Crystal structure of 1-acetylamino-4-(4-bromophenyl)-2-(4-ethoxycarbonylpiperazino)imidazole, $C_3HN_2(C_6H_4Br)[C_4H_8N_2(COOC_2H_5)](NHCOCH_3)$

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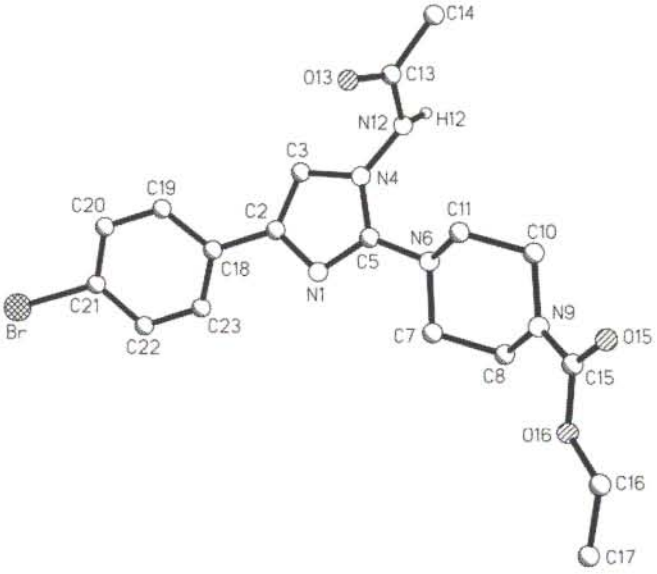

Abstract

$C_{18}H_{22}BrN_5O_3$, monoclinic, $P12_1/n1$ (No. 14), a = 11.773(1) Å, b = 5.665(1) Å, c = 30.413(3) Å, β = 94.426(7)°, V = 2022.3 Å^3, Z = 4, $R_{gt}(F)$ = 0.069, $wR(F)$ = 0.061, T = 293 K.

Source of material

The title compound was synthesized by reaction of 2-amino-3-(4-bromophenacyl)-5-methyl-1,3,4-oxadiazolium bromide with 1-ethoxycarbonylpiperazine.

Discussion

An intermolecular hydrogen bridge, H12···N1 (198 pm), forms a zigzag chain parallel [010].

Table 1. Data collection and handling.

Crystal:	colourless lath, size 0.02 × 0.25 × 1.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	20.60 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5307, 4593
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\ \sigma(F_{obs})$, 2783
$N(param)_{refined}$:	248
Program:	SHELXTL-plus [2]

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

Atom	Site	x	y	z	U_{iso}
H(3)	4e	0.2044(5)	−0.834(1)	−0.0079(2)	0.08
H(7A)	4e	0.4305(5)	−0.383(1)	−0.1455(2)	0.08
H(7B)	4e	0.5188(5)	−0.511(1)	−0.1123(2)	0.08
H(8A)	4e	0.5719(5)	−0.758(1)	−0.1684(2)	0.08
H(8B)	4e	0.5842(5)	−0.496(1)	−0.1842(2)	0.08
H(10A)	4e	0.3109(5)	−0.844(1)	−0.2314(2)	0.08
H(10B)	4e	0.3967(5)	−0.979(1)	−0.1983(2)	0.08
H(11A)	4e	0.2442(5)	−0.857(1)	−0.1605(2)	0.08
H(11B)	4e	0.2621(5)	−0.596(1)	−0.1753(2)	0.08
H(12)	4e	0.272(5)	−1.200(9)	−0.079(2)	0.06(2)
H(14A)	4e	0.1429(5)	−1.424(1)	−0.1083(2)	0.08
H(14B)	4e	0.0498(5)	−1.316(1)	−0.1420(2)	0.08
H(14C)	4e	0.0221(5)	−1.363(1)	−0.0931(2)	0.08
H(16A)	4e	0.4792(8)	−0.181(2)	−0.3007(2)	0.08
H(16B)	4e	0.5614(8)	−0.374(2)	−0.3173(2)	0.08
H(17A)	4e	0.6466(7)	−0.020(2)	−0.3156(3)	0.08
H(17B)	4e	0.7122(7)	−0.189(2)	−0.2817(3)	0.08
H(17C)	4e	0.6299(7)	0.003(2)	−0.2651(3)	0.08
H(19)	4e	0.1397(5)	−0.470(1)	0.0305(2)	0.08
H(20)	4e	0.1329(5)	−0.205(1)	0.0884(2)	0.08
H(22)	4e	0.4457(5)	0.036(1)	0.0651(2)	0.08
H(23)	4e	0.4510(5)	−0.230(1)	0.0071(2)	0.08

