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2-Amino-5-(4-carboxylatophenyl)-pyridinium monohydrate

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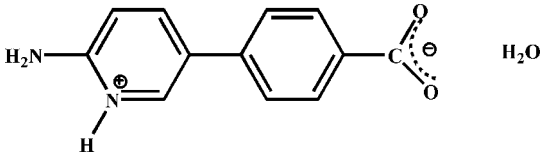
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.080; wR factor = 0.208; data-to-parameter ratio = 16.0.

The title compound, $C_{12}H_{10}N_2O_2\cdot H_2O$, crystallizes as a zwitterion in which the pyridine N atom is protonated and the carboxy –OH group is deprotonated. The benzene and pyridinium rings are inclined with a dihedral angle of 6.63 (5)° between them. In the crystal, intermolecular O—H···O and N—H···O hydrogen-bonding interactions link adjacent molecules into a two-dimensional double layered supramolecular network.

Related literature

For the use of pyridinecarboxylate acid in coordination chemistry and for related structures, see: Jia *et al.* (2007); Zhang *et al.* (2011).



Experimental

Crystal data

$C_{12}H_{10}N_2O_2\cdot H_2O$
M_r = 232.24
Monoclinic, $P2_1/n$
a = 7.796 (2) Å
b = 7.808 (2) Å
c = 18.480 (5) Å
β = 95.165 (14)°
V = 1120.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.23 × 0.16 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.985
11449 measured reflections
2554 independent reflections
1505 reflections with $I > 2\sigma(I)$
R_{int} = 0.090

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.208
S = 1.01
2554 reflections
160 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	1.82	2.648 (3)	160
N2—H2A···O2^{i}	0.86	2.07	2.911 (4)	167
N2—H2B···O3	0.86	2.09	2.921 (4)	163
O3—H3C···O2^{ii}	0.86 (2)	1.99 (2)	2.849 (4)	178 (4)
O3—H3D···O1^{iii}	0.86 (2)	1.91 (2)	2.768 (4)	176 (5)

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2150).

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supporting information

Acta Cryst. (2012). E**68**, o2749 [doi:10.1107/S1600536812035854]

2-Amino-5-(4-carboxylatophenyl)pyridinium monohydrate

Xiao-Hong Wei, Hong Yan and Wei-Gong Lin

S1. Comment

Rigid pyridinecarboxylate ligands have been extensively employed to react with metal ions and generate coordination polymers with fascinating structures and properties(Jia *et al.*, 2007; Zhang *et al.*, 2011). We attempted to synthesize a Zn^{II}complex with the ligand in hydrothermal synthesis conditions. However the title compound was obtained, its structure is reported here.

The asymmetric unit comprises one 2-amino-5-(4-carboxylatophenyl)pyridinium molecule and one lattice water. The dihedral angel between the benzene ring and pyridinium ring is 6.63 (5)°, while the deprotonated carboxylate COO(O1—C12—O2) group is slightly twisted with an angle of 13.74 (3) ° (Fig. 1). Intermolecular O—H···O and N—H···O hydrogen- bonding interactions (Table 1)) link adjacent molecules into a two-dimensional double layered supramolecular network (Fig. 2).

S2. Experimental

A mixture of 4-(6-aminopyridin-3-yl)benzoic acid (0.0214 g, 0.1 mmol), $Zn(CH_3COO)_2.2H_2O$ (0.0219 g, 0.1 mmol) and water (8 ml) was stired vigorously for 30 min and then sealed in a Teflon-lined stainless-steel autoclave. The autoclave was heated and maintained at 393 K for 2 days, and then cooled to room temperature at 5 K h^{-1} to obtain colorless prism crystals suitable for X-ray analysis.

S3. Refinement

The H atoms bonded to C and N atoms were positioned geometrically (C—H = 0.93 Å, N—H = 0.86 Å) and allowed to ride on their parent atoms, with U_{iso}(H) value equal to 1.2U_{eq}(C or N). The H atoms bonded to water O atoms were located in a difference Fourier map and refined with O—H distance restraint of 0.85±0.02 Å, U_{iso}(H) = 1.5U_{eq}(O).

