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Benzaldehyde *O*-[(*E*)-(6-chloropyridin-3-yl)methyl]oxime

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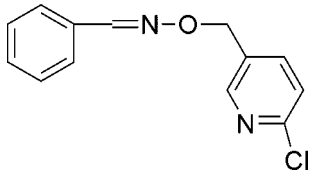
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.069; wR factor = 0.172; data-to-parameter ratio = 15.8.

The title compound, $C_{13}H_{11}ClN_2O$, was obtained as the product of our attempted synthesis of biologically active compounds containing oxime ether and pyridyl groups. Intermolecular C—H···N hydrogen bonds link molecules into a linear structure and contribute to the stability of the molecular configuration. In addition, C—H···π hydrogen bonds are observed in the crystal structure.

Related literature

The biological and pharmaceutical activities of pyridine have been described by Liu *et al.* (1996), Finkelstein *et al.* (1997), Li *et al.* (2006) and Jo *et al.* (2004). The preparation of the potentially active oxime ether has been described by Mohammad *et al.* (2005). For related literature, see: Liu *et al.*, (2000); Shimizu & Hakogi (2006).



Experimental

Crystal data

$C_{13}H_{11}ClN_2O$
M_r = 246.69
Monoclinic, $P2_1/n$
a = 7.6265 (7) Å
b = 6.1724 (6) Å
c = 26.559 (3) Å
β = 95.571 (2)°
V = 1244.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 291 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.944, T_{max} = 0.972
6565 measured reflections
2434 independent reflections
1812 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.173
S = 1.08
2434 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1^{i}	0.93	2.48	3.407 (3)	175
C10—H10···$Cg1^{ii}$	0.93	2.93	3.755 (3)	149
C15—H15···$Cg1^{iii}$	0.97	2.97	3.690 (4)	136

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.
Note: $Cg1$ and $Cg2$ are the centroids of the pyridyl and phenyl rings, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: BQ2025).

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supplementary materials

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Benzaldehyde *O*-[(*E*)-(6-chloropyridin-3-yl)methyl]oxime

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Comment

Many pyridyl-containing compounds are known to possess a wide range of biological and pharmacological activities, as well as low toxicity toward mammals. The study of oxime ether derivatives has become of much interest in recent years due to their anticholinergic, insecticidal and acaricidal activities. Different oxime ether derivatives have also been reported to possess antiprotozoan, antibacterial activity, antienteroviral, antifungal, antineoplastic, anticonvulsant, and antimicrobial activities. (Mohammad *et al.*, 2005)

In the crystal, intermolecular C—H···N hydrogen bonds link molecules into a line along the *b* axis and produce one dimensional structure. Of course, it contributes strongly to the stability of the molecular configuration. (Fig2) In addition, two weak C—H···π hydrogen bonds are observed in the crystal structure of (I). It has been known that aromatic H atoms can also function as hydrogen-bond donors towards aromatic π systems. The C10 benzene hydrogen is involved in C—H···π interactions with the C1—C6 pyridine ring, while C12 with C8—C13 benzene ring.

Experimental

Benzaldehyde oxime(2 mmol) in CH_2Cl_2(5 ml)and NaOH powder (2 mmol) was stirred vigorously for 5 min, then 2-chloro-5-(chloromethyl)- pyridine (2 mmol) was added. The mixture was stirred at room temperature until the reaction was complete (monitored by thin-layer chromatography), the solid was filtered off and the filtrate was concentrated under vacuum. The residue was purified by column chromatography on a silica gel using (20:1 *v*/*v*) petroleum ether/ethyl acetate as the eluent, giving a colourless solid (yield 67%, m.p. 331 K). A colorless crystal grown from carbon tetrachloride and petroleum ether (1:4 *v*/*v*) was selected for X-ray structure analysis.

Refinement

H atoms bonded to C were placed at calculated positions, with C—H distances of 0.97 and 0.93Å for H atoms bonded to sp^3 and sp^2 C atoms, respectively. They were refined using a riding model, with U_{iso}(H)=1.2 U_{eq}(C).

