Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Methoxyphenyl)pyrido[2,3-*b*]-pyrazine

Cui-ping Wang, Jing-bo Yan, Hai-Jun Chi, Yan Dong and Zhi-qiang Zhang*

School of Chemical Engineering, University of Science and Technology Liaoning, Anshan, 114051, People's Republic of China
Correspondence e-mail: zhao_submit@yahoo.com.cn

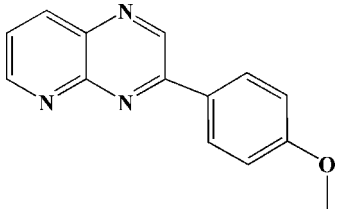
Received 13 September 2010; accepted 22 September 2010

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.146; data-to-parameter ratio = 16.2.

In the title molecule, $C_{14}H_{11}N_3O$, the benzene ring is twisted by 14.0 (2)° from the plane through the fused ring system. In the crystal, π–π interactions [centroid–centroid distances = 3.609 (1), 3.639 (1) and 3.735 (1) Å] form stacks of molecules propagating along the b axis. The crystal packing is further stabilized by weak intermolecular C—H···O and C—H···N hydrogen bonds.

Related literature

For a related structure, see: Koch *et al.* (2009). For the pharmacological properties of quinoxaline compounds, see: Kleim *et al.* (1995); Abasolo *et al.* (1987); Rodrigo *et al.* (2002).



Experimental

Crystal data

$C_{14}H_{11}N_3O$
M_r = 237.26
Monoclinic, $P2_1/c$
a = 6.4486 (13) Å
b = 7.3265 (15) Å
c = 24.216 (6) Å
β = 99.31 (3)°
V = 1129.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 K
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.982, T_{max} = 0.989
9650 measured reflections
2677 independent reflections
2221 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.09
2677 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N3^{i}	0.95	2.54	3.361 (2)	145
C3—H3···O1^{ii}	0.95	2.44	3.123 (2)	129

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author is indebted to Beijing Amber Tech Co. Ltd for the offer of some reagents.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2765).

References

Abasolo, M. I., Gaozza, C. H. & Fernandez, B. M. (1987). *J. Heterocycl. Chem.* **24**, 1771–1775.
Kleim, J. P., Bender, R., Kirsch, R., Meichsner, C., Paessens, A., Rosner, M., Rubsamen Waigmann, H., Kaiser, R., Wichers, M., Schneweis, K. E., Winkler, I. & Riess, G. (1995). *Antimicrob. Agents Chemother.* **39**, 2253–2257.
Koch, P., Schollmeyer, D. & Laufer, S. (2009). *Acta Cryst.* E**65**, o2512.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan.
Rodrigo, G. A., Robinshon, A. E., Hedrera, M. E., Kogan, M., Sicardi, S. M. & Fernaandez, B. M. (2002). *Trends Heterocycl. Chem.* **8**, 137–143.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o2650 [**doi:10.1107/S1600536810037943**]

3-(4-Methoxyphenyl)pyrido[2,3-*b*]pyrazine

C. Wang, J. Yan, H.-J. Chi, Y. Dong and Z. Zhang

Comment

Functionalized quinoxalines represent an important class of nitrogen-containing heterocycle which display a broad spectrum of biological activity. Similar structure had been reported by Koch (Koch *et al.*, 2009). Quinoxaline derivatives were found to exhibit antimicrobial (Kleim *et al.* 1995), antitumor (Abasolo *et al.*,1987), and antituberculous activity (Rodrigo *et al.*, 2002). Here, we report the synthesis and crystal structure of the title compound, (I) (Fig. 1).

The molecular structure of title compound (I) is as shown in Fig.1. The dihedral angle between the pyrido[2,3-*b*]pyrazine ring and benzene ring is 14.0 (2)°. The O atom attached to the phenyl ring don't deviate the phenyl ring with an r.m.s deviation of 0.0047 (3) Å. As a result of π-π conjugation, the C_{sp}^2-O bond [O1—C9 = 1.3656 (13) Å] is significantly shorter than the C_{sp}^3-O bond [O1—C14 = 1.4266 (15) Å]. The crystal structure is stabilized by weak C—H···N and C—H···O intermolecular interactions and π-π interactions between the *Cg*1 (centroid of N1/C1—C5) and *Cg*2 (centroid of C1/C2/N3/C6/C7/N2). Selected geometric parameters are shown in Table 1.

