

## 2-Amino-4-methylpyridinium hexa-2,4-dienoate dihydrate

Madhukar Hemamalini and Hoong-Kun Fun\*‡

X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: hkfun@usm.my

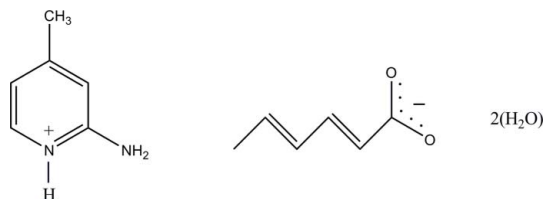
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(C-C) = 0.001$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.140; data-to-parameter ratio = 31.5.

In the title salt,  $C_6H_9N_2^+ \cdot C_6H_7O_2^- \cdot 2H_2O$ , the non-H atoms of the 2-amino-4-methylpyridinium cation are coplanar, with a maximum deviation of 0.010 (1) Å. In the crystal structure, the pyridinium N atom and the 2-amino group of the cation are hydrogen bonded to the carboxylate O atoms of the anion *via* a pair of  $N-H \cdots O$  hydrogen bonds, forming an  $R_2^2(8)$  ring motif. The sorbate anions and water molecules are linked through  $O-H \cdots O$  hydrogen bonds, forming  $R_{10}^{10}(28)$  and  $R_6^4(12)$  ring motifs. The motifs form part of a three-dimensional framework.

## Related literature

For the role of hydrogen bonding in crystal engineering, see: Goswami & Ghosh (1997); Goswami *et al.* (1998); Lehn (1992). For applications of pyridinium derivatives, see: Akkurt *et al.* (2005). For details of hydrogen bonding, see: Jeffrey & Saenger (1991); Jeffrey (1997); Scheiner (1997). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

## Crystal data

$C_6H_9N_2^+ \cdot C_6H_7O_2^- \cdot 2H_2O$   
 $M_r = 256.30$   
 Monoclinic,  $P2_1/c$

$a = 8.8233$  (4) Å  
 $b = 12.6783$  (6) Å  
 $c = 13.1647$  (6) Å

‡ Thomson Reuters ResearcherID: A-3561-2009.

$\beta = 108.279$  (1)°  
 $V = 1398.35$  (11) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation

$\mu = 0.09$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.66 \times 0.28 \times 0.25$  mm

## Data collection

Bruker APEXII DUO CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2009)  
 $T_{min} = 0.942$ ,  $T_{max} = 0.978$

23001 measured reflections  
 6087 independent reflections  
 4840 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.031$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.140$   
 $S = 1.05$   
 6087 reflections  
 193 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{max} = 0.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.24$  e Å<sup>-3</sup>

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1N1 \cdots O2^i$	0.97 (2)	1.72 (2)	2.6875 (9)	175 (1)
$N2-H1N2 \cdots O1^i$	0.91 (2)	2.01 (2)	2.9139 (10)	173 (1)
$N2-H2N2 \cdots O1W$	0.94 (2)	1.92 (2)	2.8453 (11)	166 (1)
$O2W-H1W2 \cdots O2^{ii}$	0.85 (2)	1.91 (2)	2.7510 (10)	167 (2)
$O2W-H2W2 \cdots O1$	0.87 (2)	1.96 (2)	2.8140 (9)	168 (2)
$O1W-H1W1 \cdots O1^{iii}$	0.84 (2)	2.05 (2)	2.8777 (10)	168 (2)
$O1W-H2W1 \cdots O2W$	0.86 (2)	1.88 (2)	2.7425 (11)	173 (2)

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); 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 PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5155).