Figures

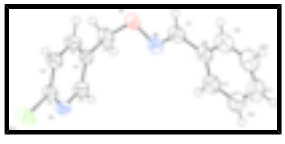

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

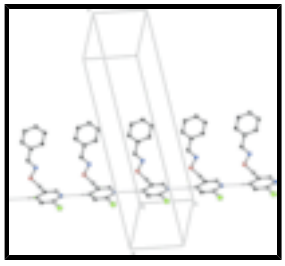

Fig. 2. Crystal Packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Benzaldehyde *O*-[(*E*)-(6-chloropyridin-3-yl)methyl]oxime

Crystal data

$C_{13}H_{11}ClN_2O$	F_{000} = 512
M_r = 246.69	D_x = 1.317 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1488 reflections
a = 7.6265 (7) Å	θ = 2.7–23.0º
b = 6.1724 (6) Å	μ = 0.29 mm^{-1}
c = 26.559 (3) Å	T = 291 (2) K
β = 95.571 (2)º	Block, colorless
V = 1244.4 (2) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1812 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.046
Monochromator: graphite	θ_{max} = 26.0º
T = 291(2) K	θ_{min} = 2.7º
φ and ω scans	h = −7→9
Absorption correction: none	k = −7→7
6565 measured reflections	l = −32→32
2434 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H-atom parameters constrained
$wR(F^2)$ = 0.173	$w = 1/[\sigma^2(F_o^2) + (0.0981P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
2434 reflections	$\Delta\rho_{max}$ = 0.46 e Å^{-3}

154 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Cl1	1.33608 (9)	0.63372 (13)	0.08131 (3)	0.0606 (3)
N1	0.9975 (3)	0.5817 (3)	0.06336 (8)	0.0430 (5)
C1	1.1464 (3)	0.4739 (4)	0.07219 (8)	0.0388 (6)
C2	1.1623 (3)	0.2523 (4)	0.07433 (9)	0.0444 (6)
H2	1.2711	0.1856	0.0816	0.053*
C3	1.0098 (3)	0.1334 (4)	0.06520 (10)	0.0465 (7)
H3	1.0141	−0.0171	0.0660	0.056*
N2	0.5987 (3)	0.0913 (4)	0.12441 (8)	0.0476 (6)
O1	0.6497 (2)	−0.0338 (3)	0.08380 (7)	0.0536 (5)
C4	0.8504 (3)	0.2383 (4)	0.05489 (8)	0.0380 (6)
C6	0.6820 (4)	0.1122 (5)	0.04346 (10)	0.0531 (7)
H6A	0.5841	0.2126	0.0379	0.064*
H6B	0.6884	0.0300	0.0126	0.064*
C7	0.5999 (3)	−0.0236 (5)	0.16416 (10)	0.0485 (7)
H7	0.6367	−0.1671	0.1632	0.058*
C5	0.8517 (3)	0.4599 (4)	0.05535 (8)	0.0416 (6)
H5	0.7441	0.5311	0.0497	0.050*
C8	0.5447 (3)	0.0640 (5)	0.21148 (9)	0.0443 (6)
C13	0.4649 (4)	0.2660 (5)	0.21383 (11)	0.0541 (7)
H13	0.4416	0.3482	0.1846	0.065*
C9	0.5771 (4)	−0.0548 (6)	0.25566 (11)	0.0601 (8)
H9	0.6287	−0.1909	0.2543	0.072*
C12	0.4203 (4)	0.3442 (6)	0.25976 (12)	0.0680 (9)
H12	0.3659	0.4786	0.2613	0.082*
C10	0.5348 (5)	0.0231 (6)	0.30130 (12)	0.0759 (10)
H10	0.5591	−0.0586	0.3306	0.091*
C11	0.4565 (5)	0.2227 (7)	0.30346 (12)	0.0750 (10)
H11	0.4276	0.2765	0.3343	0.090*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0421 (5)	0.0550 (5)	0.0831 (6)	−0.0231 (3)	−0.0027 (3)	0.0001 (4)
N1	0.0381 (13)	0.0328 (12)	0.0580 (13)	−0.0045 (10)	0.0043 (9)	−0.0007 (9)
C1	0.0313 (13)	0.0386 (15)	0.0462 (13)	−0.0081 (11)	0.0015 (10)	−0.0016 (11)
C2	0.0314 (14)	0.0379 (16)	0.0639 (16)	0.0001 (11)	0.0038 (11)	0.0048 (12)
C3	0.0434 (16)	0.0316 (14)	0.0641 (16)	−0.0043 (12)	0.0042 (12)	−0.0005 (12)
N2	0.0323 (12)	0.0466 (14)	0.0650 (14)	−0.0066 (10)	0.0100 (9)	−0.0024 (11)
O1	0.0454 (12)	0.0485 (12)	0.0693 (12)	−0.0202 (9)	0.0177 (8)	−0.0094 (9)
C4	0.0316 (13)	0.0397 (15)	0.0432 (13)	−0.0088 (11)	0.0057 (10)	−0.0031 (11)
C6	0.0422 (16)	0.0635 (19)	0.0537 (15)	−0.0211 (14)	0.0048 (12)	−0.0085 (14)
C7	0.0300 (14)	0.0422 (16)	0.0726 (18)	−0.0032 (11)	0.0019 (12)	0.0056 (14)
C5	0.0279 (13)	0.0432 (15)	0.0534 (15)	0.0019 (11)	0.0030 (10)	−0.0028 (12)
C8	0.0279 (14)	0.0481 (16)	0.0559 (16)	−0.0070 (11)	−0.0009 (10)	0.0038 (13)
C13	0.0407 (16)	0.0585 (19)	0.0631 (17)	0.0008 (14)	0.0048 (12)	0.0064 (14)
C9	0.0481 (18)	0.061 (2)	0.0693 (19)	0.0012 (15)	−0.0018 (14)	0.0123 (16)
C12	0.056 (2)	0.064 (2)	0.085 (2)	0.0030 (16)	0.0147 (16)	−0.0041 (18)
C10	0.082 (3)	0.083 (3)	0.062 (2)	−0.001 (2)	0.0035 (16)	0.0179 (19)
C11	0.071 (2)	0.097 (3)	0.0577 (19)	−0.011 (2)	0.0127 (15)	−0.0069 (19)

