

Bis[2-(2-pyridylamino)pyridinium] squarate dihydrate

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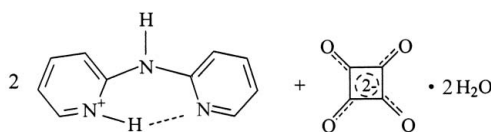
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Key indicators: single-crystal X-ray study; $T = 297$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 15.0.

In the title compound, $2\text{C}_{10}\text{H}_{10}\text{N}_3^+ \cdot \text{C}_4\text{O}_4^{2-} \cdot 2\text{H}_2\text{O}$, the squarate dianion is centrosymmetric. The organic cation shows an unusual, approximately symmetrical, intramolecular $\text{N} \cdots \text{H} \cdots \text{N}$ hydrogen bond. The other hydrogen bonds are conventional $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ links, resulting in chains.

Related literature

For related literature, see: Bertolasi *et al.* (1996, 2001); Farrugia (1999); Gilli & Gilli (2000); Gilli *et al.* (1994); Köroglu *et al.* (2005); Liebeskind *et al.* (1993); Mathew *et al.* (2002); Reetz *et al.* (1994); Seitz & Imming (1992); Steiner *et al.* (2000); Uçar *et al.* (2004, 2005).



Experimental

Crystal data

$2\text{C}_{10}\text{H}_{10}\text{N}_3^+ \cdot \text{C}_4\text{O}_4^{2-} \cdot 2\text{H}_2\text{O}$

$M_r = 492.50$

Triclinic, $P\bar{1}$

$a = 8.072$ (2) Å

$b = 8.493$ (3) Å

$c = 8.833$ (2) Å

$\alpha = 74.34$ (3)°

$\beta = 87.26$ (2)°

$\gamma = 71.85$ (4)°

$V = 553.6$ (3) Å³

$Z = 1$

Mo $K\alpha$ radiation

$\mu = 0.11$ mm⁻¹

$T = 297$ (2) K

$0.35 \times 0.24 \times 0.18$ mm

Data collection

Stoe IPDSII diffractometer

Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)

$T_{\min} = 0.947$, $T_{\max} = 0.981$

6024 measured reflections

2634 independent reflections

2027 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.122$

$S = 1.02$

2634 reflections

176 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.27$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N2}-\text{H2A} \cdots \text{O1}^{\text{i}}$	0.86	1.84	2.7008 (17)	178
$\text{O3}-\text{H3A} \cdots \text{O1}^{\text{ii}}$	0.832 (17)	2.031 (18)	2.8382 (19)	163 (2)
$\text{N3}-\text{H1A} \cdots \text{N1}$	1.28 (2)	1.415 (19)	2.5857 (18)	147.8 (15)
$\text{O3}-\text{H3B} \cdots \text{O2}$	0.834 (17)	1.951 (18)	2.765 (2)	165 (3)

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP III* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2459).

References

- Bertolasi, V., Gilli, P., Ferretti, V. & Gilli, G. (2001). *Acta Cryst.* **B57**, 591–598.
- Bertolasi, V., Gilli, P., Ferretti, V. & Gilli, G. (1996). *Chem. Eur. J.* **2**, 925–934.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Gilli, G. & Gilli, P. (2000). *J. Mol. Struct.* **552**, 1–15.
- Gilli, P., Ferretti, V., Bertolasi, V. & Gilli, G. (1994). *J. Am. Chem. Soc.* **116**, 909–915.
- Köroglu, A., Bulut, A., Uçar, I., Nichol, G. S., Harrington, R. W. & Clegg, W. (2005). *Acta Cryst.* **C61**, o678–o680.
- Liebeskind, L. S., Yu, M. S., Yu, R. H., Wang, J. & Glidewell, C. (1993). *J. Am. Chem. Soc.* **115**, 9048–9055.
- Mathew, S., Paul, G., Shivasankar, K., Choudhury, A. & Rao, C. N. R. (2002). *J. Mol. Struct.* **641**, 263–279.
- Reetz, M. T., Höger, S. & Harms, K. (1994). *Angew. Chem. Int. Ed. Engl.* **33**, 181–183.
- Seitz, G. & Imming, P. (1992). *Chem. Rev.* **92**, 1227–1260.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Steiner, T., Schreurs, A. M. M., Lutz, M. & Kroon, J. (2000). *Acta Cryst.* **C56**, 577–579.
- Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
- Uçar, I., Bulut, A. & Büyükgüngör, O. (2005). *Acta Cryst.* **C61**, m266–m268.
- Uçar, I., Bulut, A., Yeşilel, O. Z. & Büyükgüngör, O. (2004). *Acta Cryst.* **C60**, o585–o588.