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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}
Br	4*e*	0.27751(6)	0.1589(1)	0.12812(2)	0.0830(6)	0.0977(6)	0.0722(5)	–0.0032(5)	0.0144(4)	–0.0356(4)
N(1)	4*e*	0.3545(3)	–0.4935(7)	–0.0618(1)	0.039(3)	0.048(3)	0.038(2)	0.000(2)	0.005(2)	0.001(2)
C(2)	4*e*	0.3000(4)	–0.547(1)	–0.0241(2)	0.038(3)	0.048(3)	0.038(3)	0.005(3)	0.002(2)	0.001(2)
C(3)	4*e*	0.2497(5)	–0.758(1)	–0.0287(2)	0.048(4)	0.053(3)	0.044(3)	0.002(3)	0.011(3)	0.007(3)
N(4)	4*e*	0.2744(4)	–0.8433(8)	–0.0691(1)	0.047(3)	0.039(3)	0.044(2)	–0.001(2)	0.008(2)	0.001(2)
C(5)	4*e*	0.3365(4)	–0.6762(9)	–0.0878(2)	0.034(3)	0.045(3)	0.038(3)	0.007(3)	0.001(2)	0.002(3)
N(6)	4*e*	0.3809(4)	–0.7068(8)	–0.1288(1)	0.040(3)	0.062(3)	0.039(2)	–0.006(2)	0.003(2)	–0.000(2)
C(7)	4*e*	0.4669(5)	–0.531(1)	–0.1380(2)	0.062(4)	0.073(4)	0.040(3)	–0.019(4)	0.005(3)	0.000(3)
C(8)	4*e*	0.5312(5)	–0.616(1)	–0.1767(2)	0.056(4)	0.118(6)	0.045(3)	–0.024(4)	0.008(3)	0.003(4)
N(9)	4*e*	0.4513(4)	–0.662(1)	–0.2145(1)	0.059(3)	0.096(4)	0.039(3)	–0.020(3)	0.004(2)	0.005(3)
C(10)	4*e*	0.3630(5)	–0.828(1)	–0.2057(2)	0.074(5)	0.089(5)	0.044(3)	–0.019(4)	0.006(3)	–0.008(3)
C(11)	4*e*	0.2997(5)	–0.742(1)	–0.1675(2)	0.049(4)	0.079(4)	0.043(3)	–0.016(3)	0.005(3)	0.000(3)
N(12)	4*e*	0.2350(4)	–1.0541(8)	–0.0870(1)	0.041(3)	0.040(3)	0.055(3)	0.002(2)	0.006(2)	0.001(2)
C(13)	4*e*	0.1196(5)	–1.074(1)	–0.0991(2)	0.055(4)	0.052(4)	0.048(3)	0.001(3)	0.015(3)	0.001(3)
O(13)	4*e*	0.0590(4)	–0.9003(8)	–0.1001(1)	0.054(3)	0.066(3)	0.096(4)	0.011(3)	0.009(2)	–0.004(2)
C(14)	4*e*	0.0803(5)	–1.316(1)	–0.1118(2)	0.056(4)	0.062(4)	0.081(4)	–0.005(4)	0.002(3)	–0.003(4)
C(15)	4*e*	0.4538(5)	–0.558(1)	–0.2539(2)	0.049(4)	0.074(4)	0.054(4)	0.002(4)	0.007(3)	0.000(3)
O(15)	4*e*	0.3892(4)	–0.6020(9)	–0.2854(1)	0.066(3)	0.126(4)	0.054(3)	–0.013(3)	–0.003(2)	0.009(3)
O(16)	4*e*	0.5391(4)	–0.4009(9)	–0.2543(1)	0.075(3)	0.114(4)	0.052(3)	–0.024(3)	0.004(2)	0.014(2)
C(16)	4*e*	0.5486(8)	–0.267(2)	–0.2937(2)	0.115(7)	0.162(8)	0.074(5)	–0.046(7)	–0.001(5)	0.050(5)
C(17)	4*e*	0.6422(7)	–0.105(2)	–0.2885(3)	0.125(8)	0.141(9)	0.131(8)	–0.033(7)	0.021(6)	0.051(6)
C(18)	4*e*	0.2973(5)	–0.379(1)	0.0126(2)	0.044(3)	0.053(4)	0.041(3)	0.003(3)	0.005(3)	0.003(3)
C(19)	4*e*	0.2029(5)	–0.366(1)	0.0375(2)	0.056(4)	0.071(4)	0.069(4)	–0.018(3)	0.018(3)	–0.022(3)
C(20)	4*e*	0.1985(5)	–0.210(1)	0.0716(2)	0.053(4)	0.075(5)	0.067(4)	–0.006(4)	0.025(3)	–0.019(3)
C(21)	4*e*	0.2863(5)	–0.062(1)	0.0817(2)	0.053(4)	0.063(4)	0.046(3)	0.003(3)	0.007(3)	–0.009(3)
C(22)	4*e*	0.3826(5)	–0.068(1)	0.0577(2)	0.046(4)	0.068(4)	0.054(3)	–0.003(3)	0.003(3)	–0.005(3)
C(23)	4*e*	0.3853(5)	–0.226(1)	0.0239(2)	0.047(4)	0.064(4)	0.040(3)	0.008(3)	0.007(3)	–0.002(3)

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References

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