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Molecular packing in (5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)acetamide

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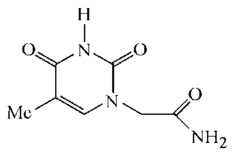
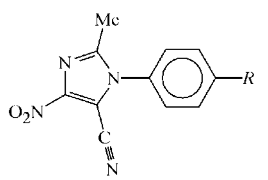
In the title compound, $C_7H_9N_3O_3$, the primary packing motif, *viz.* an infinite tape, is formed *via* intermolecular hydrogen bonds of different strengths. In the formation of the tapes, only inversion centres are used; the other symmetry elements of $P2_1/c$ connect the tapes into a three-dimensional structure through only weak hydrogen bonds.

Comment

In the course of studies of weak interactions in molecular crystals (Kubicki *et al.*, 2001, 2002), the crystal structure of (1-thyminyl)acetamide, (I) (Fig. 1), has been determined. In this simple molecule, the three carbonyl groups can potentially be involved in intermolecular carbonyl–carbonyl interactions that are able to compete successfully with hydrogen bonds (Allen *et al.*, 1998). On the other hand, the primary acetamide group and the secondary amine group, as well as the carbonyl groups, can form intermolecular hydrogen bonds of different energies; moreover, weak C—H···O and C—H···N hydrogen bonds can be formed, and these can influence the supramolecular packing motif.



(I)



(II) R=H
(III) R=Cl

The molecule of (I) contains planar thyminyl and acetamide moieties, which make a dihedral angle of 87.05 (3)°. Of the several possible tautomeric forms for the flat uracyl ring, the diketo tautomer has been found in the solid state. Appreciable differences have been observed in the values of the C═O bond lengths [1.2436 (11) and 1.2304 (10) Å for C2═O2 and C4═O4, respectively]; however, the differences in their lengths are less pronounced than in thymine itself (Portalone *et al.*, 1999). The existence of C═O groups of different lengths can be easily explained by observing the respective crystal structures. In thymine (Portalone *et al.*, 1999), as well as in the crystals of (I), centrosymmetric dimers are formed *via* N3—H3···O2═C2 hydrogen bonds. In (I), the second carbonyl group, C4═O4, is involved in a weak C—H···O hydrogen bond only (Table 1), and for this reason the C4═O4 bond is shorter. This geometrical perturbation is mainly due to self-association and confirms the fundamental role of conjugative stabilization of the intermolecular hydrogen bonding.

Intermolecular hydrogen bonds, the main driving force for crystal packing, connect the molecules of (I) into infinite tapes. Only inversion centres participate in the formation of the tape and no other symmetry operations are used in creating this principal packing motif. This mimics the packing of thymine molecules in the solid state (Portalone *et al.*, 1999). In (I), one type of centrosymmetric dimer is formed *via* almost linear and

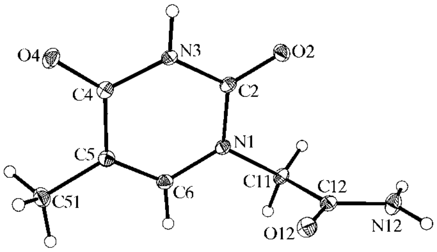


Figure 1
A view of the molecule of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are depicted as spheres of arbitrary radii.

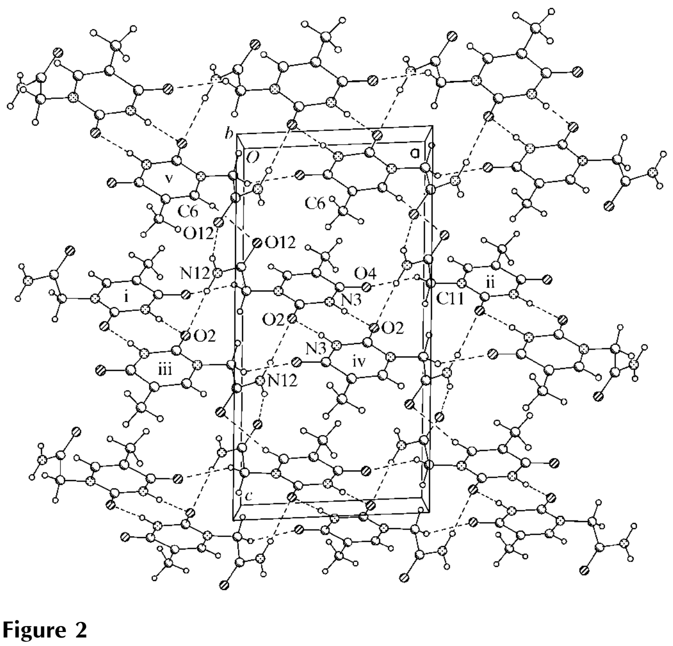


Figure 2
The molecular tape connected by hydrogen bonds (dashed lines), viewed approximately along the [100] direction. [Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x, -y+1, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.]

