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1,10-Phenanthrolin-1-ium pamoate *N*,*N*-dimethylformamide solvate

Tong-Ming Shang,* Quan-Fa Zhou and Jian-Hua Sun

Jiangsu Key Laboratory of Precious Metals Chemistry, Jiangsu Teachers' University of Technology, Changzhou 213001, People's Republic of China

Correspondence e-mail: shangtm@jstu.edu.cn

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In the title compound [systematic name: 1,10-phenanthrolin-1-ium 4-(3-carboxy-2-hydroxynaphthylmethyl)-3-hydroxy-2-naphthoate *N*,*N*-dimethylformamide solvate], $C_{12}H_9N_2^+\cdot C_{23}H_{15}O_6^-\cdot C_3H_7NO$, the two naphthyl ring systems of the pamoate monoanion are perpendicular to each other. O—H···O, N—H···O and C—H···O hydrogen-bonding interactions and π–π stacking interactions stabilize the crystal structure.

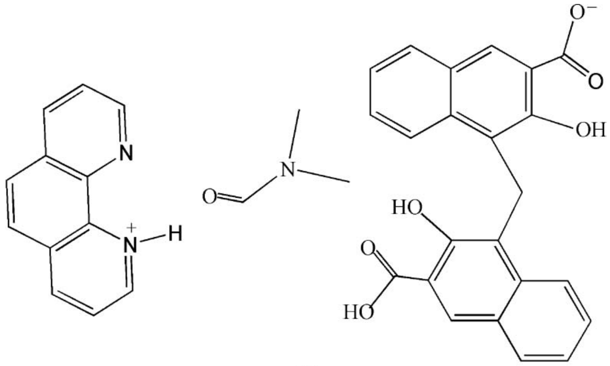
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.089
wR factor = 0.198
Data-to-parameter ratio = 12.3

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

Comment

Pamoic acid is a well known aromatic dicarboxylic acid. It has been used as a means of masking unpleasant tastes and for obtaining prolonged therapeutic action by forming slightly soluble salts with certain drugs (Dryden & Ridley, 1999; Jorgensen, 1998; Morovjan *et al.* 1998). In the construction of metal–organic coordination polymers, pamoic acid is a potential multidentate ligand, and it is also of fundamental interest because of the possibility of extensive hydrogen bonding in the solid state (Blackburn *et al.*, 1996; Haynes *et al.*, 2005; Ma *et al.*, 2006). During an attempt to synthesize a new coordination polymer with pamoic acid and $La(NO_3)_3\cdot 6H_2O$, we unexpectedly obtained the title compound, (I). We report its crystal structure here.



(I)

The asymmetric unit of (I) contains a pamoate monoanion, a 1,10-phenanthrolinium cation and an *N*,*N*-dimethylformamide molecule (Fig. 1). In the pamoate anion, the carboxyl and carboxylate groups are almost coplanar with the attached rings, and the two naphthyl ring systems are perpendicular to each other [dihedral angle 89.99 (6)°]. These orientations are influenced by intramolecular O—H···O and C—H···O hydrogen bonds (Table 2).

The stability of the solid-state structure of (I) is enhanced significantly by hydrogen-bonding interactions (Table 2). The pamoate anions are linked to a chain along the *c* axis through strong O3—H3$\cdots$O6^{i} hydrogen bonds. The 1,10-phenanthrolinium cations are attached to the chain *via* C25—H25$\cdots$O5^{i} interactions [symmetry code: (i) $x, y, z-1$]. The N2—H2*N*$\cdots$O7 hydrogen bond links the *N*,*N*-dimethylformamide molecule to the 1,10-phenanthrolinium cation. In addition, the crystal structure is stabilized by π–π interactions involving the C5–C10 (centroid *Cg*1), C12–C16/C21 (centroid *Cg*2) and N1/C24–C27/C35 (centroid *Cg*3) rings, with $Cg1\cdots Cg1^{ii}$ and $Cg2\cdots Cg3^{iii}$ distances of 3.553 (2) and 3.662 (2) Å, respectively [symmetry codes: (ii) $1-x, 2-y, 1-z$; (iii) $1-x, 1-y, 1-z$].

Experimental

An aqueous solution (10 ml) containing $La(NO_3)_3\cdot 6H_2O$ (0.20 mmol, 0.086 g) was added slowly to a solution (10 ml) of *N*,*N*-dimethylformamide containing 1,10-phenanthroline (0.20 mmol, 0.036 g) and pamoic acid (0.30 mmol, 0.110 g). Yellow crystals of (I) suitable for X-ray analysis were obtained on allowing the solution to stand at room temperature for 14 d.