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**supplementary materials**

*Acta Cryst.* (2010). E66, o2397-o2398 [ doi:10.1107/S1600536810033076 ]

## 2-Amino-4-methylpyridinium hexa-2,4-dienoate dihydrate

M. Hemamalini and H.-K. Fun

### Comment

Hydrogen bonding plays a key role in molecular recognition (Goswami & Ghosh, 1997) and crystal engineering research (Goswami *et al.*, 1998). The design of highly specific solid-state compounds is of considerable significance in organic chemistry due to important applications of these compounds in the development of new optical, magnetic and electronic systems (Lehn, 1992). Pyridinium derivatives often possess antibacterial and antifungal activities (Akkurt *et al.*, 2005). They are often involved in hydrogen-bonding interactions (Jeffrey & Saenger, 1991; Jeffrey, 1997; Scheiner, 1997). In order to study some hydrogen bonding interactions, the synthesis and structure of the title salt, (I), is presented here.

The asymmetric unit of (I) contains one 2-amino-4-methylpyridinium cation, one sorbate anion and two water molecules (Fig. 1). The non-H atoms of the 2-amino-4-methylpyridinium cation are coplanar, with a maximum deviation of 0.010 (1) Å for atom N1. The protonation of atom N1 has led to a slight increase in the C1—N1—C5 angle to 121.96 (6)°. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges.

In the crystal packing (Fig. 2), the protonated N1 atom and one of the 2-amino group hydrogen (H1N2) are hydrogen-bonded to the carboxylate oxygen atoms (O1 and O2) via a pair of intermolecular N1—H1N1...O2 and N2—H1N2...O1 hydrogen bonds forming an  $R_2^2(8)$  ring motif (Bernstein *et al.*, 1995). The sorbate anion and two water molecules are linked through O2W—H1W2...O2, O2W—H2W2...O1, O1W—H1W1...O1 and O1W—H2W1...O2W (Table 1) hydrogen-bonds, forming  $R_{10}^{10}(28)$  and  $R_6^4(12)$  ring motifs (Fig. 3).

### Experimental

A hot methanol solution (20 ml) of 2-amino-4-methylpyridine (54 mg, Aldrich) and sorbic acid (56 mg, Merck) were mixed and warmed over a heating magnetic stirrer hotplate for a few minutes. The resulting solution was allowed to cool slowly at room temperature and crystals of the title compound appeared after a few days.

### Refinement

Atoms H1N1, H1N2, H2N2, H1W2, H2W2, H1W1 and H2W1 were located in a difference Fourier map and were refined freely [N—H = 0.911 (18)–0.967 (17) Å and O—H = 0.84 (18)–0.87 (2) Å]. The remaining H atoms were positioned geometrically [C—H = 0.93 or 0.96 Å] and were refined using a riding model, with  $U_{iso}(H) = 1.2$  or  $1.5 U_{eq}(C)$ . A rotating group model was used for the methyl group.

## Figures

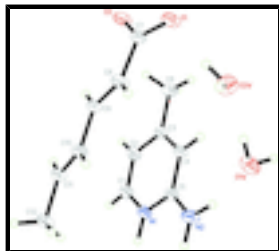


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

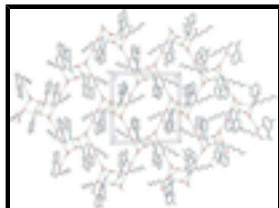


Fig. 2. The crystal packing of the title compound, showing part of a hydrogen-bonded (dashed lines) three-dimensional network. H atoms not involved in the interactions have been omitted for clarity.

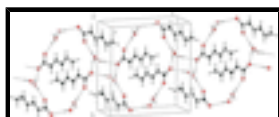
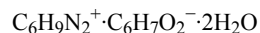


Fig. 3. Part of a hydrogen-bonded (dashed lines) two-dimensional network made up of anions and water molecules.

## 2-Amino-4-methylpyridinium hexa-2,4-dienoate dihydrate

### Crystal data



$M_r = 256.30$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 8.8233\ (4)\ \text{\AA}$

$b = 12.6783\ (6)\ \text{\AA}$

$c = 13.1647\ (6)\ \text{\AA}$

$\beta = 108.279\ (1)^\circ$

$V = 1398.35\ (11)\ \text{\AA}^3$

$Z = 4$

$F(000) = 552$

$D_x = 1.217\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 7645 reflections

$\theta = 2.9\text{--}34.9^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Needle, brown

$0.66 \times 0.28 \times 0.25\ \text{mm}$

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)