Experimental

A suspension of 2-(4-methoxyphenyl)-2-oxoacetaldehyde (2.0 mmol) and pyridine-2,3-diamine (3.0 mmol) in ethanol (5 ml) was stirred at room temperature. The reaction progress was monitored *via* TLC. The resulting precipitate was filtered off, washed with cold ethanol, dried and purified to give the target product as light yellow solid in 93% yield. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform-ethanol (1:1).

Refinement

All H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2-1.5U_{eq} of the parent atom.

Figures

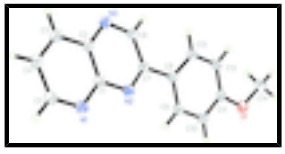


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

3-(4-Methoxyphenyl)pyrido[2,3-*b*]pyrazine

Crystal data

$C_{14}H_{11}N_3O$ $F(000) = 496$

M_r = 237.26	D_x = 1.396 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 428 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 6.4486 (13) Å	Cell parameters from 3162 reflections
b = 7.3265 (15) Å	θ = 2.6–27.9°
c = 24.216 (6) Å	μ = 0.09 mm^{-1}
β = 99.31 (3)°	T = 153 K
V = 1129.0 (4) Å^3	Prism, colourless
Z = 4	0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer	2677 independent reflections
Radiation source: rotating anode	2221 reflections with $I > 2\sigma(I)$
multilayer	R_{int} = 0.034
Detector resolution: 7.31 pixels mm^{-1}	θ_{max} = 27.9°, θ_{min} = 1.7°
φ and ω scans	h = −8→8
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)	k = −9→9
T_{min} = 0.982, T_{max} = 0.989	l = −19→31
9650 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.146	$w = 1/[\sigma^2(F_o^2) + (0.0916P)^2 + 0.0926P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.001
2677 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
165 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.194 (16)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-

factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71204 (14)	0.63090 (12)	0.31035 (3)	0.0269 (3)
N1	1.25315 (15)	0.85321 (13)	0.01789 (4)	0.0217 (3)
N2	1.03617 (15)	0.75236 (12)	0.07944 (4)	0.0194 (3)
N3	0.73020 (15)	0.63878 (13)	−0.01163 (4)	0.0212 (3)
C1	1.06896 (17)	0.77325 (15)	0.02545 (5)	0.0180 (3)
C2	0.91672 (17)	0.71404 (15)	−0.02001 (5)	0.0187 (3)
C3	0.95826 (18)	0.73760 (16)	−0.07480 (5)	0.0221 (3)
H3	0.8603	0.6979	−0.1061	0.027*
C4	1.14169 (19)	0.81838 (16)	−0.08199 (5)	0.0237 (3)
H4	1.1734	0.8377	−0.1185	0.028*
C5	1.28488 (19)	0.87344 (16)	−0.03427 (5)	0.0228 (3)
H5	1.4127	0.9288	−0.0402	0.027*
C6	0.70072 (18)	0.62433 (15)	0.04042 (5)	0.0211 (3)
H6	0.5715	0.5753	0.0477	0.025*
C7	0.85538 (17)	0.67952 (15)	0.08691 (5)	0.0181 (3)
C8	0.81251 (17)	0.65886 (15)	0.14497 (5)	0.0193 (3)
C9	0.93848 (19)	0.75321 (17)	0.18866 (5)	0.0245 (3)
H9	1.0513	0.8266	0.1806	0.029*
C10	0.90077 (19)	0.74085 (17)	0.24297 (5)	0.0253 (3)
H10	0.9865	0.8063	0.2719	0.030*
C11	0.73669 (19)	0.63212 (15)	0.25539 (5)	0.0210 (3)
C12	0.61082 (19)	0.53616 (16)	0.21299 (5)	0.0235 (3)
H12	0.4993	0.4616	0.2213	0.028*
C13	0.65008 (18)	0.55069 (16)	0.15829 (5)	0.0227 (3)
H13	0.5640	0.4852	0.1294	0.027*
C14	0.5489 (2)	0.52103 (19)	0.32631 (5)	0.0320 (3)
H14A	0.4121	0.5671	0.3081	0.048*
H14B	0.5564	0.5260	0.3670	0.048*
H14C	0.5662	0.3945	0.3147	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0318 (5)	0.0324 (5)	0.0180 (5)	−0.0071 (4)	0.0082 (3)	−0.0017 (3)
N1	0.0205 (5)	0.0225 (5)	0.0226 (5)	−0.0010 (4)	0.0050 (4)	−0.0004 (4)
N2	0.0200 (5)	0.0199 (5)	0.0185 (5)	−0.0010 (4)	0.0034 (4)	−0.0008 (4)
N3	0.0191 (5)	0.0233 (5)	0.0204 (5)	−0.0008 (4)	0.0013 (4)	0.0005 (4)
C1	0.0182 (5)	0.0172 (5)	0.0186 (6)	0.0012 (4)	0.0024 (4)	−0.0007 (4)
C2	0.0189 (5)	0.0167 (5)	0.0203 (6)	0.0017 (4)	0.0026 (4)	0.0005 (4)
C3	0.0245 (6)	0.0225 (6)	0.0185 (6)	0.0018 (4)	0.0008 (4)	0.0003 (4)
C4	0.0280 (6)	0.0241 (6)	0.0201 (6)	0.0021 (5)	0.0069 (4)	0.0019 (5)
C5	0.0218 (6)	0.0223 (6)	0.0253 (6)	−0.0002 (4)	0.0069 (4)	0.0002 (4)

