Crystal structure of 4-aminopyrimidine, $C_4H_5N_3$

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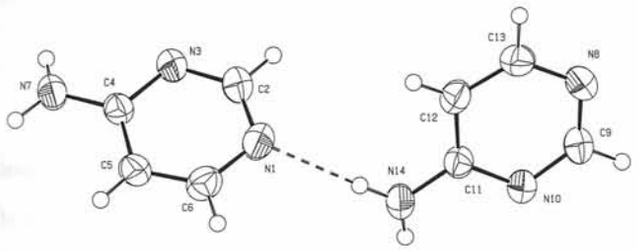

Abstract

$C_4H_5N_3$, 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)	8c	1.030(2)	0.489(2)	0.328(2)	0.058
H(5)	8c	0.829(2)	0.785(2)	0.417(1)	0.050
H(6)	8c	0.756(2)	0.616(2)	0.452(2)	0.056
H(71)	8c	1.088(2)	0.831(2)	0.292(2)	0.057
H(72)	8c	0.992(2)	0.894(2)	0.345(2)	0.057
H(9)	8c	0.758(2)	–0.009(2)	0.314(2)	0.054
H(12)	8c	0.942(2)	0.287(2)	0.430(1)	0.050
H(13)	8c	1.025(2)	0.112(2)	0.457(2)	0.052
H(141)	8c	0.690(3)	0.334(2)	0.300(2)	0.060
H(142)	8c	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)	8c	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)	8c	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)	8c	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)	8c	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)	8c	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)	8c	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)	8c	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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