$T_{\min} = 0.942$ ,  $T_{\max} = 0.978$

23001 measured reflections

6087 independent reflections

4840 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 35.1^\circ$ ,  $\theta_{\min} = 2.9^\circ$

$h = -14 \rightarrow 14$

$k = -20 \rightarrow 20$

$l = -21 \rightarrow 21$

*Refinement*

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.140$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 0.1516P]$
6087 reflections	where $P = (F_o^2 + 2F_c^2)/3$
193 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	1.07997 (7)	0.26852 (5)	0.19290 (5)	0.02127 (12)
N2	1.01177 (8)	0.43659 (6)	0.12630 (6)	0.02585 (14)
C1	1.04257 (9)	0.16859 (7)	0.21363 (7)	0.02539 (15)
H1A	1.1237	0.1224	0.2494	0.030*
C2	0.88836 (10)	0.13495 (7)	0.18292 (7)	0.02690 (16)
H2A	0.8638	0.0664	0.1974	0.032*
C3	0.76591 (9)	0.20597 (7)	0.12849 (6)	0.02333 (14)
C4	0.80544 (8)	0.30662 (6)	0.10894 (6)	0.02151 (14)
H4A	0.7257	0.3538	0.0734	0.026*
C5	0.96682 (8)	0.33929 (6)	0.14240 (6)	0.01984 (13)
C6	0.59508 (10)	0.17064 (8)	0.09388 (8)	0.03179 (18)
H6A	0.5284	0.2258	0.0535	0.048*
H6B	0.5638	0.1549	0.1558	0.048*
H6C	0.5836	0.1087	0.0502	0.048*
O1	0.35573 (6)	0.47026 (5)	0.19351 (5)	0.02451 (12)

## supplementary materials

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O2	0.39446 (7)	0.30966 (5)	0.26595 (6)	0.02668 (13)
C7	0.44389 (8)	0.40024 (6)	0.25192 (6)	0.02007 (13)
C8	0.61399 (8)	0.42857 (6)	0.30428 (7)	0.02356 (15)
H8A	0.6422	0.4993	0.3054	0.028*
C9	0.72932 (8)	0.35883 (6)	0.34995 (6)	0.02082 (13)
H9A	0.7010	0.2886	0.3538	0.025*
C10	0.89651 (8)	0.38771 (7)	0.39373 (6)	0.02347 (14)
H10A	0.9226	0.4589	0.3960	0.028*
C11	1.01497 (9)	0.31857 (7)	0.43086 (6)	0.02396 (15)
H11A	0.9882	0.2476	0.4307	0.029*
C12	1.18754 (9)	0.34726 (8)	0.47266 (7)	0.02996 (18)
H12A	1.2317	0.3219	0.5446	0.045*
H12B	1.1986	0.4226	0.4719	0.045*
