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4-Amino-5-fluoropyrimidin-2(1H)-one–2-amino-5-fluoropyrimidin-4(3H)-one–water (1/1/1)

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Key indicators

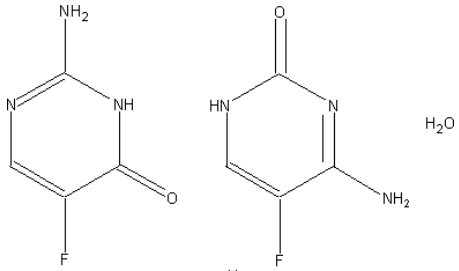
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.123
Data-to-parameter ratio = 11.3

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

The title co-crystal, $C_4H_4FN_3O\cdot C_4H_4FN_3O\cdot H_2O$, has one molecule of 4-amino-5-fluoropyrimidin-2(1*H*)-one, one molecule of its isomer 2-amino-5-fluoropyrimidin-4(3*H*)-one and a molecule of water in the asymmetric unit. 4-Amino-5-fluoropyrimidin-2(1H)-one is commonly known as 5-fluorocytosine.

Comment

The title co-crystal, (I) (Fig. 1), was grown by evaporation of a 50% aqueous solution of ethanol saturated with 5-fluorocytosine. Two different crystal forms were obtained from this solution. The major crystallisation product exhibited a block morphology and was the known monohydrate of 5-fluorocytosine (Louis *et al.*, 1982). A small number of needle-shaped crystals were observed as the minor crystallization product. These crystals proved to be the co-crystal, (I). The isomer of 5-fluorocytosine was assumed to have been present in the commercial sample of 5-fluorocytosine purchased from Fluorochem (98% pure, Old Glossop, UK) that was used to prepare the initial solution.



(I)

The simplest hydrogen-bonded subunit observed is a two-molecule unit, containing one molecule of each isomer. Each molecule of 5-fluorocytosine forms three hydrogen bonds to a

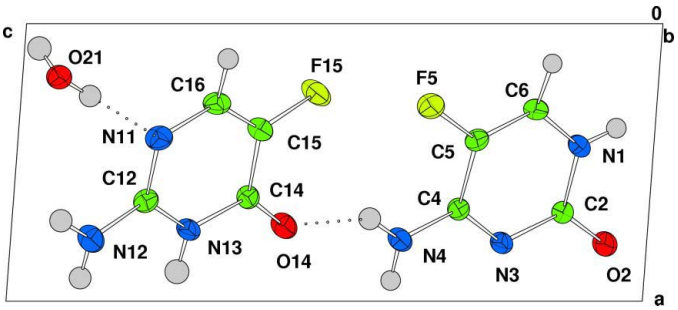


Figure 1
The asymmetric unit of the title co-crystal. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres. Dotted lines indicate hydrogen bonds.

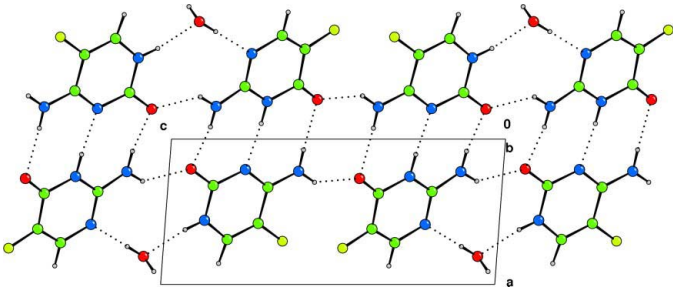


Figure 2
The hydrogen bonded ribbon present in the title structure. Dotted lines indicate hydrogen bonds.

molecule of the isomer (N4—H2···O14, N13—H13···N3 and N12—H12···O2), forming two adjoining $R_2^2(8)$ hydrogen bond rings (Table 1). Two different $R_2^4(8)$ hydrogen-bond rings join these subunits together to form a ribbon (Fig. 2).

The role of the water molecules in the structure is to join together the ribbons into a hydrogen-bonded sheet. The water hydrogen bonds to two molecules from one ribbon, acting both as donor and acceptor, and as a donor to a third molecule, from a different ribbon (Table 1). The ribbons form stepped sheets, parallel to the $01\overline{1}$ planes (Fig. 3).