supplementary materials

Acta Cryst. (2007). E63, o3377 [doi:10.1107/S160053680703139X]

Bis[2-(2-pyridylamino)pyridinium] squarate dihydrate

I. Uçar, A. Bulut and O. Büyükgüngör

Comment

Squaric acid, H₂Sq, is a very strong dibasic acid and has been studied for potential application to xerographic photoreceptors, organic solar cells and optical recording (Seitz & Imming, 1992; Liebeskind *et al.*, 1993). It is also a useful tool for constructing crystalline architecture because of its rigid and flat four-membered ring framework (Reetz *et al.*, 1994). Squaric acid (H₂Sq) can be found in three forms, *viz.* (a) as uncharged H₂Sq, (b) as the HSq⁻ monoanion and (c) as Sq²⁻ dianions on deprotonation by amines. These forms have been observed to crystallize with various types of hydrogen bonding, as summarized by Bertolasi *et al.* (2001). Our ongoing research on metallic and organic salts of squaric acid (Uçar *et al.*, 2004; Uçar *et al.*, 2005; Köroğlu *et al.*, 2005), we have synthesized the title compounds, (I), in which the dianion form of squaric acid is observed.

Each squaric acid molecule donates both its H atoms to the pyridine N atom of two 2,2'-dipyridylamine molecules, forming the bis(2,2'-dipyridiniumamine) squarate dihydrate salt. The C₄O₄²⁻ anion is centrosymmetric. (Fig. 1). The most noteworthy aspect of the structure of (I) concerns the hydrogen bonding (Table 1). Intermolecular hydrogen bonding is conventional (in terms of geometry), with each of the H atoms being donated. However, the N—H...N intramolecular hydrogen bond associated with the pyridine nitrogen atoms has much more unusual behaviour. The freely refined N—H bond length of 1.28 (2) Å is very long for an N—H covalent bond, which would be expected to be around 0.87 Å in an X-ray crystallographic analysis. Consequently, the H...N distance is 1.42 (2) Å, which is rather short. Given that the overall N...N distance is relatively short at 2.586 (2) Å, these values indicate a strong hydrogen bond, which nevertheless display unusual disorder or thermal motion. A difference Fourier map (Fig. 2; Farrugia, 1999) of the electron density associated with this H atom shows this to be smeared out between the dipyridinium N atoms, with the maximum lying closer to the N3 atom. These type hydrogen bonds have been called "positive charge assisted hydrogen bonds (N⁺—H...N or N...H—N⁺)" by Gilli and co-workers [Gilli *et al.*, 1994; Bertolasi *et al.*, 1996; Gilli & Gilli, 2000;] and found in organic amines and carboxylic acids [Steiner *et al.*, 2000; Mathew *et al.*, 2002].

In the crystal of (I), both intermolecular H bonds and van der Waals interactions combine to stabilize the extended structure (Fig. 3). The crystal water molecule and amine nitrogen atom link cations to dianions, acting as hydrogen-bond donors to the squarate oxygen atoms. These interactions mediate the formation of chains in the *ac* plane (Fig. 3) and adjacent chains are linked by van der Waals interactions.

Experimental

Compound (I) was prepared by mixing squaric acid and 2,2'-dipyridylamine in a 1:2 molar ratio in a mixed solution of methanol and water (1:1 *v/v*, 50 ml), with stirring at 333 K for 1 h. Crystals of (I) were obtained by slow evaporation of the solvent in about a week. The crystals were filtered off, washed with methanol and dried *in vacuo*.