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quite strong N3—H3$\cdots$O2^{iv} hydrogen bonds (symmetry codes are given in Table 1 and Fig. 2), which form eight-membered rings. The same O2 atoms participate in bifurcated hydrogen bonds to the amide groups, O2$^{iii}\cdots$H12*B*—N12, thus forming the second kind of centrosymmetric dimer, featuring 14-membered rings. The molecular tapes also contain weak C—H$\cdots$O hydrogen bonds (Fig. 2 and Table 1), but these are secondary interactions only. The molecular tapes in the crystal structure of (I) are further connected into a three-dimensional structure by weak bifurcated hydrogen bonds to O12, *viz*. N12—H12*A*$\cdots$O12^{v} and C6—H6$\cdots$O12^{vi} (Table 1 and Fig. 2). No carbonyl–carbonyl interactions have been found.

There are also some similarities in the crystal-packing modes of (I) and two imidazole derivatives, namely 2-methyl-4-nitro-1-phenyl-1*H*-imidazole-5-carbonitrile, (II), and 1-(4-chlorophenyl)-2-methyl-4-nitro-1*H*-imidazole-5-carbonitrile, (III) (Kubicki, 2004). These two imidazole derivatives likewise form infinite tapes in their crystal structures, using two consecutive inversion centres in the space group $P2_1/n$, and the molecular conformations in the crystals are similar to that in (I), with dihedral angles between the two planar fragments of 76.29 (4) and 87.64 (6)° in (II) and (III), respectively. On the other hand, the differences between the crystal structures of (I), (II) and (III) are determined by the intermolecular interactions. There are intermolecular hydrogen bonds in (I); in (II), dipole–dipole interactions between antiparallel cyano groups connect molecules into centrosymmetric dimers, while in (III), the dimers are connected by C≡N$\cdots$Cl—C interactions together with weak C—H$\cdots$O(N) hydrogen bonds. This diversity of interactions can be understood on the basis of a simple electrostatic model; moreover, the halogen bond is an analogue of the hydrogen bond (Legon, 1999).

Experimental

The synthesis of (1-thyminyl)acetamide was described by Spychała (1997). Crystals suitable for data collection were grown from hot water by slow cooling.

Crystal data

$C_7H_9N_3O_3$
$M_r = 183.17$
Monoclinic, $P2_1/c$
$a = 8.0388$ (1) Å
$b = 6.1476$ (1) Å
$c = 15.8390$ (1) Å
$\beta = 92.923$ (1)°
$V = 781.74$ (2) Å^3
$Z = 4$
$D_x = 1.556$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 100$ (1) K
Prism, colourless
0.55 × 0.25 × 0.10 mm

Data collection

Kuma KM-4 CCD four-circle diffractometer
ω scans
30900 measured reflections
2287 independent reflections
2262 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.056$
$\theta_{\rm max} = 30.0°$

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$\cdots$O2^{iv}	0.93 (2)	1.93 (2)	2.855 (1)	173 (1)
N12—H12*B*$\cdots$O2^{iii}	0.89 (2)	2.14 (2)	3.024 (1)	175 (2)
N12—H12*A*$\cdots$O12^{v}	0.90 (2)	2.14 (2)	3.003 (1)	160 (1)
C6—H6$\cdots$O12^{vi}	0.96 (1)	2.52 (1)	3.362 (1)	146 (1)
C11—H11*A*$\cdots$O4^{i}	0.96 (1)	2.40 (1)	3.175 (1)	138 (1)

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

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.06$
2287 reflections
155 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.3534P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.42$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.021 (4)

All H atoms were freely refined, giving C—H distances in the range 0.959 (14)–1.003 (15) Å and N—H distances in the range 0.887 (17)–0.931 (16) Å.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Stereochemical Workstation Operation Manual* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD3012). Services for accessing these data are described at the back of the journal.

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