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1-(Pyrazin-2-yl)pyridin-2(1*H*)-one

Shi-Guo Zhang,[a] Hai-Yan Xu[b] and Jing-Min Shi[b]*

[a]Department of Chemistry and Chemical Engineering, Institute of Materials Chemistry, Binzhou University, Binzhou 256603, People's Republic of China, and [b]Department of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China
Correspondence e-mail: shijingmin@beelink.com

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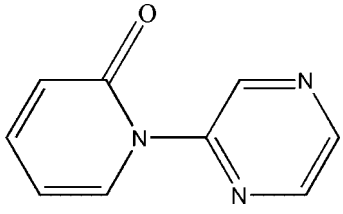
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.108; data-to-parameter ratio = 9.5.

In the crystal structure of the title compound, $C_9H_7N_3O$, the molecules are held together by C—H···N and C—H···O nonclassical hydrogen bonds. The dihedral angle between pyridine ring and pyrazine ring is 46.45 (14)°.

Related literature

For a related structure, see: McMorran & Steel (2002).



Experimental

Crystal data

$C_9H_7N_3O$
M_r = 173.18
Orthorhombic, $P2_12_12_1$
a = 3.7885 (12) Å
b = 13.939 (4) Å
c = 15.191 (5) Å
V = 802.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.45 × 0.16 × 0.13 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.957, T_{max} = 0.987
4919 measured reflections
1116 independent reflections
877 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.109
S = 1.06
1116 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N2^{i}	0.93	2.60	3.512 (3)	167
C7—H7···O1	0.93	2.54	2.846 (3)	100
C9—H9···O1^{ii}	0.93	2.53	3.450 (3)	169

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2398).

References

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supplementary materials

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1-(Pyrazin-2-yl)pyridin-2(1*H*)-one

S.-G. Zhang, H.-Y. Xu and J.-M. Shi

Comment

Pyridine, pyrazine and their derivatives are very useful ligands. Geometric parameters of the title compound are in the usual ranges. The dihedral angle between the pyridine ring and pyrazine ring is 46.45 (14) °. In the crystal the packing is stabilized by non-classic hydrogen bonds.

Experimental

The yellow single-crystal of the title compound was obtained by recrystallization of crude prodeuct in ethyl acetate. The IR spectrum displays the strong and sharp peaks at 1674 cm^{-1}, 1604 cm^{-1}, 1539 cm^{-1} and 1416 $^{-1}$, which may be attributed to the vibrations of C=O, C=C and C=N bonds.

Refinement

In the absence of anomalous scatterers Friedel pairs had been merged and the absolute structure had been arbitrarily set. The H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å, U_{iso}(H) = 1.2$_{eq}$(C).

Figures

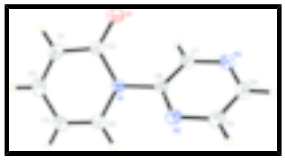

Fig. 1. The molecular structure of (I), showing the the atom numbering scheme with thermal ellipsoids drawn at the 30% probability level.

1-(Pyrazin-2-yl)pyridin-2(1*H*)-one

Crystal data

$C_9H_7N_3O$	F_{000} = 360
M_r = 173.18	D_x = 1.434 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 915 reflections
a = 3.7885 (12) Å	θ = 2.7–21.5º
b = 13.939 (4) Å	μ = 0.10 mm^{-1}
c = 15.191 (5) Å	T = 298 (2) K
V = 802.2 (4) $Å^3$	Prism, yellow
Z = 4	0.45 × 0.16 × 0.13 mm

Data collection

Bruker SMART APEX CCD diffractometer	1116 independent reflections
Radiation source: fine-focus sealed tube	877 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.050$
$T = 298(2)$ K	$\theta_{max} = 27.8^{o}$
φ and ω scans	$\theta_{min} = 2.0^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -4\rightarrow4$
$T_{min} = 0.957$, $T_{max} = 0.987$	$k = -17\rightarrow18$
4919 measured reflections	$l = -13\rightarrow19$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.0218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.109$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
1116 reflections	Extinction correction: none
118 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C3	0.0141 (7)	0.39124 (17)	0.78163 (15)	0.0360 (6)
C6	0.1437 (7)	0.47805 (14)	0.91863 (13)	0.0319 (5)
N1	0.1543 (6)	0.39158 (12)	0.86787 (11)	0.0326 (5)

