Crystal structure of 4-aminopyrimidine, $C_4H_5N_3$

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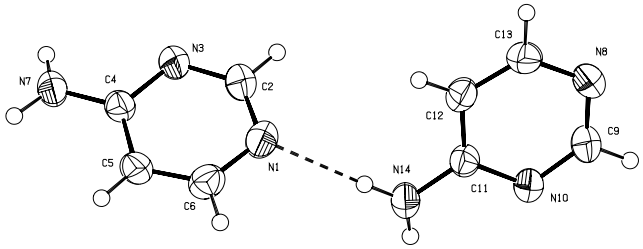

Abstract

$C_4H_5N_3$, orthorhombic, *Pcab* (No. 61), a = 10.983(2) Å, b = 12.287(3) Å, c = 14.052(3) Å, V = 1896.3 Å^3, Z = 16, $R_{gt}(F)$ = 0.054, $wR_{ref}(F^2)$ = 0.146, T = 289 K.

Source of material

4-Aminopyrimidine was commercially available from Aldrich Europe. The compound was dissolved in methanol for recrystallisation.

Discussion

The H-bonding interactions of 4-aminopyrimidine (4APM) with water have been investigated by matrix-isolation FT-IR studies and ab initio calculations [1]. A closed N7-H···O-H···N3 structure containing two H-bonds, together with H-bonds N1···H–OH, N7–H···OH2 are observed and the 4APM molecule exists exclusively in the amino form. 4APM crystallises with two molecules in the asymmetric unit (r.m.s. deviation fit between two molecules: 0.006 Å). Both molecules are linked by a H-bond N1···H142–N14 (d(N1···N14) = 2.996(3) Å, d(N1···H142) = 2.13(2) Å, d(H14—N14: 0.86(2) Å, ∠N1···H142–N14 = 174(2)°). The angle between the two pyrimidine rings is 62.5(1)°. The other H-bonds in the packing N7–H71···N10(1/2+x, 1–y, 1/2–z), N7–H72···N8(x, 1+y, z), N14–H141···N3(–1/2+x, 1–y, 1/2–z) mimic the hydrogen bonding interactions between 4APM and water described in [1]. There are no voids in the crystal packing for possible solvent molecules.

Table 1. Data collection and handling.

Crystal:	white block, size 0.15 × 0.20 × 0.35 mm
Wavelength:	Cu K_α radiation (1.54178 Å)
μ:	7.44 cm^{-1}
Diffractometer, scan mode:	Siemens P4-PC, $\theta/2\theta$
$2\theta_{max}$:	108.4°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1625, 1149
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 875
$N(param)_{refined}$:	158
Programs:	SHELXS-97 [2], SHELXL-97 [3], PLATON [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	8*c*	1.030(2)	0.489(2)	0.328(2)	0.058
H(5)	8*c*	0.829(2)	0.785(2)	0.417(1)	0.050
H(6)	8*c*	0.756(2)	0.616(2)	0.452(2)	0.056
H(71)	8*c*	1.088(2)	0.831(2)	0.292(2)	0.057
H(72)	8*c*	0.992(2)	0.894(2)	0.345(2)	0.057
H(9)	8*c*	0.758(2)	–0.009(2)	0.314(2)	0.054
H(12)	8*c*	0.942(2)	0.287(2)	0.430(1)	0.050
H(13)	8*c*	1.025(2)	0.112(2)	0.457(2)	0.052
H(141)	8*c*	0.690(3)	0.334(2)	0.300(2)	0.060
H(142)	8*c*	0.786(2)	0.391(2)	0.356(2)	0.060

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	8*c*	0.8857(2)	0.5335(2)	0.3946(1)	0.047(1)	0.040(1)	0.060(1)	–0.009(1)	0.004(1)	–0.0017(9)
C(2)	8*c*	0.9886(2)	0.5503(2)	0.3479(2)	0.048(2)	0.034(1)	0.064(2)	0.001(1)	0.002(1)	–0.007(1)
N(3)	8*c*	1.0400(2)	0.6439(1)	0.3234(1)	0.040(1)	0.033(1)	0.057(1)	0.0012(8)	0.0048(9)	–0.0033(9)
C(4)	8*c*	0.9804(2)	0.7352(2)	0.3503(2)	0.037(1)	0.033(1)	0.041(1)	0.002(1)	–0.0026(9)	–0.004(1)
C(5)	8*c*	0.8706(2)	0.7262(2)	0.4018(2)	0.039(1)	0.038(1)	0.049(1)	0.005(1)	0.001(1)	–0.007(1)
C(6)	8*c*	0.8285(2)	0.6256(2)	0.4209(2)	0.041(1)	0.050(2)	0.049(2)	–0.006(1)	0.007(1)	–0.004(1)
N(7)	8*c*	1.0281(2)	0.8308(2)	0.3264(1)	0.046(1)	0.031(1)	0.067(1)	0.002(1)	0.012(1)	0.001(1)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(8)	8*c*	0.8979(2)	0.0344(1)	0.3879(1)	0.045(1)	0.036(1)	0.056(1)	0.0070(9)	–0.002(1)	–0.0014(9)
C(9)	8*c*	0.7957(2)	0.0526(2)	0.3401(2)	0.050(2)	0.032(1)	0.054(2)	–0.001(1)	0.000(1)	–0.006(1)
N(10)	8*c*	0.7428(2)	0.1471(1)	0.3203(1)	0.041(1)	0.032(1)	0.051(1)	–0.0022(8)	–0.0035(9)	–0.0009(8)
C(11)	8*c*	0.7992(2)	0.2367(2)	0.3538(2)	0.038(1)	0.032(1)	0.042(1)	–0.002(1)	0.004(1)	0.001(1)
C(12)	8*c*	0.9076(2)	0.2270(2)	0.4063(2)	0.041(1)	0.037(1)	0.048(1)	–0.007(1)	–0.004(1)	–0.001(1)
C(13)	8*c*	0.9520(2)	0.1252(2)	0.4209(2)	0.037(1)	0.046(2)	0.048(2)	0.001(1)	–0.004(1)	0.003(1)
N(14)	8*c*	0.7491(2)	0.3336(2)	0.3355(2)	0.047(1)	0.030(1)	0.072(2)	–0.0025(9)	–0.013(1)	0.003(1)

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