Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,10-Phenanthroline pyridinium perchlorate

Xi-Shi Tai,[a]* Jie Yin[b] and Yi-Min Feng[a]

[a]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, People's Republic of China

Correspondence e-mail: taixishi@lzu.edu.cn

Received 25 January 2007
Accepted 26 January 2007

Key indicators

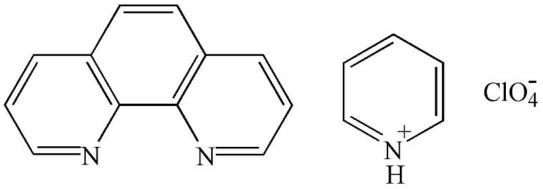
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.139
Data-to-parameter ratio = 12.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In 1,10-phenanthroline pyridinium perchlorate, $C_{12}H_8N_2\cdot C_5H_6N^+\cdot ClO_4^-$, intra- and intermolecular hydrogen bonding interactions dominate the crystal packing. The phenanthroline molecule, the cation and anion lie on crystallographic twofold rotation axes.

Comment

Phenanthroline and its derivative ligands and their complexes with metal ions have received considerable attention over the past three decades (Summers, 1978; Weijnen *et al.*, 1991; Guo *et al.*, 2004). In the title compound, (I), the bond lengths and angles are within normal ranges.



(I)

The phenanthroline molecule, the cation and anion all lie on crystallographic twofold rotation axes. The dihedral angles formed by plane N1/C1–C5 with N1A/C1A–C5A and C7/C8/C9/C8A/C7A/N2 are 0.9 and 5.4°, respectively, indicating that the three planes in the molecule are approximately coplanar, probably as a result of the hydrogen-bonding requirement. The perchlorate anion plays an important role in forming this structure, *viz.* it forms a chain structure *via* hydrogen bonding. In the crystal structure, strong intra- and intermolecular hydrogen bonds result in a two-dimensional structure (Fig. 2).

Experimental

All commercially available reagents were used as supplied. Magnesium perchlorate (5 mmol) was added to a solution of 1,10-phenanthroline (10 mmol) in pyridine (10 ml). The mixture was stirred continuously for 3 h under reflux and then filtered. Single crystals suitable for X-ray analysis were obtained, after two weeks, by evaporation of the filtrate.

Crystal data

$C_{12}H_8N_2\cdot C_5H_6N^+\cdot ClO_4^-$
M_r = 359.76
Monoclinic, $C2/c$
a = 10.534 (3) Å
b = 22.884 (8) Å
c = 6.811 (2) Å
β = 95.403 (6)°
V = 1634.5 (9) Å^3

Z = 4
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 294 (2) K
Block, colourless
0.26 × 0.22 × 0.18 mm

doi:10.1107/S160053680700431X

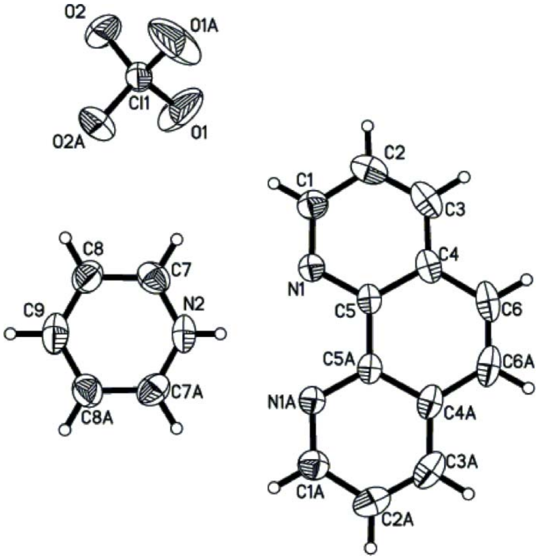


Figure 1

The structure of the components of (I) with 30% probabiility displacement ellipsoids. In the cation and the organic molecule, symmetry code: (A) $2 - x, y, \frac{1}{2} - z$. In the anion, symmetry code: (A) $1 - x, y, \frac{1}{2} - z$.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.935$, $T_{\max} = 0.954$
4107 measured reflections
1445 independent reflections
835 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.139$
$S = 1.03$
1445 reflections
117 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.9324P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.28$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1$^{\rm i}$	0.75 (5)	2.34 (4)	2.984 (5)	144.0 (8)
N2—H2A···N1	0.75 (5)	2.34 (4)	2.984 (5)	144.0 (7)

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

All H atoms were positioned geometrically. Atom H2*A* on N2 was refined freely.

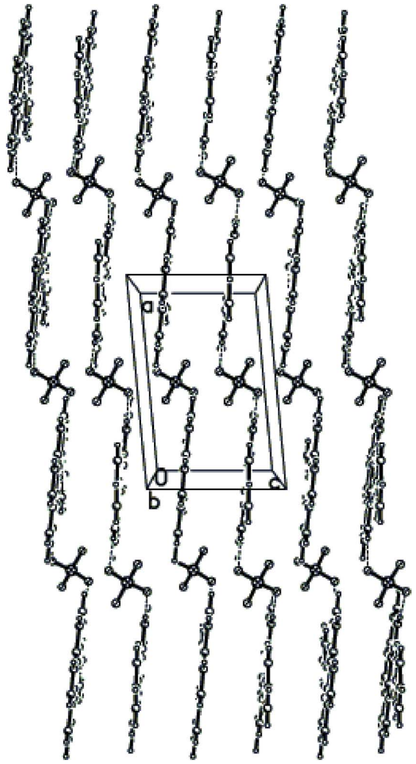


Figure 2

The packing of (I). Hydrogen bonds are indicated by dashed lines.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (No. 20671073), NingXia Natural Gas Transfer Key Laboratory (No. 2004007) and the Science and Technology Foundation of Weifang and Weifang University for research grants.

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Guo, D. F., He, J. & Zeng, Z. Z. (2004). *J. Chin. Rare Earth Soc.* **22**, 55–60.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Summers, L. A. (1978). *Advances in Hetrocyclic Chemistry*, Vol. 22, pp. 1–69. New York: Academic Press.

Weijnen, J. G. J., Koudijs, A. & Engberse, J. F. J. (1991). *J. Chem. Soc. Perkin Trans. 2*, pp. 1121–1126.