Refinement

H atoms attached to C atoms and amine N atoms were placed in calculated positions (N—H = 0.86 Å, C—H = 0.93 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The remaining H atoms were located in a difference map. The H atoms of water molecule were refined with the O—H distance restrained to 0.82 (2) Å.

Figures

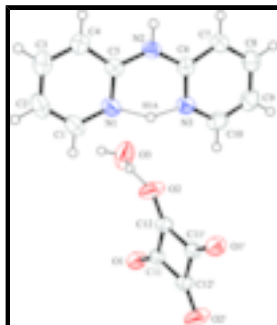


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry code: (i) $1 - x, 1 - y, -z$. Dashed lines indicate the hydrogen bonds.

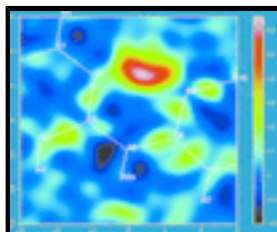


Fig. 2. A difference Fourier map of the electron density associated with the intramolecular N...H...N interaction. The diffuse nature of the electron density is clear, with the largest concentration of electron density located closer to the atom N3 than atom N1.

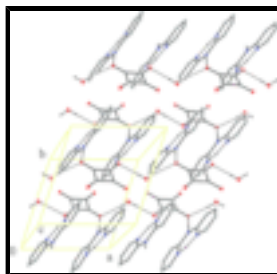


Fig. 3. The hydrogen-bonding and van der Waals interactions of (I) in the unit cell (dashed lines indicate the hydrogen bonds).

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$M_r = 492.50$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.072$ (2) Å

$b = 8.493$ (3) Å

$c = 8.833$ (2) Å

$Z = 1$

$F_{000} = 258.0$

$D_x = 1.477$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71069$ Å

Cell parameters from 1875 reflections

$\theta = 2.6\text{--}27.8^\circ$

$\mu = 0.11$ mm⁻¹

$\alpha = 74.34 (3)^\circ$
 $\beta = 87.26 (2)^\circ$
 $\gamma = 71.85 (4)^\circ$
 $V = 553.6 (3) \text{ \AA}^3$

$T = 297 (2) \text{ K}$
 Block, colourless
 $0.35 \times 0.24 \times 0.18 \text{ mm}$

Data collection

Stoe IPDS II diffractometer
 Radiation source: fine-focus sealed tube
 Monochromator: graphite
 Detector resolution: $6.67 \text{ pixels mm}^{-1}$
 $T = 297(2) \text{ K}$
 ω scans
 Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
 $T_{\min} = 0.947, T_{\max} = 0.981$
 6024 measured reflections

2634 independent reflections
 2027 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\max} = 28.2^\circ$
 $\theta_{\min} = 2.6^\circ$
 $h = -9 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.122$
 $S = 1.02$
 2634 reflections
 176 parameters
 2 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
 $w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 0.0549P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.27 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick, 1997),
 $F_c^* = kFc[1 + 0.001 \times Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.079 (12)

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 $F^2 > 2\sigma(F^2)$ 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.

