Crystal structure of 2-methyl-4-phenyl-5-(4-methoxyphenyl)-7-pyrid-3-yl-methylaminoimidazo[1,5-*b*]pyridazine, $C_6HN_3(CH_3)(C_6H_5)(C_6H_4OCH_3)(NHCH_2C_5H_4N)$

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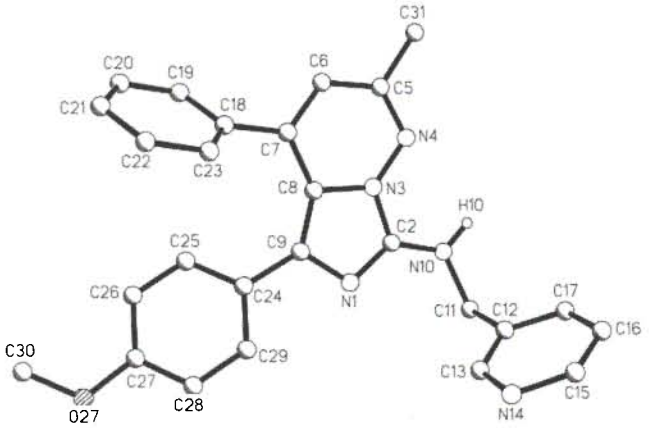

Abstract

$C_{26}H_{23}N_5O$, monoclinic, $P12_1/n1$ (No. 14), $a = 9.857(1)$ Å, $b = 18.907(2)$ Å, $c = 11.705(2)$ Å, $\beta = 101.93(1)°$, $V = 2134.3$ Å^3, $Z = 4$, $R_{gt}(F) = 0.062$, $wR(F) = 0.058$, $T = 293$ K.

Source of material

The title compound was synthesized by reaction of 1-amino-4-(4-methyloxyphenyl)-2-pyrid-3-ylmethylaminoimidazole with benzoylacetone [1].

Table 1. Data collection and handling.

Crystal:	red needle, size 0.2 × 0.3 × 1.7 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.80 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5346, 4903
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\ \sigma(F_{obs})$, 3447
$N(param)_{refined}$:	293
Program:	SHELXTL-plus [2]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(6)	4*e*	0.2631(3)	0.9327(1)	0.6447(2)	0.08
H(10)	4*e*	-0.071(3)	0.969(2)	0.190(2)	0.059(9)
H(11A)	4*e*	-0.0385(3)	1.0795(2)	0.0500(2)	0.08
H(11B)	4*e*	-0.1391(3)	1.0159(2)	0.0097(2)	0.08
H(13)	4*e*	-0.1202(3)	1.1823(2)	0.1270(3)	0.08
H(15)	4*e*	-0.5062(4)	1.1952(2)	0.1735(3)	0.08
H(16)	4*e*	-0.5449(3)	1.0777(2)	0.1255(3)	0.08
H(17)	4*e*	-0.3641(3)	1.0102(2)	0.0817(2)	0.08
H(19)	4*e*	0.5244(3)	0.9853(1)	0.6585(2)	0.08
H(20)	4*e*	0.6764(3)	1.0479(2)	0.8040(2)	0.08
H(21)	4*e*	0.6077(3)	1.1554(2)	0.8711(2)	0.08
H(22)	4*e*	0.3929(3)	1.2043(2)	0.7860(2)	0.08
H(23)	4*e*	0.2412(3)	1.1435(2)	0.6371(2)	0.08
H(25)	4*e*	0.4888(3)	1.1200(1)	0.4867(2)	0.08
H(26)	4*e*	0.6327(3)	1.2187(1)	0.5103(2)	0.08
H(28)	4*e*	0.3416(3)	1.3267(1)	0.2781(2)	0.08
H(29)	4*e*	0.1924(3)	1.2300(1)	0.2637(2)	0.08
H(30A)	4*e*	0.7563(3)	1.3882(2)	0.4715(3)	0.08
H(30B)	4*e*	0.7695(3)	1.3062(2)	0.4581(3)	0.08
H(30C)	4*e*	0.7003(3)	1.3371(2)	0.5565(3)	0.08
H(31A)	4*e*	0.1214(3)	0.8312(1)	0.6002(3)	0.08
H(31B)	4*e*	0.0892(3)	0.8085(1)	0.4686(3)	0.08
H(31C)	4*e*	-0.0249(3)	0.8464(1)	0.5218(3)	0.08

