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Diaminopyrimidinium squarate 1.394-hydrate

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Key indicators

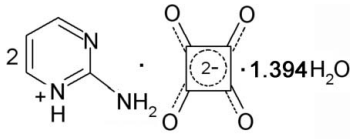
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.104
Data-to-parameter ratio = 10.1

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

In the title compound, $2C_4H_5N_3^{+}\cdot C_4O_4^{2-}\cdot 1.394H_2O$, both the squarate and the aminopyrimidinium molecules lie on a crystallographic mirror plane and the water molecules are located between the mirror planes. The inversion-related aminopyrimidine molecules are linked through N—H···N hydrogen bonds [N···N = 2.975 (3) Å] to form dimers. The dimers and the squarate dianions are alternately arranged and linked *via* N—H···O hydrogen bonds [N···O = 2.621 (2) and 2.811 (2) Å] to form a chain along the *c* axis. Chains lying on the adjacent planes are linked *via* O—H···O hydrogen bonds [O···O = 2.713 (2) Å] involving the water molecules to form a three-dimensional network.

Comment

The crystal structure determination of the title compound, (I), was carried out as part of a project investigating the structural and physical properties of organic compounds containing squaric acid, since they have potential applications in the development of new optical, magnetic and electronic systems (Lehn, 1990). In this context, the crystal structures of dinicotinamidium squarate (Bulut *et al.*, 2003), picolinamidium squarate and di-*p*-toluidinium squarate dihydrate (Uçar *et al.*, 2004), and 4-carbamoylpyridinium squarate (Köroglu *et al.*, 2005) have already been published.



(I)

The asymmetric unit of (I) contains one aminopyrimidinium cation, half of a centrosymmetric squarate dianion (SQ^{2-}) and a water molecule with partial occupancy. Both the squarate and the aminopyrimidinium molecules lie on a crystallographic mirror plane. The inversion-related aminopyrimidine molecules are linked through N—H···N hydrogen bonds to form dimers. The dimers and the squarate dianions are alternately arranged and linked *via* N—H···O hydrogen bonds to form a chain along the *c* axis (Fig. 1). O—H···O hydrogen bonds involving the water molecules located between the crystallographic mirror planes link the molecular chains to form a three-dimensional network (Fig. 2). The hydrogen-bonding geometry is given in Table 2.

Experimental

Aminopyrimidine and squaric acid in a 1:1 molar ratio were mixed in a solution of methanol (50%) and water (50%) and stirred at 333 K

for 12 h. Crystals of (I) were obtained by slow evaporation of the resulting solution. The crystals formed were filtered, washed in water and methanol, and dried in vacuum.

Crystal data

$2C_4H_6N_3^+\cdot C_4O_4^{2-}\cdot 1.394H_2O$
$M_r = 329.39$
Orthorhombic, *Cmca*
$a = 6.4881\ (7)$ Å
$b = 18.0686\ (19)$ Å
$c = 12.7422\ (18)$ Å
$V = 1493.8\ (3)$ Å^3
$Z = 4$
$D_x = 1.465$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2140 reflections
$\theta = 2.3$–$27.9°$
$\mu = 0.12$ mm^{-1}
$T = 296\ (2)$ K
Prismatic plate, pale yellow
$0.44 \times 0.42 \times 0.09$ mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.940$, $T_{max} = 0.989$
2140 measured reflections
964 independent reflections
701 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 27.8°$
$h = -8 \rightarrow 8$
$k = -23 \rightarrow 23$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.104$
$S = 1.03$
964 reflections
95 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.2353P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N3	1.303 (3)	C2—N1	1.315 (3)
C1—N1	1.350 (2)	C5—C6	1.459 (3)
C1—N2	1.353 (3)	C6—O2	1.245 (2)
N1—C2—C3	124.1 (2)	O2—C6—C5	133.87 (19)
C4—C3—C2	116.7 (2)	C2—N1—C1	117.52 (19)
N2—C4—C3	120.5 (2)	C4—N2—C1	120.41 (19)
O1—C5—C6	134.96 (18)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···N1^{ii}	0.91 (3)	2.06 (3)	2.975 (3)	179 (2)
O5—H5···O2^{iv}	0.84 (2)	1.88 (2)	2.713 (2)	168 (3)
N2—H2A···O1	0.95 (3)	1.68 (3)	2.621 (2)	168 (2)
N3—H3A···O2	0.89 (2)	1.94 (3)	2.811 (2)	168 (2)

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

All H atoms were located in a difference map and refined isotropically.

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: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

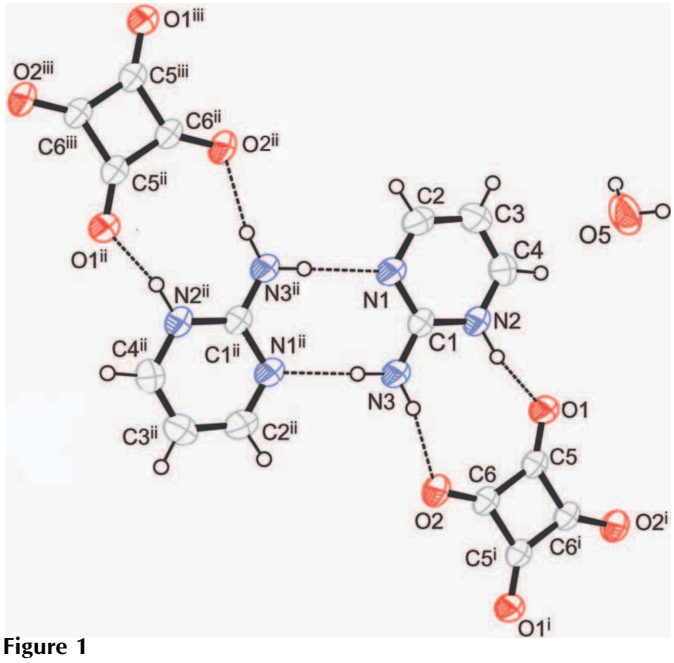


Figure 1
ORTEPIII (Burnett & Johnson, 1996) plot of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms are shown as small spheres of arbitrary radii and hydrogen bonds are indicated by dashed lines. [Symmetry code: (i) $x, 1-y, 2-z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, y, z-1$.]

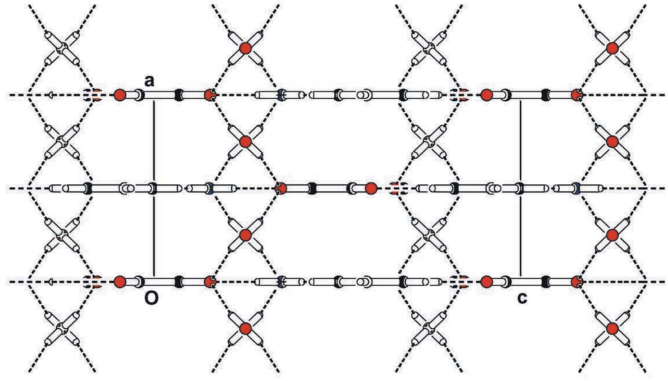


Figure 2
The crystal packing of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

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