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(*E*)-1-(Pyridin-4-yl)propan-1-one oxime

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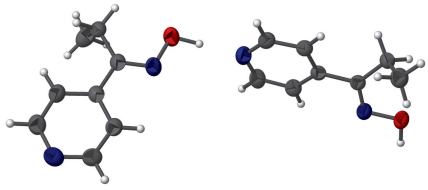
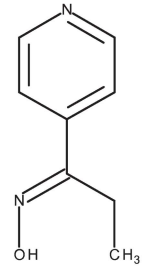
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_8H_{10}N_2O$, contains two crystallographically independent molecules of slightly different conformation, which are linked *via* an intermolecular O—H···N hydrogen bond. The dihedral angle between the pyridine ring and the oxime plane of molecule *A* [2.09 (19)°] is smaller than in molecule *B* [16.50 (18)°].

3D view



Chemical scheme



Structure description

The title compound, $C_8H_{10}N_2O$, was synthesized by the reaction of 4-propionylpyridine and hydroxylamine. The asymmetric unit contains two crystallographically independent molecules (*A* and *B*, Fig. 1) of slightly different conformation, which are linked *via* an intermolecular O—H···N hydrogen bond (Table 1). The dihedral angle between the pyridine ring and the oxime plane of molecule *A* [2.09 (19)°] is smaller than in molecule *B* [16.50 (18)°]. Both molecules are in an *E* orientation.

In the crystal, each *A* molecule is connected with two *B* molecules and *vice versa* via further O—H···N hydrogen bonds, resulting in a zigzag chain parallel to the *c* axis.

Synthesis and crystallization

An aqueous solution of sodium hydroxide (20%, 20 ml) was added to hydroxylamine hydrochloride (3.70 g, 53.27 mmol) in water (50 ml). After addition of 4-propionylpyridine (5.72 g, 44.39 mmol) at 273 K, the reaction was stirred for 2.5 h at 298 K. Then, the product was extracted by ethyl acetate and the solvent was evaporated under reduced pressure. The title compound was obtained by crystallization in hot ethanol as white crystals in 87% yield. ^{1}H NMR (400 MHz, DMSO-d_6): δ 1.03 (*t*, ^3J = 7.6 Hz, 3H, CH_3), 2.71 (*q*, ^3J = 7.6 Hz, 2H, CH_2), 7.60 (*d*, ^3J = 5.3 Hz, 2H, CH), 8.58 (*d*, ^3J = 5.2 Hz, 2H, CH),

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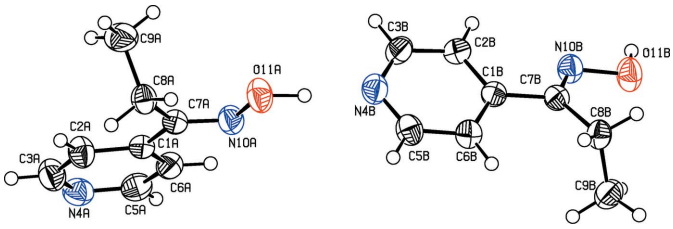

Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

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

D—H···A	D—H	H···A	D···A	D—H···A
O11A—H11A···N4B	1.06	1.68	2.729 (2)	175
O11B—H11B···N4A^{i}	1.02	1.69	2.708 (2)	172

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

11.68 (*s*, 1H, OH); ^{13}C-{^{1}H}-NMR (100 MHz, DMSO-d_6): δ 10.6, 17.7, 120.0, 142.9, 150.0, 156.2. For a similar preparation of the title compound, see Huang *et al.* (2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_{10}N_2O$
M_r	150.18
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	213
a, b, c (Å)	7.9149 (3), 9.3676 (4), 21.6431 (8)
V (Å^3)	1604.70 (11)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.69
Crystal size (mm)	0.70 × 0.40 × 0.20
Data collection	
Diffractometer	Stoe IPDS 2T
Absorption correction	Integration (*X-RED*; Stoe & Cie, 2011)
T_{min}, T_{max}	0.684, 0.888
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15705, 2797, 2734
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.599
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.088, 1.12
No. of reflections	2797
No. of parameters	201
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.15
Absolute structure	Flack x determined using 1114 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter	0.01 (6)

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2011), *SIR2004* (Burla *et al.*, 2005), *SHELXL2013* and *XP* (Sheldrick, 2015).