H12C	1.2434	0.3158	0.4284	0.045*
O1W	0.75170 (8)	0.57495 (6)	0.03208 (6)	0.03181 (15)
O2W	0.51394 (8)	0.62847 (5)	0.11569 (6)	0.03052 (14)
H1N1	1.192 (2)	0.2876 (12)	0.2177 (14)	0.047 (4)*
H1N2	1.118 (2)	0.4529 (13)	0.1473 (14)	0.049 (4)*
H2N2	0.9370 (19)	0.4873 (12)	0.0898 (13)	0.042 (4)*
H1W2	0.529 (2)	0.6833 (14)	0.1552 (15)	0.051 (4)*
H2W2	0.468 (2)	0.5855 (14)	0.1483 (13)	0.049 (4)*
H1W1	0.7068 (19)	0.5623 (12)	-0.0331 (14)	0.041 (4)*
H2W1	0.672 (2)	0.5876 (14)	0.0553 (16)	0.061 (5)*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0137 (2)	0.0268 (3)	0.0213 (3)	0.0011 (2)	0.00269 (19)	-0.0009 (2)
N2	0.0161 (3)	0.0250 (3)	0.0347 (4)	0.0000 (2)	0.0054 (2)	0.0003 (3)
C1	0.0194 (3)	0.0278 (3)	0.0252 (3)	0.0014 (2)	0.0017 (3)	0.0030 (3)
C2	0.0219 (3)	0.0289 (4)	0.0267 (3)	-0.0031 (3)	0.0031 (3)	0.0042 (3)
C3	0.0158 (3)	0.0327 (4)	0.0203 (3)	-0.0031 (2)	0.0038 (2)	0.0002 (3)
C4	0.0125 (3)	0.0294 (3)	0.0216 (3)	0.0009 (2)	0.0038 (2)	-0.0002 (2)
C5	0.0139 (3)	0.0252 (3)	0.0199 (3)	0.0011 (2)	0.0046 (2)	-0.0023 (2)
C6	0.0178 (3)	0.0439 (5)	0.0312 (4)	-0.0086 (3)	0.0041 (3)	0.0033 (3)
O1	0.0151 (2)	0.0244 (3)	0.0303 (3)	0.00155 (18)	0.00176 (19)	0.0031 (2)
O2	0.0139 (2)	0.0262 (3)	0.0363 (3)	-0.00069 (18)	0.0026 (2)	0.0061 (2)
C7	0.0130 (2)	0.0238 (3)	0.0224 (3)	0.0010 (2)	0.0039 (2)	-0.0004 (2)
C8	0.0134 (3)	0.0252 (3)	0.0292 (3)	-0.0009 (2)	0.0027 (2)	0.0005 (3)
C9	0.0137 (3)	0.0264 (3)	0.0218 (3)	0.0000 (2)	0.0047 (2)	0.0005 (2)
C10	0.0134 (3)	0.0282 (3)	0.0268 (3)	-0.0005 (2)	0.0034 (2)	0.0012 (3)
C11	0.0143 (3)	0.0332 (4)	0.0230 (3)	0.0010 (2)	0.0038 (2)	0.0006 (3)
C12	0.0128 (3)	0.0450 (5)	0.0293 (4)	0.0016 (3)	0.0026 (3)	0.0013 (3)
O1W	0.0235 (3)	0.0377 (3)	0.0302 (3)	0.0067 (2)	0.0027 (2)	-0.0046 (3)
O2W	0.0328 (3)	0.0252 (3)	0.0357 (3)	-0.0037 (2)	0.0138 (3)	-0.0036 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