Geometric parameters (Å, °)

Cl1—C1	1.748 (2)	C7—C8	1.467 (4)
N1—C1	1.317 (3)	C7—H7	0.9300
N1—C5	1.341 (3)	C5—H5	0.9300
C1—C2	1.374 (4)	C8—C9	1.385 (4)
C2—C3	1.376 (3)	C8—C13	1.391 (4)
C2—H2	0.9300	C13—C12	1.385 (4)
C3—C4	1.381 (4)	C13—H13	0.9300
C3—H3	0.9300	C9—C10	1.371 (4)
N2—C7	1.271 (3)	C9—H9	0.9300
N2—O1	1.412 (3)	C12—C11	1.387 (5)
O1—C6	1.439 (3)	C12—H12	0.9300
C4—C5	1.368 (4)	C10—C11	1.373 (5)
C4—C6	1.508 (3)	C10—H10	0.9300
C6—H6A	0.9700	C11—H11	0.9300
C6—H6B	0.9700		
C1—N1—C5	115.6 (2)	C8—C7—H7	119.1
N1—C1—C2	125.5 (2)	N1—C5—C4	124.5 (2)
N1—C1—Cl1	115.30 (19)	N1—C5—H5	117.7
C2—C1—Cl1	119.16 (19)	C4—C5—H5	117.7
C1—C2—C3	117.0 (2)	C9—C8—C13	118.6 (3)
C1—C2—H2	121.5	C9—C8—C7	119.2 (3)
C3—C2—H2	121.5	C13—C8—C7	122.2 (2)
C2—C3—C4	119.8 (2)	C12—C13—C8	119.9 (3)
C2—C3—H3	120.1	C12—C13—H13	120.1