References

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full crystallographic data

IUCrData (2016). **1**, x160803 [doi:10.1107/S2414314616008038]

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Crystal data

$C_8H_{10}N_2O$
M_r = 150.18
Orthorhombic, $P2_12_12_1$
a = 7.9149 (3) Å
b = 9.3676 (4) Å
c = 21.6431 (8) Å
V = 1604.70 (11) Å^3
Z = 8
$F(000)$ = 640
D_x = 1.243 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 42392 reflections
θ = 4.1–68.6°
μ = 0.69 mm^{-1}
T = 213 K
Plate, colourless
0.70 × 0.40 × 0.20 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: Incoatec microSource Cu
X-ray mirror monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED*; Stoe & Cie, 2011)
T_{min} = 0.684, T_{max} = 0.888
15705 measured reflections
2797 independent reflections
2734 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 67.5°, θ_{min} = 4.1°
h = −9→9
k = −11→11
l = −25→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.088
S = 1.12
2797 reflections
201 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.2424P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack x determined using 1114 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter: 0.01 (6)

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.4400 (3)	0.8985 (2)	0.69902 (8)	0.0352 (4)
C2A	0.4013 (3)	1.0058 (2)	0.74113 (10)	0.0463 (5)
H2A	0.4815	1.0766	0.7505	0.056*
C3A	0.2444 (3)	1.0079 (3)	0.76919 (10)	0.0507 (6)
H3A	0.2219	1.0809	0.7979	0.061*
N4A	0.1234 (2)	0.9129 (2)	0.75800 (9)	0.0475 (4)
C5A	0.1604 (3)	0.8092 (2)	0.71751 (10)	0.0458 (5)
H5A	0.0769	0.7407	0.7089	0.055*
C6A	0.3135 (3)	0.7972 (2)	0.68773 (9)	0.0409 (4)
H6A	0.3329	0.7217	0.6600	0.049*
C7A	0.6061 (3)	0.8934 (2)	0.66701 (8)	0.0359 (4)
C8A	0.7356 (3)	1.0078 (2)	0.67723 (9)	0.0401 (5)
H8A	0.8478	0.9702	0.6671	0.048*
H8B	0.7358	1.0350	0.7209	0.048*
C9A	0.7009 (4)	1.1392 (3)	0.63795 (11)	0.0576 (6)
H9A	0.7926	1.2069	0.6428	0.086*
H9B	0.5958	1.1830	0.6511	0.086*
H9C	0.6921	1.1114	0.5949	0.086*
N10A	0.6241 (2)	0.7873 (2)	0.62925 (8)	0.0441 (4)
O11A	0.7815 (2)	0.78887 (17)	0.60004 (7)	0.0515 (4)
H11A	0.7795	0.6997	0.5702	0.077*
C1B	0.7775 (2)	0.3235 (2)	0.44265 (8)	0.0339 (4)
C2B	0.6914 (3)	0.4473 (2)	0.42528 (9)	0.0403 (5)
H2B	0.6315	0.4502	0.3878	0.048*
C3B	0.6946 (3)	0.5650 (2)	0.46333 (10)	0.0462 (5)
H3B	0.6366	0.6475	0.4506	0.055*
N4B	0.7761 (2)	0.56832 (19)	0.51765 (8)	0.0454 (4)
C5B	0.8581 (3)	0.4508 (2)	0.53451 (10)	0.0439 (5)
H5B	0.9157	0.4512	0.5725	0.053*
C6B	0.8631 (3)	0.3273 (2)	0.49901 (9)	0.0398 (4)
H6B	0.9236	0.2471	0.5128	0.048*
C7B	0.7755 (2)	0.1927 (2)	0.40380 (8)	0.0344 (4)
C8B	0.8959 (2)	0.0715 (2)	0.41461 (9)	0.0391 (4)
H8C	0.9967	0.1076	0.4358	0.047*
H8D	0.9316	0.0324	0.3747	0.047*
C9B	0.8171 (3)	−0.0472 (2)	0.45324 (11)	0.0487 (5)
H9D	0.7127	−0.0783	0.4340	0.073*
H9E	0.7936	−0.0117	0.4945	0.073*
H9F	0.8949	−0.1270	0.4558	0.073*
N10B	0.6582 (2)	0.19141 (18)	0.36239 (8)	0.0404 (4)
O11B	0.6592 (2)	0.06524 (17)	0.32787 (7)	0.0495 (4)
H11B	0.5572	0.0810	0.2998	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0400 (10)	0.0344 (10)	0.0313 (9)	0.0014 (8)	−0.0010 (8)	0.0027 (7)
C2A	0.0467 (12)	0.0458 (12)	0.0463 (11)	−0.0048 (9)	0.0032 (9)	−0.0100 (9)
C3A	0.0525 (13)	0.0518 (12)	0.0477 (12)	−0.0006 (10)	0.0092 (10)	−0.0078 (10)
N4A	0.0448 (10)	0.0517 (10)	0.0459 (9)	0.0019 (8)	0.0059 (8)	0.0071 (8)
C5A	0.0432 (12)	0.0435 (11)	0.0506 (11)	−0.0044 (10)	−0.0005 (9)	0.0060 (10)
C6A	0.0447 (11)	0.0369 (10)	0.0412 (10)	−0.0004 (9)	−0.0011 (9)	0.0005 (9)
C7A	0.0408 (10)	0.0349 (10)	0.0321 (9)	0.0019 (8)	−0.0019 (8)	0.0008 (8)
C8A	0.0370 (10)	0.0433 (11)	0.0402 (10)	0.0006 (8)	−0.0026 (8)	−0.0072 (8)
C9A	0.0737 (16)	0.0494 (12)	0.0498 (12)	−0.0184 (12)	−0.0048 (12)	0.0044 (10)
N10A	0.0474 (10)	0.0413 (9)	0.0435 (9)	−0.0013 (8)	0.0098 (8)	−0.0044 (8)
O11A	0.0491 (9)	0.0512 (9)	0.0543 (9)	−0.0032 (7)	0.0163 (7)	−0.0141 (7)
C1B	0.0308 (9)	0.0345 (9)	0.0363 (9)	−0.0022 (8)	0.0039 (7)	0.0006 (8)
C2B	0.0442 (11)	0.0369 (10)	0.0399 (10)	0.0004 (9)	0.0011 (9)	0.0037 (8)
C3B	0.0547 (12)	0.0325 (10)	0.0515 (12)	0.0013 (10)	0.0074 (10)	0.0023 (9)
N4B	0.0482 (10)	0.0390 (9)	0.0490 (10)	−0.0052 (8)	0.0103 (8)	−0.0063 (7)
C5B	0.0401 (10)	0.0487 (12)	0.0430 (11)	−0.0042 (9)	0.0004 (9)	−0.0078 (9)
C6B	0.0361 (10)	0.0410 (10)	0.0424 (10)	0.0013 (9)	−0.0020 (8)	−0.0027 (8)
C7B	0.0327 (9)	0.0361 (9)	0.0343 (9)	−0.0011 (8)	0.0010 (7)	−0.0003 (8)
C8B	0.0364 (10)	0.0385 (10)	0.0423 (10)	0.0040 (8)	−0.0016 (8)	−0.0061 (8)
C9B	0.0537 (13)	0.0387 (11)	0.0537 (12)	0.0045 (10)	−0.0024 (10)	0.0012 (9)
N10B	0.0420 (9)	0.0391 (9)	0.0400 (8)	0.0017 (8)	−0.0030 (7)	−0.0055 (7)
O11B	0.0524 (9)	0.0488 (8)	0.0474 (8)	0.0067 (7)	−0.0113 (7)	−0.0158 (7)