supplementary materials

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1787 (2)	-0.0003 (2)	0.20087 (18)	0.0525 (4)
H1	0.1856	0.0817	0.1086	0.063*
C2	0.1266 (2)	-0.1349 (2)	0.1916 (2)	0.0562 (4)
H2	0.1019	-0.1468	0.0942	0.067*
C3	0.1108 (2)	-0.2539 (2)	0.3286 (2)	0.0518 (4)
H3	0.0732	-0.3457	0.3243	0.062*
C4	0.15007 (19)	-0.23637 (18)	0.46912 (19)	0.0440 (3)
H4	0.1387	-0.3145	0.5625	0.053*
C5	0.20815 (17)	-0.09827 (17)	0.47064 (16)	0.0372 (3)
C6	0.30437 (17)	0.05217 (16)	0.63285 (16)	0.0367 (3)
C7	0.3349 (2)	0.05677 (19)	0.78463 (17)	0.0436 (3)
H7	0.3259	-0.0310	0.8710	0.052*
C8	0.3784 (2)	0.1927 (2)	0.8039 (2)	0.0519 (4)
H8	0.3975	0.1990	0.9048	0.062*
C9	0.3944 (2)	0.3214 (2)	0.6754 (2)	0.0535 (4)
H9	0.4246	0.4142	0.6884	0.064*
C10	0.3654 (2)	0.30938 (19)	0.5314 (2)	0.0495 (4)
H10	0.3760	0.3954	0.4440	0.059*
C11	0.38626 (17)	0.57812 (16)	-0.05777 (14)	0.0344 (3)
C12	0.43433 (18)	0.42336 (17)	0.07214 (15)	0.0371 (3)
N1	0.22009 (17)	0.01827 (15)	0.33788 (14)	0.0430 (3)
N2	0.25340 (16)	-0.07779 (14)	0.60874 (13)	0.0392 (3)
H2A	0.2493	-0.1574	0.6917	0.047*
N3	0.32133 (16)	0.17666 (14)	0.50969 (14)	0.0415 (3)
O1	0.24748 (14)	0.67258 (13)	-0.12805 (13)	0.0494 (3)
O2	0.35589 (16)	0.33000 (16)	0.15768 (15)	0.0639 (4)
O3	0.0043 (2)	0.4689 (2)	0.2011 (2)	0.0858 (5)
H3A	-0.058 (3)	0.426 (3)	0.163 (3)	0.088 (8)*
H3B	0.105 (3)	0.435 (3)	0.171 (3)	0.095 (8)*
H1A	0.282 (3)	0.132 (2)	0.392 (2)	0.064 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0580 (10)	0.0630 (10)	0.0364 (7)	-0.0161 (8)	0.0007 (7)	-0.0158 (7)
C2	0.0512 (9)	0.0726 (11)	0.0480 (9)	-0.0113 (8)	-0.0037 (7)	-0.0297 (8)
C3	0.0442 (8)	0.0512 (8)	0.0648 (10)	-0.0109 (7)	-0.0037 (7)	-0.0270 (7)
C4	0.0410 (8)	0.0397 (7)	0.0498 (8)	-0.0097 (6)	-0.0012 (6)	-0.0125 (6)
C5	0.0327 (7)	0.0379 (7)	0.0375 (7)	-0.0040 (5)	0.0010 (5)	-0.0123 (5)
C6	0.0325 (6)	0.0347 (6)	0.0405 (7)	-0.0050 (5)	0.0017 (5)	-0.0126 (5)
C7	0.0462 (8)	0.0453 (7)	0.0390 (7)	-0.0134 (6)	0.0009 (6)	-0.0116 (6)
C8	0.0545 (9)	0.0564 (9)	0.0519 (9)	-0.0162 (7)	0.0005 (7)	-0.0269 (7)
C9	0.0591 (10)	0.0446 (8)	0.0655 (10)	-0.0202 (7)	0.0059 (8)	-0.0249 (7)
C10	0.0568 (9)	0.0376 (7)	0.0554 (9)	-0.0172 (7)	0.0075 (7)	-0.0124 (6)

C11	0.0396 (7)	0.0343 (6)	0.0293 (6)	-0.0137 (5)	-0.0012 (5)	-0.0055 (5)
C12	0.0409 (7)	0.0361 (6)	0.0326 (6)	-0.0146 (5)	0.0004 (5)	-0.0031 (5)
N1	0.0483 (7)	0.0452 (6)	0.0355 (6)	-0.0138 (5)	0.0023 (5)	-0.0116 (5)
N2	0.0465 (7)	0.0348 (6)	0.0340 (6)	-0.0124 (5)	-0.0001 (5)	-0.0052 (4)
N3	0.0472 (7)	0.0363 (6)	0.0398 (6)	-0.0117 (5)	0.0026 (5)	-0.0101 (5)
O1	0.0410 (6)	0.0464 (6)	0.0497 (6)	-0.0138 (5)	-0.0091 (5)	0.0074 (4)
O2	0.0490 (7)	0.0599 (7)	0.0655 (8)	-0.0244 (5)	0.0033 (5)	0.0200 (6)
O3	0.0617 (9)	0.1184 (13)	0.1131 (13)	-0.0447 (9)	0.0245 (9)	-0.0735 (11)