C6	0.0183 (5)	0.0229 (6)	0.0220 (6)	−0.0020 (4)	0.0029 (4)	0.0001 (4)
C7	0.0185 (5)	0.0164 (5)	0.0194 (6)	0.0005 (4)	0.0032 (4)	−0.0010 (4)
C8	0.0203 (5)	0.0194 (5)	0.0183 (6)	−0.0003 (4)	0.0032 (4)	−0.0011 (4)
C9	0.0241 (6)	0.0278 (6)	0.0218 (6)	−0.0078 (5)	0.0046 (4)	−0.0012 (4)
C10	0.0277 (6)	0.0283 (7)	0.0192 (6)	−0.0066 (5)	0.0015 (5)	−0.0032 (5)
C11	0.0244 (6)	0.0216 (6)	0.0178 (6)	0.0007 (4)	0.0058 (4)	0.0000 (4)
C12	0.0242 (6)	0.0230 (6)	0.0247 (6)	−0.0053 (4)	0.0080 (5)	−0.0017 (5)
C13	0.0247 (6)	0.0229 (6)	0.0209 (6)	−0.0045 (4)	0.0048 (4)	−0.0041 (4)
C14	0.0340 (7)	0.0412 (8)	0.0241 (6)	−0.0085 (6)	0.0141 (5)	−0.0009 (5)

Geometric parameters (Å, °)