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)	4*e*	0.1343(2)	1.0965(1)	0.2530(2)	0.044(1)	0.046(1)	0.037(1)	0.003(1)	0.0008(9)	0.0002(9)
C(2)	4*e*	0.0675(2)	1.0362(1)	0.2570(2)	0.039(1)	0.044(1)	0.038(1)	0.005(1)	0.000(1)	-0.002(1)
N(3)	4*e*	0.1125(2)	1.0026(1)	0.3601(2)	0.040(1)	0.041(1)	0.036(1)	-0.0006(9)	0.0009(9)	-0.0005(9)
N(4)	4*e*	0.0645(2)	0.9376(1)	0.3862(2)	0.043(1)	0.041(1)	0.047(1)	0.001(1)	0.003(1)	-0.002(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}
C(5)	4*e*	0.1227(3)	0.9139(1)	0.4896(2)	0.041(1)	0.040(1)	0.048(1)	0.004(1)	0.008(1)	0.000(1)
C(6)	4*e*	0.2248(3)	0.9528(1)	0.5697(2)	0.047(1)	0.047(2)	0.040(1)	0.005(1)	0.002(1)	0.004(1)
C(7)	4*e*	0.2703(2)	1.0176(1)	0.5437(2)	0.034(1)	0.042(1)	0.039(1)	0.006(1)	0.003(1)	–0.002(1)
C(8)	4*e*	0.2171(2)	1.0453(1)	0.4291(2)	0.035(1)	0.040(1)	0.039(1)	0.004(1)	0.003(1)	–0.004(1)
C(9)	4*e*	0.2295(2)	1.1028(1)	0.3584(2)	0.037(1)	0.043(1)	0.038(1)	0.006(1)	0.003(1)	–0.001(1)
N(10)	4*e*	–0.0280(2)	1.0055(1)	0.1712(2)	0.054(1)	0.049(1)	0.041(1)	–0.000(1)	–0.008(1)	–0.001(1)
C(11)	4*e*	–0.1031(3)	1.0473(2)	0.0732(2)	0.049(2)	0.061(2)	0.036(1)	0.004(1)	–0.001(1)	–0.002(1)
C(12)	4*e*	–0.2227(3)	1.0897(1)	0.1004(2)	0.045(1)	0.046(2)	0.030(1)	–0.001(1)	–0.001(1)	0.001(1)
C(13)	4*e*	–0.2077(3)	1.1601(2)	0.1276(3)	0.055(2)	0.059(2)	0.074(2)	–0.006(2)	0.013(2)	–0.006(2)
N(14)	4*e*	–0.3107(3)	1.2008(2)	0.1546(3)	0.086(2)	0.070(2)	0.105(2)	0.006(2)	0.020(2)	–0.018(2)
C(15)	4*e*	–0.4328(4)	1.1675(2)	0.1536(3)	0.072(2)	0.089(3)	0.064(2)	0.028(2)	0.021(2)	0.007(2)
C(16)	4*e*	–0.4559(3)	1.0985(2)	0.1264(3)	0.046(2)	0.068(2)	0.069(2)	0.006(2)	0.013(1)	0.023(2)
C(17)	4*e*	–0.3502(3)	1.0595(2)	0.1003(2)	0.051(2)	0.045(2)	0.059(2)	–0.002(1)	0.003(1)	0.006(1)
C(18)	4*e*	0.3677(2)	1.0583(1)	0.6344(2)	0.040(1)	0.043(1)	0.034(1)	0.001(1)	0.002(1)	0.005(1)
C(19)	4*e*	0.4973(3)	1.0303(1)	0.6846(2)	0.045(1)	0.048(2)	0.052(2)	0.003(1)	–0.000(1)	0.004(1)
C(20)	4*e*	0.5864(3)	1.0668(2)	0.7709(2)	0.048(2)	0.065(2)	0.056(2)	–0.004(1)	–0.010(1)	0.008(2)
C(21)	4*e*	0.5468(3)	1.1307(2)	0.8093(2)	0.064(2)	0.066(2)	0.041(1)	–0.022(2)	–0.004(1)	0.004(1)
C(22)	4*e*	0.4195(3)	1.1592(2)	0.7597(2)	0.072(2)	0.052(2)	0.048(2)	–0.004(2)	0.005(1)	–0.007(1)
C(23)	4*e*	0.3295(3)	1.1235(2)	0.6719(2)	0.054(2)	0.054(2)	0.045(2)	0.010(1)	–0.001(1)	–0.004(1)
C(24)	4*e*	0.3237(2)	1.1641(1)	0.3749(2)	0.039(1)	0.039(1)	0.038(1)	0.004(1)	0.008(1)	–0.001(1)
C(25)	4*e*	0.4565(3)	1.1628(1)	0.4459(2)	0.042(1)	0.044(2)	0.044(1)	0.004(1)	0.007(1)	0.007(1)
C(26)	4*e*	0.5436(3)	1.2210(1)	0.4584(2)	0.040(1)	0.047(2)	0.047(1)	0.000(1)	0.005(1)	0.002(1)
C(27)	4*e*	0.5013(3)	1.2822(1)	0.3962(2)	0.048(1)	0.040(1)	0.046(1)	0.001(1)	0.009(1)	–0.003(1)
O(27)	4*e*	0.5804(2)	1.3423(1)	0.4002(2)	0.061(1)	0.044(1)	0.072(1)	–0.006(1)	0.000(1)	0.0043(9)
C(28)	4*e*	0.3704(3)	1.2847(1)	0.3228(2)	0.053(2)	0.038(1)	0.051(2)	0.006(1)	0.004(1)	0.005(1)
C(29)	4*e*	0.2828(3)	1.2270(1)	0.3134(2)	0.048(2)	0.046(2)	0.043(1)	0.010(1)	0.001(1)	0.002(1)
C(30)	4*e*	0.7124(3)	1.3435(2)	0.4778(3)	0.054(2)	0.053(2)	0.076(2)	–0.006(1)	0.005(2)	–0.003(2)
C(31)	4*e*	0.0727(3)	0.8437(1)	0.5231(3)	0.055(2)	0.046(2)	0.066(2)	–0.001(1)	0.009(1)	0.003(1)

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