C4—C3—H3	120.1	C8—C13—H13	120.1
C7—N2—O1	110.4 (2)	C10—C9—C8	121.7 (3)
N2—O1—C6	107.8 (2)	C10—C9—H9	119.2
C5—C4—C3	117.5 (2)	C8—C9—H9	119.2
C5—C4—C6	121.6 (2)	C13—C12—C11	120.2 (3)
C3—C4—C6	121.0 (2)	C13—C12—H12	119.9
O1—C6—C4	112.2 (2)	C11—C12—H12	119.9
O1—C6—H6A	109.2	C9—C10—C11	119.5 (3)
C4—C6—H6A	109.2	C9—C10—H10	120.3
O1—C6—H6B	109.2	C11—C10—H10	120.3
C4—C6—H6B	109.2	C10—C11—C12	120.2 (3)
H6A—C6—H6B	107.9	C10—C11—H11	119.9
N2—C7—C8	121.8 (3)	C12—C11—H11	119.9
N2—C7—H7	119.1		
C5—N1—C1—C2	−0.8 (3)	C3—C4—C5—N1	2.4 (4)
C5—N1—C1—Cl1	178.74 (16)	C6—C4—C5—N1	−177.4 (2)
N1—C1—C2—C3	1.7 (4)	N2—C7—C8—C9	−168.9 (2)
Cl1—C1—C2—C3	−177.83 (19)	N2—C7—C8—C13	9.3 (4)
C1—C2—C3—C4	−0.5 (4)	C9—C8—C13—C12	0.3 (4)
C7—N2—O1—C6	−168.0 (2)	C7—C8—C13—C12	−178.0 (2)
C2—C3—C4—C5	−1.4 (4)	C13—C8—C9—C10	−1.0 (4)
C2—C3—C4—C6	178.5 (2)	C7—C8—C9—C10	177.3 (3)
N2—O1—C6—C4	72.9 (3)	C8—C13—C12—C11	0.6 (4)
C5—C4—C6—O1	−122.5 (3)	C8—C9—C10—C11	0.8 (5)
C3—C4—C6—O1	57.7 (3)	C9—C10—C11—C12	0.0 (5)
O1—N2—C7—C8	−177.3 (2)	C13—C12—C11—C10	−0.8 (5)
C1—N1—C5—C4	−1.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N1^{i}	0.93	2.48	3.407 (3)	175
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Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2.

Fig. 1

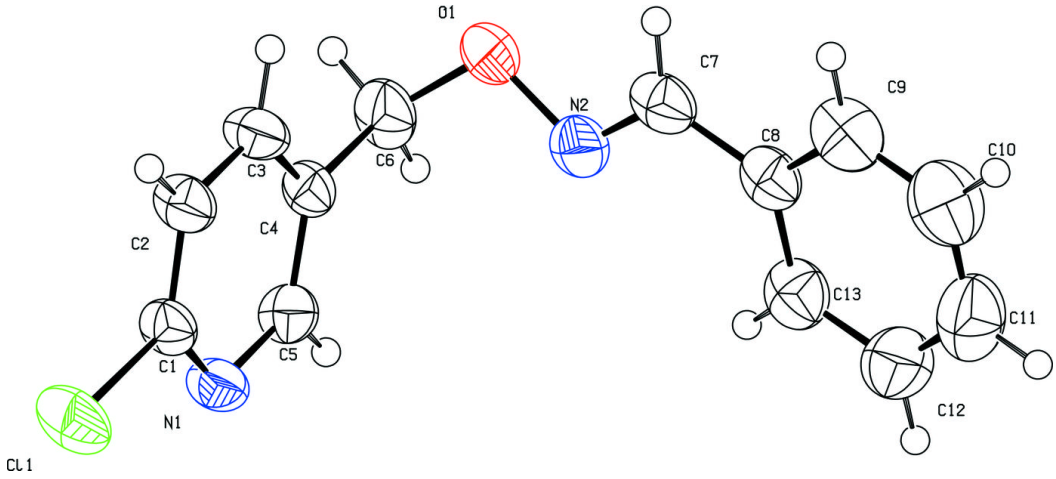

Fig. 2