Geometric parameters (Å, °)

C1—N1	1.333 (2)	C8—C9	1.380 (2)
C1—C2	1.358 (3)	C8—H8	0.9300
C1—H1	0.9300	C9—C10	1.340 (2)
C2—C3	1.382 (3)	C9—H9	0.9300
C2—H2	0.9300	C10—N3	1.3441 (19)
C3—C4	1.353 (2)	C10—H10	0.9300
C3—H3	0.9300	C11—O1	1.2335 (17)
C4—C5	1.395 (2)	C11—C12 ⁱ	1.4440 (19)
C4—H4	0.9300	C11—C12	1.4511 (17)
C5—N1	1.3366 (18)	C12—O2	1.2426 (16)
C5—N2	1.3596 (18)	C12—C11 ⁱ	1.4440 (19)
C6—N3	1.3323 (18)	N1—H1A	1.415 (19)
C6—N2	1.3605 (18)	N2—H2A	0.8600
C6—C7	1.388 (2)	N3—H1A	1.28 (2)
C7—C8	1.360 (2)	O3—H3A	0.832 (17)
C7—H7	0.9300	O3—H3B	0.834 (17)
N1—C1—C2	122.13 (16)	C10—C9—H9	120.8
N1—C1—H1	118.9	C8—C9—H9	120.8
C2—C1—H1	118.9	C9—C10—N3	121.90 (15)
C1—C2—C3	119.11 (15)	C9—C10—H10	119.0
C1—C2—H2	120.4	N3—C10—H10	119.0
C3—C2—H2	120.4	O1—C11—C12 ⁱ	134.52 (12)
C4—C3—C2	119.71 (15)	O1—C11—C12	134.30 (13)
C4—C3—H3	120.1	C12 ⁱ —C11—C12	91.18 (11)
C2—C3—H3	120.1	O1—C11—C11 ⁱ	179.69 (14)
C3—C4—C5	118.45 (15)	C12 ⁱ —C11—C11 ⁱ	45.73 (8)
C3—C4—H4	120.8	C12—C11—C11 ⁱ	45.45 (8)
C5—C4—H4	120.8	O2—C12—C11 ⁱ	135.38 (13)
N1—C5—N2	117.87 (12)	O2—C12—C11	135.79 (14)
N1—C5—C4	121.56 (13)	C11 ⁱ —C12—C11	88.82 (11)
N2—C5—C4	120.57 (13)	C1—N1—C5	118.99 (13)
N3—C6—N2	119.44 (13)	C1—N1—H1A	138.1 (8)
N3—C6—C7	120.33 (13)	C5—N1—H1A	102.9 (8)
N2—C6—C7	120.22 (12)	C5—N2—C6	128.48 (12)
C8—C7—C6	118.39 (14)	C5—N2—H2A	115.8
C8—C7—H7	120.8	C6—N2—H2A	115.8