C7	0.2634 (8)	0.56411 (14)	0.88484 (16)	0.0395 (6)
H7	0.3520	0.5661	0.8278	0.047*
C1	0.0273 (8)	0.29989 (18)	0.73926 (16)	0.0447 (7)
H1	−0.0532	0.2949	0.6816	0.054*
N2	0.0239 (6)	0.46918 (14)	0.99967 (12)	0.0417 (6)
O1	−0.1113 (6)	0.46495 (12)	0.75031 (11)	0.0524 (5)
N3	0.2542 (7)	0.64396 (13)	0.93230 (14)	0.0478 (6)
C5	0.2798 (8)	0.30965 (15)	0.90766 (15)	0.0391 (6)
H5	0.3655	0.3132	0.9649	0.047*
C8	0.1289 (9)	0.63572 (18)	1.01391 (17)	0.0493 (7)
H8	0.1149	0.6902	1.0491	0.059*
C2	0.1513 (9)	0.22094 (18)	0.77935 (18)	0.0490 (7)
H2	0.1511	0.1627	0.7494	0.059*
C4	0.2815 (8)	0.22503 (16)	0.86602 (17)	0.0469 (7)
H4	0.3668	0.1702	0.8937	0.056*
C9	0.0197 (8)	0.54941 (17)	1.04775 (17)	0.0487 (7)
H9	−0.0593	0.5467	1.1057	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.0343 (14)	0.0426 (13)	0.0312 (12)	0.0027 (12)	−0.0002 (11)	0.0019 (10)
C6	0.0334 (14)	0.0321 (11)	0.0301 (11)	0.0051 (12)	−0.0024 (11)	0.0015 (9)
N1	0.0385 (13)	0.0303 (9)	0.0290 (9)	0.0019 (10)	0.0007 (10)	0.0017 (8)
C7	0.0441 (17)	0.0365 (12)	0.0377 (13)	−0.0030 (12)	−0.0014 (12)	0.0026 (11)
C1	0.0450 (17)	0.0522 (14)	0.0370 (13)	−0.0006 (13)	0.0000 (13)	−0.0103 (12)
N2	0.0534 (15)	0.0389 (10)	0.0328 (10)	0.0003 (11)	0.0055 (11)	0.0010 (9)
O1	0.0689 (14)	0.0489 (10)	0.0393 (9)	0.0112 (11)	−0.0120 (11)	0.0048 (8)
N3	0.0613 (17)	0.0328 (10)	0.0492 (13)	−0.0007 (11)	−0.0052 (13)	0.0019 (9)
C5	0.0415 (17)	0.0380 (12)	0.0379 (12)	0.0034 (12)	0.0011 (12)	0.0058 (10)
C8	0.061 (2)	0.0388 (13)	0.0482 (16)	0.0072 (14)	−0.0080 (16)	−0.0102 (12)
C2	0.0488 (18)	0.0424 (13)	0.0557 (16)	0.0004 (14)	0.0075 (15)	−0.0143 (12)
C4	0.0518 (19)	0.0338 (12)	0.0552 (16)	0.0073 (13)	0.0011 (15)	0.0036 (11)
C9	0.062 (2)	0.0483 (15)	0.0356 (13)	0.0048 (15)	0.0041 (14)	−0.0035 (12)

Geometric parameters (Å, °)

C3—O1	1.228 (3)	N2—C9	1.336 (3)
C3—N1	1.414 (3)	N3—C8	1.332 (3)
C3—C1	1.427 (3)	C5—C4	1.338 (3)
C6—N2	1.318 (3)	C5—H5	0.9300
C6—C7	1.381 (3)	C8—C9	1.372 (4)
C6—N1	1.431 (3)	C8—H8	0.9300
N1—C5	1.377 (3)	C2—C4	1.407 (4)
C7—N3	1.327 (3)	C2—H2	0.9300
C7—H7	0.9300	C4—H4	0.9300
C1—C2	1.343 (4)	C9—H9	0.9300
C1—H1	0.9300		

O1—C3—N1	120.1 (2)	C7—N3—C8	116.3 (2)
O1—C3—C1	125.8 (2)	C4—C5—N1	121.7 (2)
N1—C3—C1	114.1 (2)	C4—C5—H5	119.2
N2—C6—C7	122.8 (2)	N1—C5—H5	119.2
N2—C6—N1	115.72 (18)	N3—C8—C9	122.1 (2)
C7—C6—N1	121.5 (2)	N3—C8—H8	118.9
C5—N1—C3	122.26 (19)	C9—C8—H8	118.9
C5—N1—C6	118.14 (17)	C1—C2—C4	120.9 (2)
C3—N1—C6	119.44 (17)	C1—C2—H2	119.5
N3—C7—C6	121.2 (2)	C4—C2—H2	119.5
N3—C7—H7	119.4	C5—C4—C2	118.4 (2)
C6—C7—H7	119.4	C5—C4—H4	120.8
C2—C1—C3	122.6 (2)	C2—C4—H4	120.8
C2—C1—H1	118.7	N2—C9—C8	121.7 (2)
C3—C1—H1	118.7	N2—C9—H9	119.1
C6—N2—C9	115.9 (2)	C8—C9—H9	119.1
O1—C3—N1—C5	176.3 (3)	C7—C6—N2—C9	0.9 (4)
C1—C3—N1—C5	−2.2 (3)	N1—C6—N2—C9	178.8 (2)
O1—C3—N1—C6	0.9 (4)	C6—C7—N3—C8	0.9 (4)
C1—C3—N1—C6	−177.5 (2)	C3—N1—C5—C4	1.2 (4)
N2—C6—N1—C5	−43.8 (3)	C6—N1—C5—C4	176.6 (3)
C7—C6—N1—C5	134.2 (3)	C7—N3—C8—C9	0.9 (5)
N2—C6—N1—C3	131.8 (2)	C3—C1—C2—C4	−1.0 (5)
C7—C6—N1—C3	−50.3 (4)	N1—C5—C4—C2	0.1 (5)
N2—C6—C7—N3	−2.0 (4)	C1—C2—C4—C5	−0.1 (5)
N1—C6—C7—N3	−179.7 (3)	C6—N2—C9—C8	0.9 (4)
O1—C3—C1—C2	−176.3 (3)	N3—C8—C9—N2	−1.9 (5)
N1—C3—C1—C2	2.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N2^{i}	0.93	2.60	3.512 (3)	167
C7—H7···O1	0.93	2.54	2.846 (3)	100
C9—H9···O1^{ii}	0.93	2.53	3.450 (3)	169

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

Fig. 1