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#### Key indicators

Single-crystal X-ray study

$T = 288\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$

$R$  factor = 0.040

$wR$  factor = 0.127

Data-to-parameter ratio = 15.6

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

## 1,10-Phenanthroline perchlorate

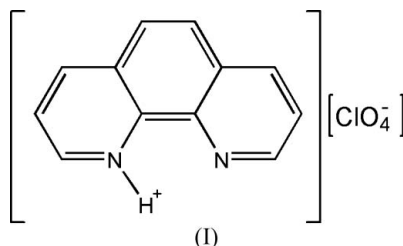
The proton-transfer title compound,  $\text{C}_{12}\text{H}_9\text{N}_2^+\cdot\text{ClO}_4^-$ , has been obtained from 1,10-phenanthroline and  $\text{HClO}_4$ . In the crystal structure, the molecules stack along the  $a$  axis *via* hydrogen-bond interactions and van der Waals forces.

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#### Comment

1,10-Phenanthroline (phen) has been recognized as a good proton acceptor and it is considered a suitable agent in the synthesis of proton-transfer systems. Some proton-transfer complexes of 1,10-phenanthroline have been obtained, such as  $(\text{pydaH}_2)(\text{phendc})$  ( $\text{pydaH}_2$  is protonated 2,6-pyridinedianine; Moghimi *et al.*, 2003) and  $(\text{phenH}^+)_2(\text{pydc}^{2-})$  ( $\text{pydc}^{2-}$  is the pyridinedicarboxylic acid dianion; Moghimi *et al.*, 2005). We report here the synthesis and characterization of the title complex, (I).



Vigorous reaction of 1,10-phenanthroline with  $\text{HClO}_4$  in water resulted in the proton-transfer compound  $(\text{phenH}^+)(\text{ClO}_4^-)$  (Fig. 1). In the compound, phen acts as proton acceptor and  $\text{HClO}_4$  acts as proton donor (Etter, 1990). Selected bond lengths and angles are shown in Table 1.

Hydrogen bonds play a very important role in the formation of proton-transfer compounds. There are two kinds of hydrogen bond in the title complex. One is formed between atom O2 of  $\text{ClO}_4^-$  and the protonated phen (N1—H1B), and the other is formed within 1,10-phen (Table 2). A one-dimensional chain along the  $a$  axis results from the  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond (Fig. 2). In the crystal structure, the mono-protonated phen cations are parallel to each other, showing  $\pi-\pi$  interactions with a centroid-centroid distance of  $3.37(1)\text{ \AA}$ .

#### Experimental

All chemicals were obtained from commercial sources and used without further purification. 1,10-Phenanthroline (0.1 mmol, 0.0198 g) was dissolved in 10 ml water and  $\text{HClO}_4$  (1 ml,  $1\text{ mol l}^{-1}$ ) was added with stirring. The resulting solution was filtered after 0.5 h, then upon slow evaporation of the filtrate at room temperature, pink crystals of (I) were obtained after three weeks. Initial and final pH values of the solution were 1.6 and 1.0, respectively.

## Crystal data

$C_{12}H_9N_2^+ \cdot ClO_4^-$   
 $M_r = 280.66$   
 Triclinic,  $P\bar{1}$   
 $a = 5.8054$  (12) Å  
 $b = 9.778$  (2) Å  
 $c = 10.628$  (2) Å  
 $\alpha = 93.16$  (3)°  
 $\beta = 101.41$  (3)°  
 $\gamma = 98.08$  (3)°

$V = 583.4$  (2) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.598$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.34$  mm<sup>-1</sup>  
 $T = 288$  (2) K  
 Block, pink  
 $0.30 \times 0.25 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.900$ ,  $T_{\max} = 0.938$

5890 measured reflections  
 2767 independent reflections  
 2345 reflections with  $I > 2\sigma I$   
 $R_{\text{int}} = 0.016$   
 $\theta_{\text{max}} = 28.3^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.128$   
 $S = 1.01$   
 2767 reflections  
 177 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0799P)^2 + 0.1598P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.43$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

C1—O3	1.4230 (15)	N2—C5	1.325 (2)
C11—O4	1.4244 (14)	N2—C12	1.359 (2)
C11—O2	1.4251 (18)	N1—C2	1.326 (2)
C11—O1	1.4249 (19)	N1—C11	1.357 (2)
O3—C11—O4	110.13 (10)	O2—C11—O1	110.53 (15)
O3—C11—O2	109.38 (11)	C5—N2—C12	116.31 (16)
O4—C11—O2	109.44 (12)	C2—N1—C11	123.35 (16)
O3—C11—O1	108.78 (12)	C2—N1—H1A	123.4 (15)
O4—C11—O1	108.57 (11)	C11—N1—H1A	113.3 (15)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1A $\cdots$ O2 <sup>i</sup>	0.84 (2)	2.32 (2)	2.944 (2)	132 (2)
N1—H1A $\cdots$ N2	0.84 (2)	2.33 (2)	2.741 (2)	111 (2)

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

H atoms on the C atoms were located in a difference Fourier map and refined as riding on their parent atoms, with  $C-H = 0.93$  Å and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ . H atoms bonded to N atoms were located in a difference Fourier map and refined with the N—H distance restrained to 0.84 (2) Å.

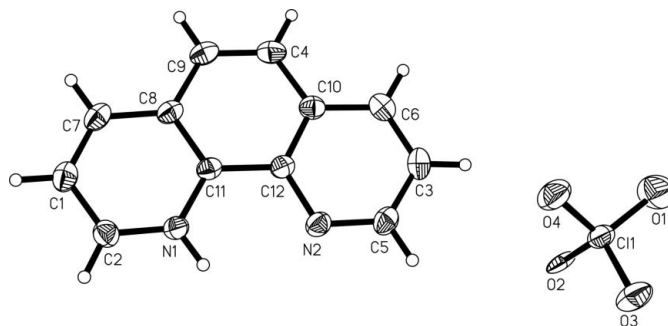


Figure 1

The asymmetric unit of the title complex, showing the atom-labelling scheme and 30% probability displacement ellipsoids.

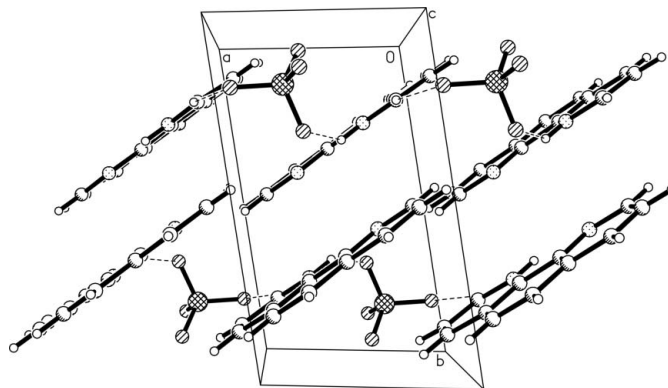


Figure 2

View along the  $c$  axis of the packing, with hydrogen bonds shown as dashed lines.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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