supplementary materials

C6—C7—H7	120.8	C6—N3—C10	120.29 (13)
C7—C8—C9	120.69 (15)	C6—N3—H1A	103.3 (8)
C7—C8—H8	119.7	C10—N3—H1A	136.4 (8)
C9—C8—H8	119.7	H3A—O3—H3B	108 (3)
C10—C9—C8	118.38 (14)		
N1—C1—C2—C3	2.0 (3)	O1—C11—C12—C11 ⁱ	179.75 (19)
C1—C2—C3—C4	-1.1 (2)	C12 ⁱ —C11—C12—C11 ⁱ	0.0
C2—C3—C4—C5	-0.9 (2)	C2—C1—N1—C5	-0.8 (2)
C3—C4—C5—N1	2.1 (2)	N2—C5—N1—C1	179.13 (13)
C3—C4—C5—N2	-178.34 (13)	C4—C5—N1—C1	-1.3 (2)
N3—C6—C7—C8	1.4 (2)	N1—C5—N2—C6	2.9 (2)
N2—C6—C7—C8	-177.22 (14)	C4—C5—N2—C6	-176.63 (13)
C6—C7—C8—C9	-1.0 (2)	N3—C6—N2—C5	-2.9 (2)
C7—C8—C9—C10	0.3 (3)	C7—C6—N2—C5	175.82 (13)
C8—C9—C10—N3	0.1 (3)	N2—C6—N3—C10	177.57 (13)
O1—C11—C12—O2	0.8 (3)	C7—C6—N3—C10	-1.1 (2)
C12 ⁱ —C11—C12—O2	-178.9 (2)	C9—C10—N3—C6	0.3 (2)
C11 ⁱ —C11—C12—O2	-178.9 (2)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A \cdots O1 ⁱⁱ	0.86	1.84	2.7008 (17)	178
O3—H3A \cdots O1 ⁱⁱⁱ	0.832 (17)	2.031 (18)	2.8382 (19)	163 (2)
N3—H1A \cdots N1	1.28 (2)	1.415 (19)	2.5857 (18)	147.8 (15)
O3—H3B \cdots O2	0.834 (17)	1.951 (18)	2.765 (2)	165 (3)

