Crystal structure of 9-methyl-(6-*N*-pyrrolyl)purine, $C_{10}H_9N_5$

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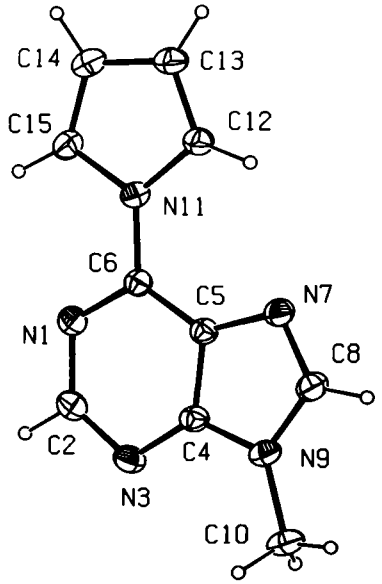

Abstract

$C_{10}H_9N_5$, monoclinic, *C*12/*c*1 (No. 15), $a = 11.053(1)$ Å, $b = 10.231(1)$ Å, $c = 16.639(2)$ Å, $\beta = 91.009(7)°$, $V = 1881.3$ Å^3, $Z = 8$, $R_{gt}(F) = 0.050$, $wR_{ref}(F^2) = 0.138$, $T = 295$ K.

Source of material

The title compound was prepared by methylation of (6-*N*-pyrrolyl)purine with methyl iodide in the presence of sodium hydride as described for 2-amino-6-chloropurine [1].

Discussion

As a part of research in our laboratories to develop novel anticancer and antiviral agents we prepared a derivative of (6-*N*-pyrrolyl)purine [2].

The observed values for bond distances and angles of the *N*-pyrrolyl and purine ring are in a good agreement with those found in the other (6-*N*-pyrrolyl)purine derivatives [2, 3].

Table 1. Data collection and handling.

Crystal:	colourless prismatic, size 0.30 × 0.40 × 0.75 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.93 cm^{-1}
Diffractometer, scan mode:	Philips PW1100 Stoe STADI, ω
$2\theta_{max}$:	60.08°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7022, 2747
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1650
$N(param)_{refined}$:	173
Programs:	SHELXS-97 [4], SHELXL-97 [5], ORTEP-3 [6]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	8*f*	–0.071(2)	0.402(2)	0.540(1)	0.072(5)
H(8)	8*f*	0.233(2)	–0.070(2)	0.431(1)	0.078(6)
H(101)	8*f*	0.079(2)	–0.025(3)	0.327(2)	0.13(1)
H(102)	8*f*	–0.034(3)	0.049(3)	0.350(2)	0.119(9)
H(103)	8*f*	0.074(3)	0.134(3)	0.317(2)	0.14(1)
H(12)	8*f*	0.326(2)	0.073(2)	0.666(1)	0.061(5)
H(13)	8*f*	0.401(2)	0.114(2)	0.808(1)	0.080(6)
H(14)	8*f*	0.274(2)	0.289(2)	0.867(1)	0.065(5)
H(15)	8*f*	0.120(2)	0.356(2)	0.756(1)	0.074(6)

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*f*	0.0543(1)	0.3232(1)	0.61096(8)	0.0551(7)	0.0557(7)	0.0523(8)	0.0091(6)	–0.0001(6)	0.0020(6)
C(2)	8*f*	–0.0114(2)	0.3344(2)	0.5427(1)	0.0560(9)	0.065(1)	0.062(1)	0.0161(8)	–0.0048(8)	0.0060(8)
N(3)	8*f*	–0.0063(1)	0.2627(1)	0.47638(8)	0.0515(7)	0.0681(8)	0.0533(8)	0.0070(6)	–0.0071(6)	0.0090(7)
C(4)	8*f*	0.0777(1)	0.1696(1)	0.48317(8)	0.0447(7)	0.0519(8)	0.0399(7)	–0.0056(6)	–0.0008(5)	0.0081(6)
C(5)	8*f*	0.1531(1)	0.1453(1)	0.55011(8)	0.0438(7)	0.0452(7)	0.0400(7)	–0.0012(6)	0.0005(6)	0.0058(6)
C(6)	8*f*	0.1369(1)	0.2279(1)	0.61550(8)	0.0426(7)	0.0441(7)	0.0414(7)	–0.0022(6)	0.0019(5)	0.0052(6)
N(7)	8*f*	0.2282(1)	0.0398(1)	0.53532(8)	0.0639(8)	0.0548(7)	0.0437(7)	0.0121(6)	–0.0034(6)	–0.0011(6)
C(8)	8*f*	0.1976(2)	0.0046(2)	0.4623(1)	0.071(1)	0.0583(9)	0.0444(9)	0.0073(8)	–0.0013(7)	–0.0009(7)
N(9)	8*f*	0.1079(1)	0.0772(1)	0.42736(7)	0.0593(8)	0.0590(8)	0.0368(6)	–0.0051(6)	–0.0027(5)	0.0032(5)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(10)	8*f*	0.0553(2)	0.0611(2)	0.3467(1)	0.075(1)	0.078(1)	0.0385(8)	–0.014(1)	–0.0088(7)	0.0032(8)
N(11)	8*f*	0.2016(1)	0.2171(1)	0.68787(7)	0.0511(7)	0.0470(6)	0.0388(6)	–0.0007(5)	–0.0019(5)	0.0008(5)
C(12)	8*f*	0.2976(2)	0.1336(2)	0.7045(1)	0.0592(9)	0.0573(9)	0.0475(9)	0.0089(7)	–0.0054(7)	0.0017(7)
C(13)	8*f*	0.3356(2)	0.1556(2)	0.7809(1)	0.065(1)	0.069(1)	0.0461(9)	0.0009(8)	–0.0097(7)	0.0075(8)
C(14)	8*f*	0.2633(2)	0.2548(2)	0.8134(1)	0.070(1)	0.066(1)	0.0412(8)	–0.0124(8)	–0.0017(7)	–0.0019(7)
C(15)	8*f*	0.1817(2)	0.2912(2)	0.75610(9)	0.0625(9)	0.0554(9)	0.0457(8)	0.0003(7)	0.0008(7)	–0.0053(7)

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