Crystal data

$C_{12}H_9N_2^{+}\cdot C_{23}H_{15}O_6^{-}\cdot C_3H_7NO$
$M_r = 641.66$
Triclinic, $P\overline{1}$
$a = 10.7047$ (12) Å
$b = 11.7544$ (14) Å
$c = 13.4577$ (15) Å
$\alpha = 82.238$ (3)°
$\beta = 72.346$ (2)°
$\gamma = 71.824$ (2)°
$V = 1531.6$ (3) Å^3
$Z = 2$
$D_x = 1.391$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 298$ (2) K
Block, yellow
0.35 × 0.31 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.967$, $T_{max} = 0.978$
8169 measured reflections
5363 independent reflections
3703 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.089$
$wR(F^2) = 0.198$
$S = 1.12$
5363 reflections
435 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2 + 0.3956P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.367 (4)	O7—C38	1.210 (5)
O2—C22	1.238 (4)	N1—C24	1.321 (5)
O3—C22	1.275 (4)	N1—C35	1.349 (5)
O4—C13	1.356 (4)	N2—C33	1.320 (5)
O5—C23	1.240 (4)	N2—C34	1.350 (5)
O6—C23	1.281 (4)		
C24—N1—C35	116.0 (4)	O3—C22—C3	116.2 (4)
C33—N2—C34	123.4 (4)	O5—C23—O6	123.0 (3)
O2—C22—O3	123.2 (3)	O6—C23—C14	116.9 (3)

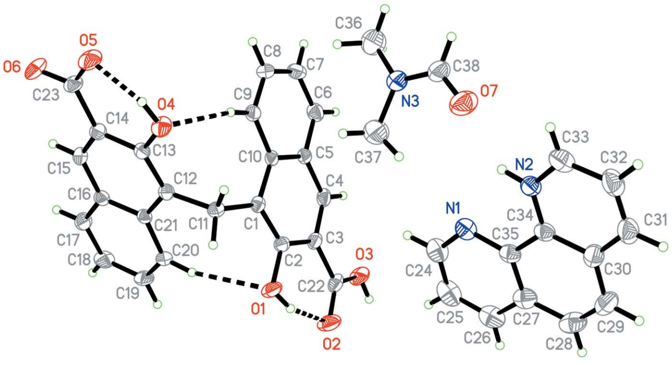


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme, showing displacement ellipsoids at the 30% probability level.

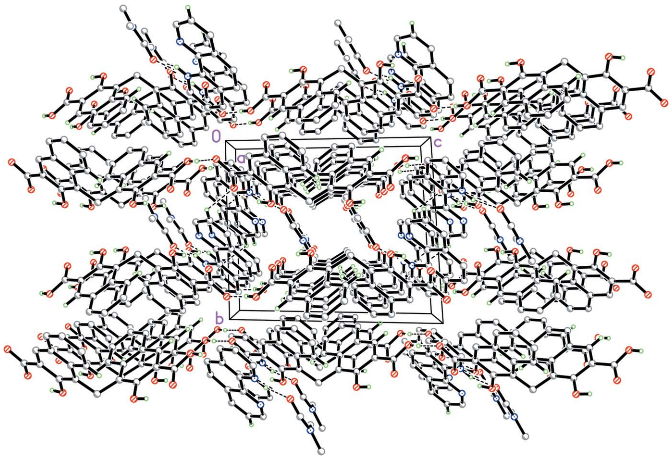


Figure 2
The crystal packing of (I). Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in hydrogen bonding have been omitted.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2*N*$\cdots$O7	0.86	1.95	2.686 (4)	143
O4—H4$\cdots$O5	0.82	1.77	2.530 (3)	154
O3—H3$\cdots$O6^{i}	0.82	1.64	2.458 (3)	176
O1—H1$\cdots$O2	0.82	1.78	2.534 (4)	152
C25—H25$\cdots$O5^{i}	0.93	2.50	3.165 (5)	129
C9—H9$\cdots$O4	0.93	2.32	3.232 (4)	165
C20—H20$\cdots$O1	0.93	2.44	3.350 (4)	167

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

H atoms were positioned geometrically and allowed to ride on their parent atoms, with O—H = 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(O)$, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$, C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}(C)$ for aromatic H atoms, C—H = 0.97 Å and $U_{iso} = 1.5U_{eq}(C)$ for methylene atoms, and C—H = 0.96 Å and $U_{iso} = 1.5U_{eq}(C)$ for methyl atoms.

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

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References

Blackburn, A. C., Dobson, A. J. & Gerkin, R. E. (1996). *Acta Cryst.* C**52**, 1269–1272.

Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Dryden, M. W. & Ridley, R. K. (1999). *Vet. Parasitol.* **82**, 311–315.

Haynes, D. A., Jones, W. & Motherwell, W. D. S. (2005). *CrystEngComm*, **7**, 538–543.

Jorgensen, M. (1998). *J. Chromatogr. B*, **716**, 315–323.

Ma, A.-Q., Jia, Z.-B. & Wang, G.-P. (2006). *Acta Cryst.* E**62**, m21–m23.

Morovjan, G., Csokan, P., Makranszki, L., Abdellah-Nagy, E. A. & Toth, K. (1998). *J. Chromatogr. A*, **797**, 237–244.

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

o508 Shang *et al.* • $C_{12}H_9N_2^+ \cdot C_{23}H_{15}O_6^- \cdot C_3H_7NO$ *Acta Cryst.* (2007). E**63**, o506–o508