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

Fig. 1

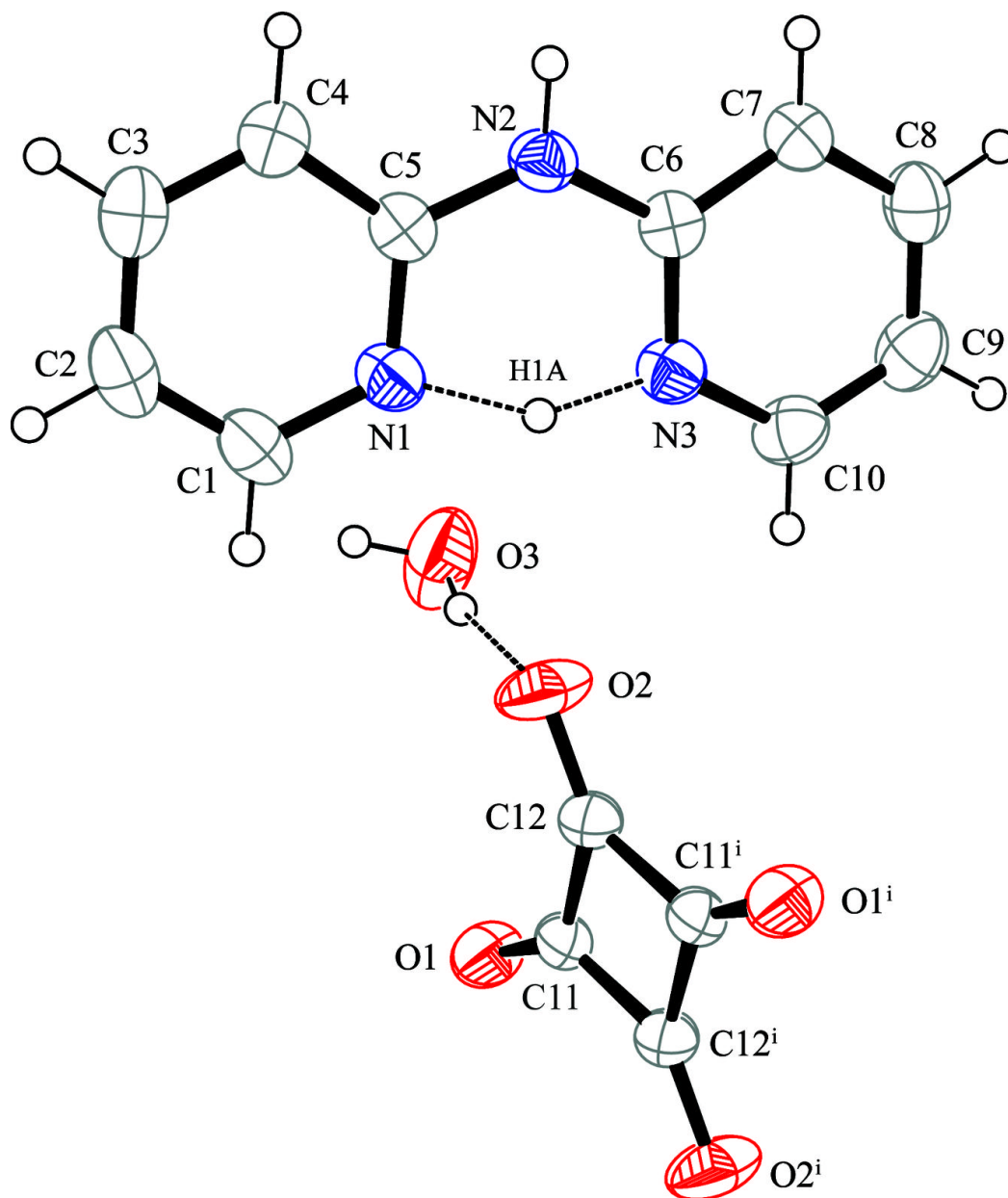


Fig. 2

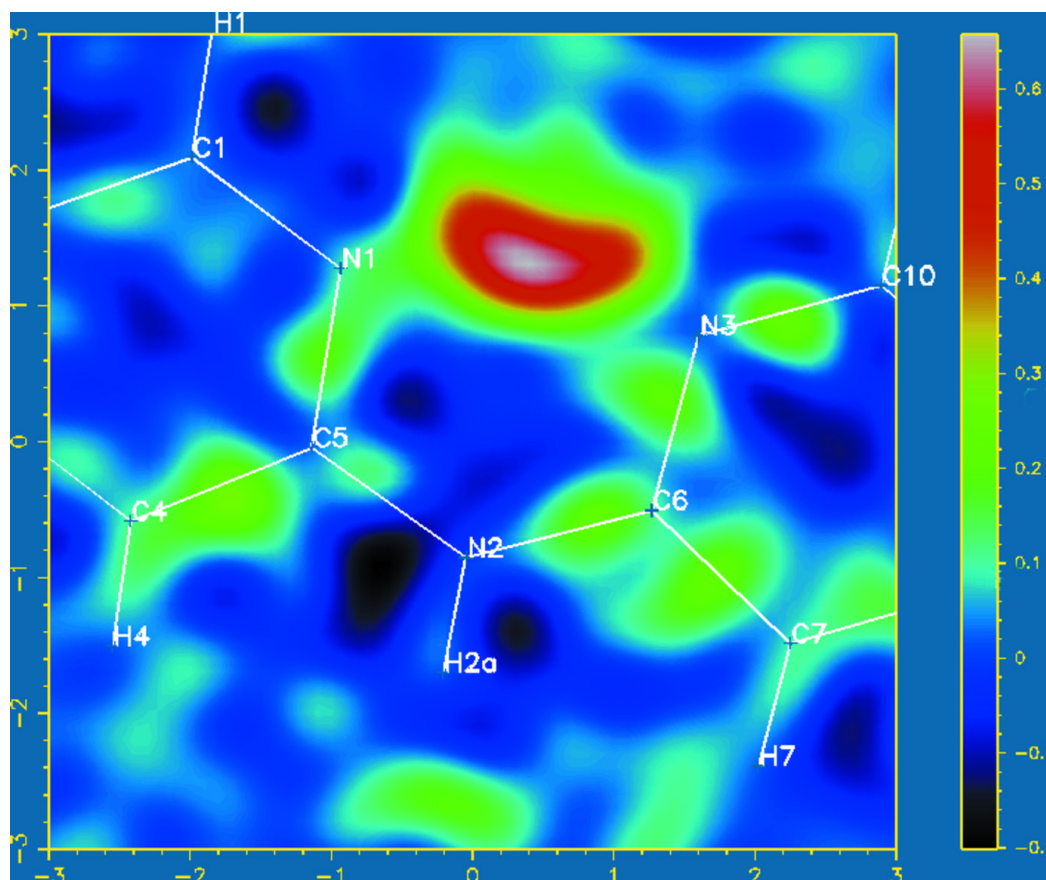


Fig. 3