Within the ribbon structure, there is also a close F···F contact, between F5 and F15, of 2.9003 (15) Å; however, this is likely to have arisen as a consequence of the adjacent $R_2^4(8)$ hydrogen-bond ring.

Experimental

Crystals were grown from a 50% aqueous ethanol solution, by evaporation at room temperature. The crystal form reported was the minor crystallisation product.

Crystal data

$C_4H_4FN_3O{\cdot}C_4H_4FN_3O{\cdot}H_2O$
M_r = 276.22
Triclinic, $P\overline{1}$
a = 5.4122 (16) Å
b = 8.447 (2) Å
c = 12.083 (4) Å
α = 89.454 (5)°
β = 85.718 (5)°
γ = 77.096 (4)°
V = 536.9 (3) Å^3
Z = 2
D_x = 1.708 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1511 reflections
θ = 3.0–28.1°
μ = 0.16 mm^{-1}
T = 150 (2) K
Needle, colourless
0.44 × 0.14 × 0.11 mm

Data collection

Bruker SMART APEX diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.934, T_{max} = 0.984
4532 measured reflections
2405 independent reflections
1884 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.3°
$h = -6 \rightarrow 6$
$k = -11 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.123
S = 1.05
2405 reflections
212 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.0364P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

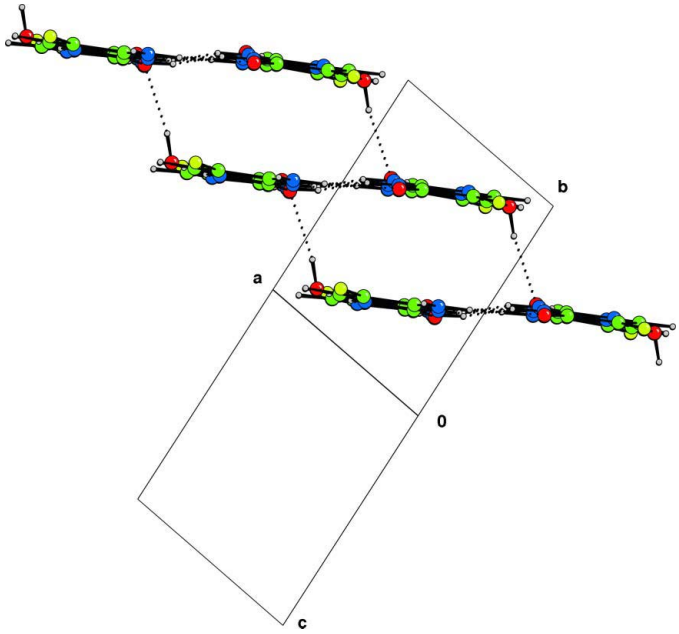


Figure 3
The stepped structure of the sheet, comprising ribbons which are hydrogen bonded (dotted lines) *via* water molecules.

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

D—H···A	D—H	H···A	D···A	D—H···A
N12—H11···O2^{i}	0.86 (3)	2.13 (3)	2.870 (2)	143 (2)
N12—H12···O2^{ii}	0.91 (2)	1.99 (2)	2.889 (2)	172 (2)
N13—H13···N3^{ii}	0.91 (3)	2.01 (3)	2.922 (2)	175 (2)
N1—H1···O21^{iii}	0.83 (2)	1.95 (2)	2.775 (2)	173 (2)
N4—H2···O14^{ii}	0.88 (2)	2.07 (2)	2.9482 (19)	177 (2)
N4—H3···O14	0.91 (3)	2.01 (2)	2.8285 (19)	149 (2)
O21—H21···N11	0.84 (3)	1.94 (3)	2.785 (2)	177 (2)
O21—H22···O2^{iv}	0.81 (3)	2.03 (3)	2.826 (2)	170 (2)

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

All H atoms were located [C—H = 0.95 (2)–0.96 (2), N—H = 0.83 (2)–0.91 (3) and O—H = 0.95 (2)] in a difference map and were refined isotropically.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL97*.

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