O1—C11	1.3656 (13)	C6—H6	0.9500
O1—C14	1.4266 (15)	C7—C8	1.4838 (15)
N1—C5	1.3203 (15)	C8—C13	1.3924 (16)
N1—C1	1.3630 (14)	C8—C9	1.4069 (16)
N2—C7	1.3210 (14)	C9—C10	1.3786 (16)
N2—C1	1.3662 (14)	C9—H9	0.9500
N3—C6	1.3089 (15)	C10—C11	1.3955 (16)
N3—C2	1.3678 (15)	C10—H10	0.9500
C1—C2	1.4192 (16)	C11—C12	1.3921 (17)
C2—C3	1.4061 (15)	C12—C13	1.3922 (16)
C3—C4	1.3588 (17)	C12—H12	0.9500
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.4161 (17)	C14—H14A	0.9800
C4—H4	0.9500	C14—H14B	0.9800
C5—H5	0.9500	C14—H14C	0.9800
C6—C7	1.4361 (16)		
Cg1···Cg2^{i}	3.639 (1)	Cg2···Cg2^{ii}	3.735 (1)
Cg1···Cg2^{ii}	3.609 (1)		
C11—O1—C14	118.35 (9)	C13—C8—C9	118.02 (11)
C5—N1—C1	116.75 (10)	C13—C8—C7	122.69 (10)
C7—N2—C1	116.94 (10)	C9—C8—C7	119.28 (10)
C6—N3—C2	116.34 (9)	C10—C9—C8	121.05 (11)
N1—C1—N2	116.73 (10)	C10—C9—H9	119.5
N1—C1—C2	122.39 (11)	C8—C9—H9	119.5
N2—C1—C2	120.88 (10)	C9—C10—C11	120.00 (11)
N3—C2—C3	119.72 (10)	C9—C10—H10	120.0
N3—C2—C1	121.51 (11)	C11—C10—H10	120.0
C3—C2—C1	118.75 (11)	O1—C11—C12	124.73 (11)
C4—C3—C2	118.49 (11)	O1—C11—C10	115.19 (10)
C4—C3—H3	120.8	C12—C11—C10	120.08 (11)
C2—C3—H3	120.8	C11—C12—C13	119.28 (11)
C3—C4—C5	119.06 (11)	C11—C12—H12	120.4
C3—C4—H4	120.5	C13—C12—H12	120.4
C5—C4—H4	120.5	C12—C13—C8	121.56 (11)
N1—C5—C4	124.56 (11)	C12—C13—H13	119.2
N1—C5—H5	117.7	C8—C13—H13	119.2

C4—C5—H5	117.7	O1—C14—H14A	109.5
N3—C6—C7	122.78 (11)	O1—C14—H14B	109.5
N3—C6—H6	118.6	H14A—C14—H14B	109.5
C7—C6—H6	118.6	O1—C14—H14C	109.5
N2—C7—C6	121.51 (11)	H14A—C14—H14C	109.5
N2—C7—C8	118.35 (10)	H14B—C14—H14C	109.5
C6—C7—C8	120.13 (10)		
C5—N1—C1—N2	−179.99 (9)	N3—C6—C7—N2	1.49 (17)
C5—N1—C1—C2	−0.10 (17)	N3—C6—C7—C8	−179.77 (10)
C7—N2—C1—N1	178.19 (9)	N2—C7—C8—C13	−166.08 (10)
C7—N2—C1—C2	−1.70 (16)	C6—C7—C8—C13	15.13 (16)
C6—N3—C2—C3	−178.71 (10)	N2—C7—C8—C9	14.63 (16)
C6—N3—C2—C1	−0.13 (17)	C6—C7—C8—C9	−164.15 (11)
N1—C1—C2—N3	−178.12 (9)	C13—C8—C9—C10	−0.79 (17)
N2—C1—C2—N3	1.77 (17)	C7—C8—C9—C10	178.54 (10)
N1—C1—C2—C3	0.47 (17)	C8—C9—C10—C11	0.59 (18)
N2—C1—C2—C3	−179.64 (9)	C14—O1—C11—C12	1.36 (17)
N3—C2—C3—C4	177.79 (10)	C14—O1—C11—C10	−179.27 (10)
C1—C2—C3—C4	−0.83 (17)	C9—C10—C11—O1	−179.45 (10)
C2—C3—C4—C5	0.83 (17)	C9—C10—C11—C12	−0.05 (18)
C1—N1—C5—C4	0.10 (17)	O1—C11—C12—C13	179.06 (10)
C3—C4—C5—N1	−0.48 (18)	C10—C11—C12—C13	−0.28 (17)
C2—N3—C6—C7	−1.43 (16)	C11—C12—C13—C8	0.06 (17)
C1—N2—C7—C6	0.18 (16)	C9—C8—C13—C12	0.46 (17)
C1—N2—C7—C8	−178.59 (9)	C7—C8—C13—C12	−178.84 (10)

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*; (ii) −*x*+2, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N3^{iii}	0.95	2.54	3.361 (2)	145
C3—H3···O1^{iv}	0.95	2.44	3.123 (2)	129

Symmetry codes: (iii) −*x*+1, −*y*+1, −*z*; (iv) *x*, −*y*+3/2, *z*−1/2.

Fig. 1