Geometric parameters (Å, º)

C1A—C2A	1.391 (3)	C1B—C6B	1.396 (3)
C1A—C6A	1.400 (3)	C1B—C2B	1.397 (3)
C1A—C7A	1.487 (3)	C1B—C7B	1.486 (3)
C2A—C3A	1.383 (3)	C2B—C3B	1.377 (3)
C2A—H2A	0.9400	C2B—H2B	0.9400
C3A—N4A	1.330 (3)	C3B—N4B	1.341 (3)
C3A—H3A	0.9400	C3B—H3B	0.9400
N4A—C5A	1.340 (3)	N4B—C5B	1.329 (3)
C5A—C6A	1.377 (3)	C5B—C6B	1.389 (3)
C5A—H5A	0.9400	C5B—H5B	0.9400
C6A—H6A	0.9400	C6B—H6B	0.9400
C7A—N10A	1.294 (3)	C7B—N10B	1.290 (2)
C7A—C8A	1.499 (3)	C7B—C8B	1.501 (3)
C8A—C9A	1.521 (3)	C8B—C9B	1.525 (3)
C8A—H8A	0.9800	C8B—H8C	0.9800
C8A—H8B	0.9800	C8B—H8D	0.9800
C9A—H9A	0.9700	C9B—H9D	0.9700
C9A—H9B	0.9700	C9B—H9E	0.9700
C9A—H9C	0.9700	C9B—H9F	0.9700
N10A—O11A	1.397 (2)	N10B—O11B	1.398 (2)