N1—C5	1.3518 (9)	O2—C7	1.2624 (9)
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N1—C1	1.3583 (11)	C7—C8	1.4859 (10)
N1—H1N1	0.967 (17)	C8—C9	1.3397 (10)
N2—C5	1.3329 (10)	C8—H8A	0.93
N2—H1N2	0.911 (18)	C9—C10	1.4522 (10)
N2—H2N2	0.938 (16)	C9—H9A	0.93
C1—C2	1.3607 (11)	C10—C11	1.3339 (11)
C1—H1A	0.93	C10—H10A	0.93
C2—C3	1.4163 (12)	C11—C12	1.4927 (11)
C2—H2A	0.93	C11—H11A	0.93
C3—C4	1.3684 (11)	C12—H12A	0.96
C3—C6	1.4997 (11)	C12—H12B	0.96
C4—C5	1.4141 (10)	C12—H12C	0.96
C4—H4A	0.93	O1W—H1W1	0.840 (18)
C6—H6A	0.96	O1W—H2W1	0.87 (2)
C6—H6B	0.96	O2W—H1W2	0.853 (18)
C6—H6C	0.96	O2W—H2W2	0.868 (17)
O1—C7	1.2686 (9)		
C5—N1—C1	121.96 (6)	H6A—C6—H6C	109.5
C5—N1—H1N1	121.1 (9)	H6B—C6—H6C	109.5
C1—N1—H1N1	116.9 (9)	O2—C7—O1	123.44 (6)
C5—N2—H1N2	119.3 (11)	O2—C7—C8	119.81 (6)
C5—N2—H2N2	121.3 (9)	O1—C7—C8	116.75 (7)
H1N2—N2—H2N2	119.3 (14)	C9—C8—C7	124.27 (7)
N1—C1—C2	121.07 (7)	C9—C8—H8A	117.9
N1—C1—H1A	119.5	C7—C8—H8A	117.9
C2—C1—H1A	119.5	C8—C9—C10	123.08 (7)
C1—C2—C3	118.95 (8)	C8—C9—H9A	118.5
C1—C2—H2A	120.5	C10—C9—H9A	118.5
C3—C2—H2A	120.5	C11—C10—C9	124.16 (8)
C4—C3—C2	119.28 (7)	C11—C10—H10A	117.9
C4—C3—C6	120.83 (7)	C9—C10—H10A	117.9
C2—C3—C6	119.89 (8)	C10—C11—C12	124.50 (8)
C3—C4—C5	120.38 (7)	C10—C11—H11A	117.7
C3—C4—H4A	119.8	C12—C11—H11A	117.7
C5—C4—H4A	119.8	C11—C12—H12A	109.5
N2—C5—N1	118.80 (6)	C11—C12—H12B	109.5
N2—C5—C4	122.84 (7)	H12A—C12—H12B	109.5
N1—C5—C4	118.35 (7)	C11—C12—H12C	109.5
C3—C6—H6A	109.5	H12A—C12—H12C	109.5
C3—C6—H6B	109.5	H12B—C12—H12C	109.5
H6A—C6—H6B	109.5	H1W1—O1W—H2W1	102.7 (17)
C3—C6—H6C	109.5	H1W2—O2W—H2W2	102.4 (15)
C5—N1—C1—C2	0.83 (12)	C3—C4—C5—N2	-179.36 (8)
N1—C1—C2—C3	0.02 (13)	C3—C4—C5—N1	0.62 (11)
C1—C2—C3—C4	-0.51 (13)	O2—C7—C8—C9	13.47 (12)
C1—C2—C3—C6	180.00 (8)	O1—C7—C8—C9	-165.81 (8)
C2—C3—C4—C5	0.19 (12)	C7—C8—C9—C10	175.41 (7)
C6—C3—C4—C5	179.67 (7)	C8—C9—C10—C11	-173.75 (8)