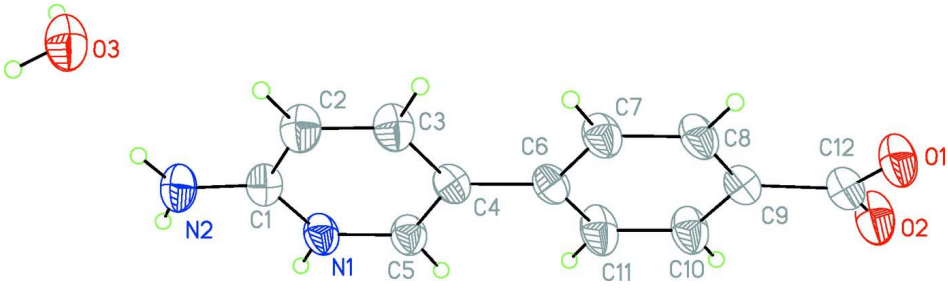

Figure 1

The structure of the title compound with the atom-numbering scheme showing displacement ellipsoids at the 30% probability level for non-H atoms.

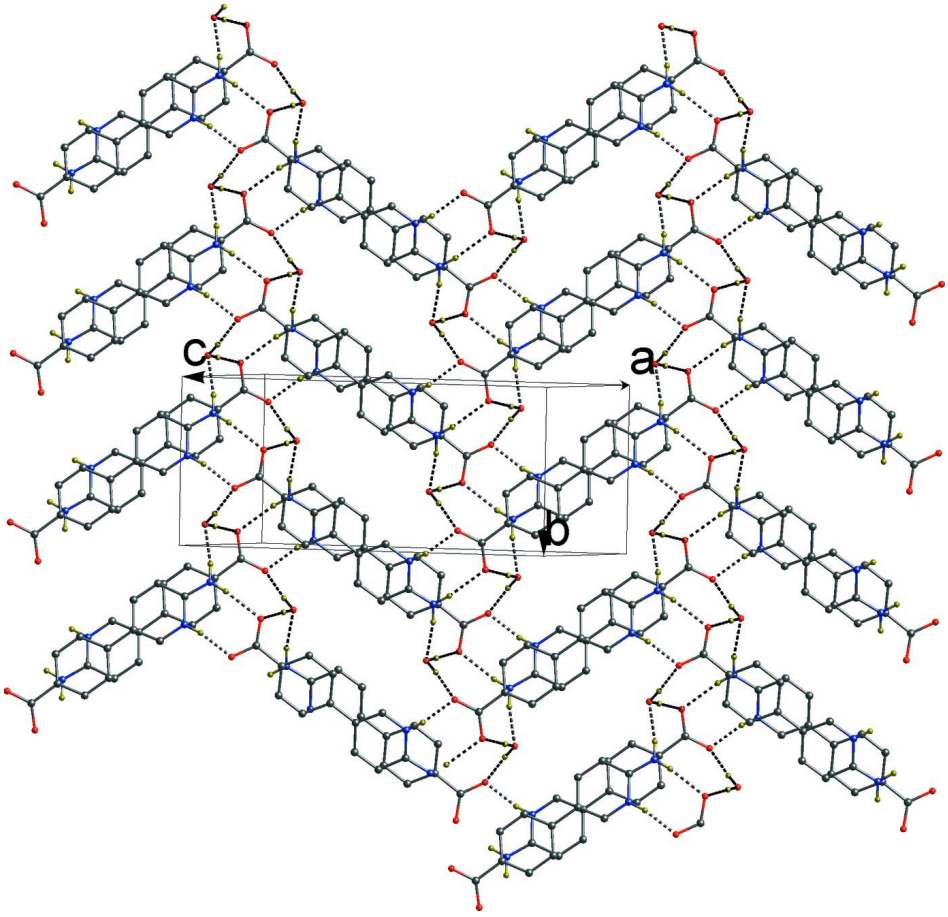

Figure 2

The two-dimensional supramolecular network formed by N—H···O and O—H···O (dashed lines) hydrogen-bonding interactions.

2-Amino-5-(4-carboxylatophenyl)pyridinium monohydrate

Crystal data

$C_{12}H_{10}N_2O_2·H_2O$
M_r = 232.24
Monoclinic, $P2_1/n$
Hall symbol: P 2yn
a = 7.796 (2) Å
b = 7.808 (2) Å
c = 18.480 (5) Å
β = 95.165 (14)°
V = 1120.4 (6) Å^3
Z = 4
$F(000)$ = 488
D_x = 1.377 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1672 reflections
θ = 2.8–27.5°
μ = 0.10 mm^{-1}
T = 296 K
Prism, colorless
0.23 × 0.16 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.985
11449 measured reflections
2554 independent reflections