O11A—H11A	1.0560	O11B—H11B	1.0215
C2A—C1A—C6A	116.51 (19)	C6B—C1B—C2B	116.79 (18)
C2A—C1A—C7A	121.52 (18)	C6B—C1B—C7B	121.40 (17)
C6A—C1A—C7A	121.96 (17)	C2B—C1B—C7B	121.80 (17)
C3A—C2A—C1A	119.7 (2)	C3B—C2B—C1B	119.67 (19)
C3A—C2A—H2A	120.1	C3B—C2B—H2B	120.2
C1A—C2A—H2A	120.1	C1B—C2B—H2B	120.2
N4A—C3A—C2A	123.9 (2)	N4B—C3B—C2B	123.5 (2)
N4A—C3A—H3A	118.1	N4B—C3B—H3B	118.3
C2A—C3A—H3A	118.1	C2B—C3B—H3B	118.3
C3A—N4A—C5A	116.54 (19)	C5B—N4B—C3B	117.15 (18)
N4A—C5A—C6A	123.9 (2)	N4B—C5B—C6B	123.5 (2)
N4A—C5A—H5A	118.1	N4B—C5B—H5B	118.3
C6A—C5A—H5A	118.1	C6B—C5B—H5B	118.3
C5A—C6A—C1A	119.48 (19)	C5B—C6B—C1B	119.41 (19)
C5A—C6A—H6A	120.3	C5B—C6B—H6B	120.3
C1A—C6A—H6A	120.3	C1B—C6B—H6B	120.3
N10A—C7A—C1A	114.60 (17)	N10B—C7B—C1B	114.11 (17)
N10A—C7A—C8A	124.50 (18)	N10B—C7B—C8B	123.93 (17)
C1A—C7A—C8A	120.86 (17)	C1B—C7B—C8B	121.91 (16)
C7A—C8A—C9A	111.87 (17)	C7B—C8B—C9B	112.16 (17)
C7A—C8A—H8A	109.2	C7B—C8B—H8C	109.2
C9A—C8A—H8A	109.2	C9B—C8B—H8C	109.2
C7A—C8A—H8B	109.2	C7B—C8B—H8D	109.2
C9A—C8A—H8B	109.2	C9B—C8B—H8D	109.2
H8A—C8A—H8B	107.9	H8C—C8B—H8D	107.9
C8A—C9A—H9A	109.5	C8B—C9B—H9D	109.5
C8A—C9A—H9B	109.5	C8B—C9B—H9E	109.5
H9A—C9A—H9B	109.5	H9D—C9B—H9E	109.5
C8A—C9A—H9C	109.5	C8B—C9B—H9F	109.5
H9A—C9A—H9C	109.5	H9D—C9B—H9F	109.5
H9B—C9A—H9C	109.5	H9E—C9B—H9F	109.5
C7A—N10A—O11A	112.09 (17)	C7B—N10B—O11B	112.01 (16)
N10A—O11A—H11A	104.8	N10B—O11B—H11B	101.0
C6A—C1A—C2A—C3A	0.0 (3)	C6B—C1B—C2B—C3B	0.2 (3)
C7A—C1A—C2A—C3A	179.00 (19)	C7B—C1B—C2B—C3B	178.90 (18)
C1A—C2A—C3A—N4A	−0.8 (4)	C1B—C2B—C3B—N4B	−0.5 (3)
C2A—C3A—N4A—C5A	0.9 (3)	C2B—C3B—N4B—C5B	0.4 (3)
C3A—N4A—C5A—C6A	−0.2 (3)	C3B—N4B—C5B—C6B	0.1 (3)
N4A—C5A—C6A—C1A	−0.6 (3)	N4B—C5B—C6B—C1B	−0.5 (3)
C2A—C1A—C6A—C5A	0.7 (3)	C2B—C1B—C6B—C5B	0.3 (3)
C7A—C1A—C6A—C5A	−178.33 (18)	C7B—C1B—C6B—C5B	−178.43 (19)
C2A—C1A—C7A—N10A	179.88 (19)	C6B—C1B—C7B—N10B	162.62 (18)
C6A—C1A—C7A—N10A	−1.2 (3)	C2B—C1B—C7B—N10B	−16.1 (3)
C2A—C1A—C7A—C8A	−2.5 (3)	C6B—C1B—C7B—C8B	−14.8 (3)
C6A—C1A—C7A—C8A	176.47 (18)	C2B—C1B—C7B—C8B	166.50 (18)

N10A—C7A—C8A—C9A	95.8 (2)	N10B—C7B—C8B—C9B	−80.2 (2)
C1A—C7A—C8A—C9A	−81.6 (2)	C1B—C7B—C8B—C9B	97.0 (2)
C1A—C7A—N10A—O11A	179.33 (16)	C1B—C7B—N10B—O11B	−178.80 (15)
C8A—C7A—N10A—O11A	1.8 (3)	C8B—C7B—N10B—O11B	−1.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11*A*—H11*A*···N4*B*	1.06	1.68	2.729 (2)	175
O11*B*—H11*B*···N4*A*^{i}	1.02	1.69	2.708 (2)	172

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