## supplementary materials

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C1—N1—C5—N2	178.84 (8)	C9—C10—C11—C12	177.89 (8)
C1—N1—C5—C4	-1.14 (11)		

### Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1N1···O2 <sup>i</sup>	0.97 (2)	1.72 (2)	2.6875 (9)	175 (1)
N2—H1N2···O1 <sup>i</sup>	0.91 (2)	2.01 (2)	2.9139 (10)	173 (1)
N2—H2N2···O1W	0.94 (2)	1.92 (2)	2.8453 (11)	166 (1)
O2W—H1W2···O2 <sup>ii</sup>	0.85 (2)	1.91 (2)	2.7510 (10)	167 (2)
O2W—H2W2···O1	0.87 (2)	1.96 (2)	2.8140 (9)	168 (2)
O1W—H1W1···O1 <sup>iii</sup>	0.84 (2)	2.05 (2)	2.8777 (10)	168 (2)
O1W—H2W1···O2W	0.86 (2)	1.88 (2)	2.7425 (11)	173 (2)

Symmetry codes: (i)  $x+1, y, z$ ; (ii)  $-x+1, y+1/2, -z+1/2$ ; (iii)  $-x+1, -y+1, -z$ .

Fig. 1

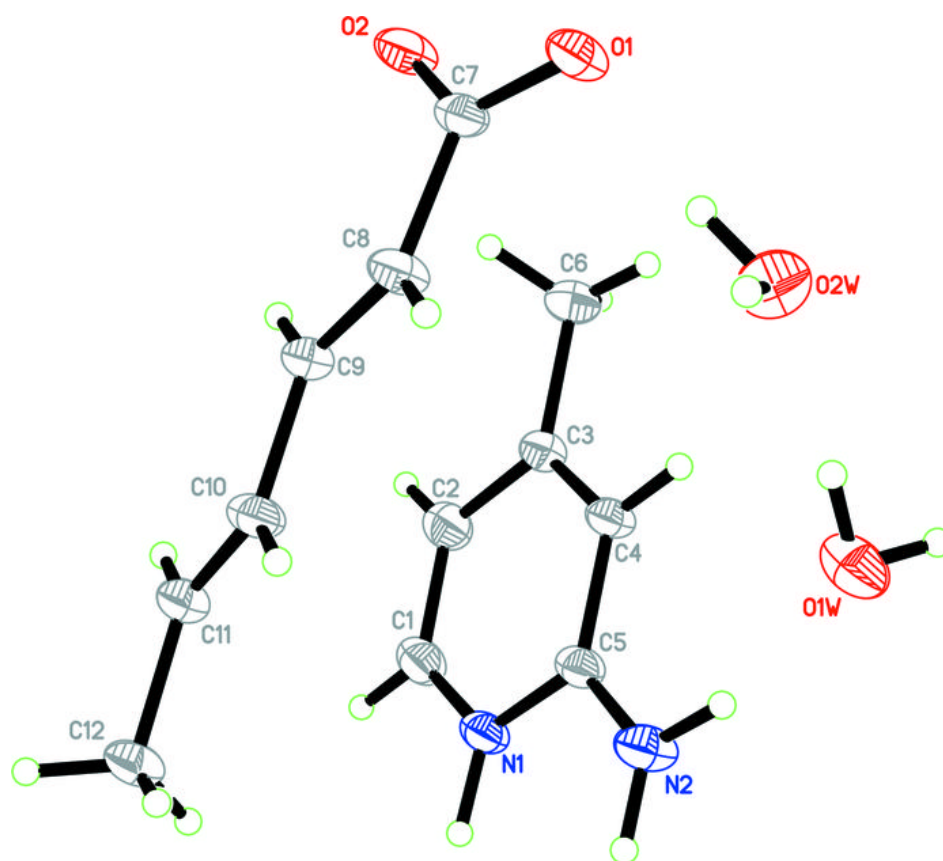


Fig. 2

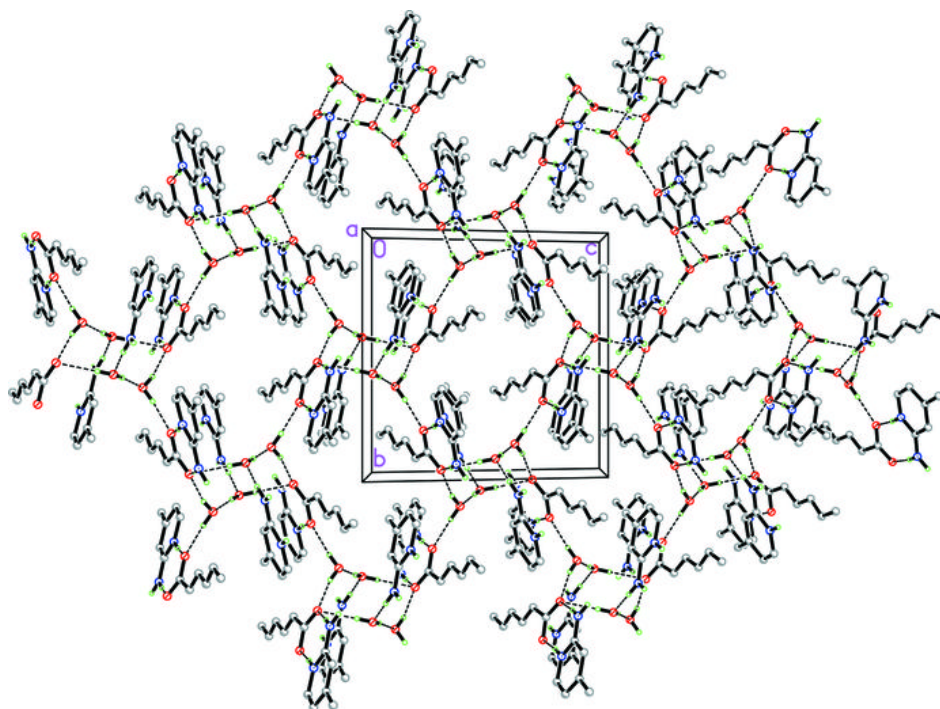


Fig. 3