1505 reflections with $I > 2\sigma(I)$
$R_{int} = 0.090$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -23 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.080$
$wR(F^2) = 0.208$
$S = 1.01$
2554 reflections
160 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2 + 0.595P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5962 (4)	0.7159 (4)	0.15326 (17)	0.0568 (8)
C2	0.6222 (4)	0.7885 (4)	0.08526 (18)	0.0669 (9)
H2C	0.6003	0.9042	0.0767	0.080*
C3	0.6796 (4)	0.6884 (4)	0.03225 (17)	0.0647 (9)
H3A	0.6927	0.7373	−0.0128	0.078*
C4	0.7203 (4)	0.5123 (4)	0.04277 (15)	0.0522 (7)
C5	0.6949 (4)	0.4505 (4)	0.11010 (16)	0.0600 (8)
H5A	0.7200	0.3362	0.1205	0.072*
C6	0.7823 (4)	0.4004 (4)	−0.01377 (15)	0.0528 (7)
C7	0.8241 (4)	0.4649 (4)	−0.08022 (16)	0.0642 (9)
H7B	0.8121	0.5815	−0.0895	0.077*
C8	0.8830 (4)	0.3594 (4)	−0.13264 (16)	0.0648 (9)
H8C	0.9119	0.4067	−0.1761	0.078*
C9	0.8999 (4)	0.1853 (4)	−0.12169 (15)	0.0555 (7)
C10	0.8584 (5)	0.1196 (4)	−0.05641 (17)	0.0728 (10)
H10A	0.8683	0.0025	−0.0478	0.087*
C11	0.8022 (5)	0.2251 (4)	−0.00347 (18)	0.0770 (11)
H11A	0.7770	0.1774	0.0404	0.092*
C12	0.9664 (4)	0.0670 (4)	−0.17777 (17)	0.0634 (8)
N1	0.6345 (3)	0.5496 (3)	0.16235 (13)	0.0606 (7)
H1A	0.6200	0.5033	0.2036	0.073*

N2	0.5351 (3)	0.8023 (4)	0.20782 (15)	0.0693 (8)
H2A	0.5210	0.7511	0.2481	0.083*
H2B	0.5100	0.9091	0.2027	0.083*
O1	1.0359 (3)	0.1364 (3)	−0.22902 (12)	0.0757 (7)
O2	0.9515 (4)	−0.0921 (3)	−0.17007 (13)	0.0853 (8)
O3	0.4085 (4)	1.1412 (3)	0.16247 (15)	0.0866 (8)
H3C	0.300 (3)	1.128 (6)	0.165 (2)	0.130*
H3D	0.447 (5)	1.207 (5)	0.1977 (19)	0.130*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0564 (17)	0.0549 (18)	0.0606 (19)	−0.0067 (14)	0.0137 (14)	−0.0057 (14)
C2	0.085 (2)	0.0504 (17)	0.068 (2)	−0.0074 (16)	0.0206 (17)	0.0030 (16)
C3	0.082 (2)	0.0570 (18)	0.0581 (19)	−0.0106 (16)	0.0216 (16)	0.0042 (15)
C4	0.0583 (17)	0.0535 (17)	0.0454 (16)	−0.0112 (14)	0.0088 (13)	0.0015 (12)
C5	0.075 (2)	0.0542 (17)	0.0516 (17)	0.0010 (16)	0.0116 (15)	0.0009 (14)
C6	0.0579 (17)	0.0570 (17)	0.0441 (16)	−0.0110 (14)	0.0079 (13)	−0.0008 (13)
C7	0.091 (2)	0.0542 (17)	0.0480 (17)	−0.0022 (17)	0.0119 (16)	0.0042 (14)
C8	0.091 (2)	0.065 (2)	0.0397 (16)	−0.0048 (18)	0.0144 (15)	0.0046 (14)
C9	0.0617 (17)	0.0595 (18)	0.0452 (16)	−0.0059 (14)	0.0042 (13)	−0.0028 (13)
C10	0.109 (3)	0.058 (2)	0.0543 (19)	0.0010 (19)	0.0242 (18)	0.0045 (15)
C11	0.124 (3)	0.058 (2)	0.0527 (18)	−0.003 (2)	0.0330 (19)	0.0092 (15)
C12	0.072 (2)	0.069 (2)	0.0497 (18)	−0.0034 (17)	0.0087 (15)	−0.0035 (16)
N1	0.0786 (17)	0.0604 (16)	0.0444 (14)	−0.0014 (13)	0.0153 (12)	0.0001 (12)
N2	0.0809 (18)	0.0634 (16)	0.0668 (17)	−0.0017 (14)	0.0254 (15)	−0.0080 (13)
O1	0.1006 (18)	0.0747 (15)	0.0557 (13)	−0.0044 (13)	0.0287 (13)	−0.0042 (11)
O2	0.130 (2)	0.0615 (15)	0.0686 (16)	−0.0009 (15)	0.0326 (15)	−0.0012 (12)
O3	0.117 (2)	0.0677 (16)	0.0786 (18)	−0.0107 (16)	0.0272 (16)	−0.0095 (13)

