C3—H3	119.9	C16—C15—H15	120.1
C5—C4—C3	118.2 (2)	C14—C15—H15	120.1
C5—C4—C9	119.1 (2)	C17—C16—C15	118.4 (3)
C3—C4—C9	122.7 (2)	C17—C16—H16	120.8
N1—C5—C4	118.6 (2)	C15—C16—H16	120.8
N1—C5—C6	120.4 (2)	C16—C17—C18	119.2 (3)
C4—C5—C6	121.0 (2)	C16—C17—H17	120.4
N2—C6—C7	123.9 (2)	C18—C17—H17	120.4
N2—C6—C5	118.3 (2)	N3—C18—C17	123.4 (3)
C7—C6—C5	117.8 (2)	N3—C18—H18	118.3
C6—C7—C10	116.8 (2)	C17—C18—H18	118.3
C6—C7—C8	120.5 (2)	O6—C19—H19A	109.5
C10—C7—C8	122.7 (2)	O6—C19—H19B	109.5
C9—C8—C7	121.2 (2)	H19A—C19—H19B	109.5
C9—C8—H8	119.4	O6—C19—H19C	109.5
C7—C8—H8	119.4	H19A—C19—H19C	109.5
C8—C9—C4	120.4 (2)	H19B—C19—H19C	109.5
C8—C9—H9	119.8	O4—C11—O3	111.0 (3)
C4—C9—H9	119.8	O4—C11—O2	111.7 (2)
C11—C10—C7	119.4 (2)	O3—C11—O2	107.0 (2)
C11—C10—H10	120.3	O4—C11—O5	108.2 (3)
C7—C10—H10	120.3	O3—C11—O5	107.6 (3)
C10—C11—C12	119.0 (2)	O2—C11—O5	111.2 (3)
C10—C11—H11	120.5	C1—N1—C5	122.6 (2)
C12—C11—H11	120.5	C1—N1—H4	113.1
N2—C12—O1	121.1 (2)	C5—N1—H4	124.3
N2—C12—C11	124.7 (2)	C12—N2—C6	116.2 (2)
O1—C12—C11	114.2 (2)	C18—N3—C14	117.6 (3)
O1—C13—C14	110.5 (2)	C12—O1—C13	119.09 (19)
O1—C13—H13A	109.5	C19—O6—H5	109.6
N1—C1—C2—C3	-0.8 (5)	C7—C10—C11—C12	-0.5 (4)
C1—C2—C3—C4	0.8 (5)	C10—C11—C12—N2	-0.8 (4)
C2—C3—C4—C5	0.1 (4)	C10—C11—C12—O1	177.9 (2)
C2—C3—C4—C9	178.2 (3)	O1—C13—C14—N3	115.5 (3)
C3—C4—C5—N1	-1.1 (4)	O1—C13—C14—C15	-63.9 (3)
C9—C4—C5—N1	-179.2 (2)	N3—C14—C15—C16	0.0 (4)
C3—C4—C5—C6	177.5 (2)	C13—C14—C15—C16	179.3 (3)
C9—C4—C5—C6	-0.6 (4)	C14—C15—C16—C17	-0.2 (5)
N1—C5—C6—N2	-0.5 (3)	C15—C16—C17—C18	0.2 (5)
C4—C5—C6—N2	-179.1 (2)	C16—C17—C18—N3	0.0 (6)
N1—C5—C6—C7	178.1 (2)	C2—C1—N1—C5	-0.1 (4)
C4—C5—C6—C7	-0.5 (4)	C4—C5—N1—C1	1.1 (4)
N2—C6—C7—C10	-0.6 (4)	C6—C5—N1—C1	-177.5 (2)
C5—C6—C7—C10	-179.1 (2)	O1—C12—N2—C6	-177.3 (2)
N2—C6—C7—C8	179.3 (2)	C11—C12—N2—C6	1.3 (4)
C5—C6—C7—C8	0.8 (4)	C7—C6—N2—C12	-0.6 (3)
C6—C7—C8—C9	-0.1 (4)	C5—C6—N2—C12	178.0 (2)
C10—C7—C8—C9	179.9 (3)	C17—C18—N3—C14	-0.2 (5)
C7—C8—C9—C4	-1.0 (4)	C15—C14—N3—C18	0.2 (4)

C5—C4—C9—C8	1.3 (4)	C13—C14—N3—C18	-179.2 (3)
C3—C4—C9—C8	-176.7 (3)	N2—C12—O1—C13	-1.8 (3)
C6—C7—C10—C11	1.1 (4)	C11—C12—O1—C13	179.4 (2)
C8—C7—C10—C11	-178.8 (2)	C14—C13—O1—C12	-90.4 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H4 \cdots O6	0.81	1.85	2.648 (3)	167
O6—H5 \cdots N3	0.89	1.85	2.738 (4)	175
C3—H3 \cdots O2	0.93	2.32	3.238 (5)	170
C13—H13B \cdots O6	0.97	2.58	3.405 (4)	143
C8—H8 \cdots Cg3 ⁱ	0.93	2.81	3.650 (2)	151

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

Fig. 1

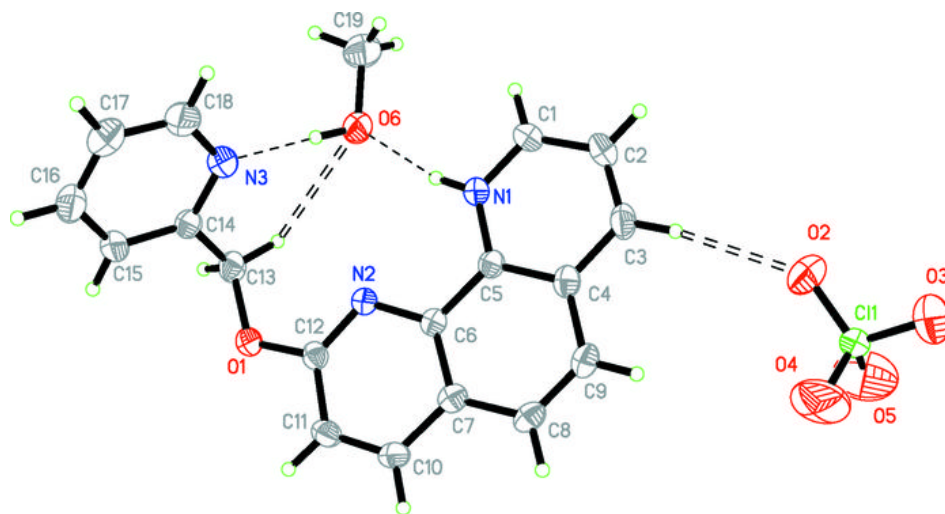


Fig. 2