Geometric parameters (Å, º)

C1—N2	1.336 (4)	C8—C9	1.379 (4)
C1—N1	1.339 (4)	C8—H8C	0.9300
C1—C2	1.410 (4)	C9—C10	1.376 (4)
C2—C3	1.360 (4)	C9—C12	1.514 (4)
C2—H2C	0.9300	C10—C11	1.380 (4)
C3—C4	1.421 (4)	C10—H10A	0.9300
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.365 (4)	C12—O1	1.256 (4)
C4—C6	1.477 (4)	C12—O2	1.257 (4)
C5—N1	1.355 (4)	N1—H1A	0.8600
C5—H5A	0.9300	N2—H2A	0.8600
C6—C11	1.389 (4)	N2—H2B	0.8600
C6—C7	1.393 (4)	O3—H3C	0.860 (18)
C7—C8	1.381 (4)	O3—H3D	0.861 (18)
C7—H7B	0.9300		

N2—C1—N1	119.0 (3)	C9—C8—H8C	119.4
N2—C1—C2	124.0 (3)	C7—C8—H8C	119.4
N1—C1—C2	117.0 (3)	C10—C9—C8	118.0 (3)
C3—C2—C1	119.6 (3)	C10—C9—C12	119.6 (3)
C3—C2—H2C	120.2	C8—C9—C12	122.3 (3)
C1—C2—H2C	120.2	C9—C10—C11	120.9 (3)
C2—C3—C4	122.8 (3)	C9—C10—H10A	119.6
C2—C3—H3A	118.6	C11—C10—H10A	119.6
C4—C3—H3A	118.6	C10—C11—C6	122.0 (3)
C5—C4—C3	114.7 (3)	C10—C11—H11A	119.0
C5—C4—C6	121.3 (3)	C6—C11—H11A	119.0
C3—C4—C6	124.0 (3)	O1—C12—O2	124.3 (3)
N1—C5—C4	122.4 (3)	O1—C12—C9	116.8 (3)
N1—C5—H5A	118.8	O2—C12—C9	119.0 (3)
C4—C5—H5A	118.8	C1—N1—C5	123.5 (3)
C11—C6—C7	116.4 (3)	C1—N1—H1A	118.2
C11—C6—C4	121.7 (3)	C5—N1—H1A	118.2
C7—C6—C4	121.8 (3)	C1—N2—H2A	120.0
C8—C7—C6	121.4 (3)	C1—N2—H2B	120.0
C8—C7—H7B	119.3	H2A—N2—H2B	120.0
C6—C7—H7B	119.3	H3C—O3—H3D	108 (3)
C9—C8—C7	121.2 (3)		

N2—C1—C2—C3	−177.8 (3)	C7—C8—C9—C10	−0.8 (5)
N1—C1—C2—C3	1.7 (5)	C7—C8—C9—C12	−179.2 (3)
C1—C2—C3—C4	−2.0 (5)	C8—C9—C10—C11	−0.3 (5)
C2—C3—C4—C5	0.9 (5)	C12—C9—C10—C11	178.1 (3)
C2—C3—C4—C6	179.8 (3)	C9—C10—C11—C6	1.1 (6)
C3—C4—C5—N1	0.4 (4)	C7—C6—C11—C10	−0.8 (5)
C6—C4—C5—N1	−178.5 (3)	C4—C6—C11—C10	179.3 (3)
C5—C4—C6—C11	6.1 (5)	C10—C9—C12—O1	−165.4 (3)
C3—C4—C6—C11	−172.8 (3)	C8—C9—C12—O1	12.9 (5)
C5—C4—C6—C7	−173.9 (3)	C10—C9—C12—O2	13.6 (5)
C3—C4—C6—C7	7.3 (5)	C8—C9—C12—O2	−168.1 (3)
C11—C6—C7—C8	−0.3 (5)	N2—C1—N1—C5	179.1 (3)
C4—C6—C7—C8	179.6 (3)	C2—C1—N1—C5	−0.4 (5)
C6—C7—C8—C9	1.2 (5)	C4—C5—N1—C1	−0.7 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.86	1.82	2.648 (3)	160
N2—H2*A*···O2^{i}	0.86	2.07	2.911 (4)	167
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Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*−1/2, −*y*+3/2, *z*+1/2.