Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(pyridin-3-yl)oxamide

Shih-Miao Liu,[a] Hsiu-Yi He[b] and Jhy-Der Chen[b]*

[a]Center for General Education, Hsin Sheng Junior College of Medical Care and Management, Longtan, Taiwan, and [b]Department of Chemistry, Chung-Yuan Christian University, Chung-Li, Taiwan
Correspondence e-mail: jdchen@cycu.edu.tw

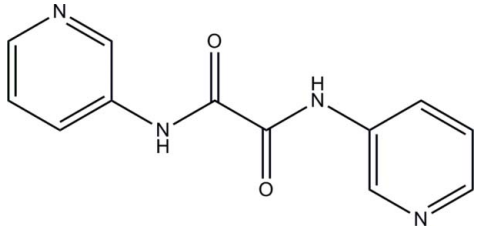
Received 12 March 2013; accepted 17 March 2013

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.126; data-to-parameter ratio = 12.8.

The title molecule, $C_{12}H_{10}N_4O_2$, located about an inversion centre, is roughly planar, with an r.m.s. deviation from the least-squares plane of all non-H atoms of 0.019 Å. In the crystal, N—H···N hydrogen bonds between the amide N—H group and the pyridine N atom connect the molecules into a corrugated layer parallel to $(10\bar{1})$.

Related literature

For *N*,*N*'-di(3-pyridyl)oxamide and its metal complexes, see: Hu *et al.* (2012).



Experimental

Crystal data

$C_{12}H_{10}N_4O_2$
M_r = 242.24
Monoclinic, $P2_1/n$
a = 3.8992 (7) Å
b = 12.662 (2) Å
c = 10.9678 (17) Å
β = 97.983 (4)°
V = 536.26 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 297 K
0.58 × 0.20 × 0.06 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 1.000, T_{max} = 1.000
2997 measured reflections
1050 independent reflections
768 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.126
S = 1.06
1050 reflections
82 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.86	2.26	3.061 (2)	156

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the National Science Council of the Republic of China for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2563).

References

Bruker (1997). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hu, H.-L., Hsu, Y.-F., Wu, C.-J., Yeh, C.-W., Chen, J.-D. & Wang, J.-C. (2012). *Polyhedron*, **33**, 280–288.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2013). E**69**, o560 [doi:10.1107/S1600536813007277]

N,N′-Bis(pyridin-3-yl)oxamide

Shih-Miao Liu, Hsiu-Yi He and Jhy-Der Chen

S1. Comment

Several Zn(II), Cd(II) and Hg(II) complexes containing *N,N′*-di(3-pyridyl)oxamide ligands have been reported, which show one-dimensional chains and metallocycles (Hu *et al.*, 2012). Within this project the crystal structure of the title compound was determined (Fig. 1). In its crystal structure intermolecular N—H···N hydrogen bonds are found (Table 1 & Fig. 2).

S2. Experimental

The title compound was prepared according to a published procedure (Hu *et al.*, 2012). Block crystals suitable for X-ray crystallography were obtained by slow evaporation of the solvent from a solution of the title compound in methanol.

S3. Refinement

H atoms bound to C and N atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C/N).

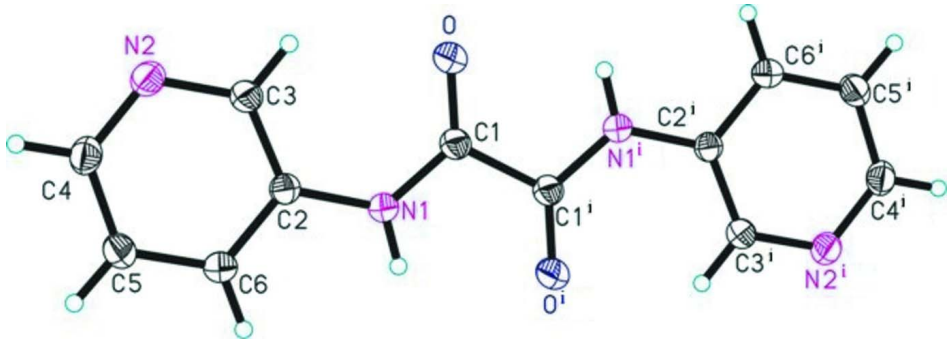


Figure 1

Molecular structure of the title compound with atom labeling and displacement ellipsoids drawn at the 30% probability level.

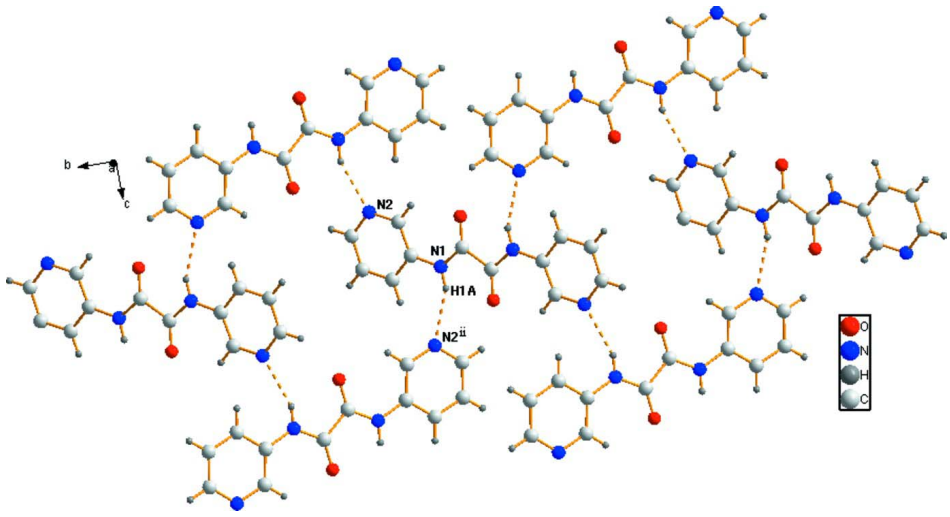


Figure 2

Hydrogen bonding interactions in the title compound.

N,N′-Bis(pyridin-3-yl)oxamide

Crystal data

$C_{12}H_{10}N_4O_2$
$M_r = 242.24$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 3.8992$ (7) Å
$b = 12.662$ (2) Å
$c = 10.9678$ (17) Å
$\beta = 97.983$ (4)°
$V = 536.26$ (16) Å^3
$Z = 2$
$F(000) = 252$
$D_x = 1.500$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1108 reflections
$\theta = 2.5$–25.6°
$\mu = 0.11$ mm^{-1}
$T = 297$ K
Parallelepiped, colorless
0.58 × 0.20 × 0.06 mm

Data collection

Bruker SMART 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 1.000$, $T_{max} = 1.000$
2997 measured reflections
1050 independent reflections
768 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.5°$
$h = -4 \rightarrow 4$
$k = -15 \rightarrow 14$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.126$
$S = 1.06$
1050 reflections
82 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O	0.1096 (4)	0.96926 (10)	1.15577 (12)	0.0530 (5)
N1	0.2264 (4)	0.87848 (10)	0.98550 (13)	0.0342 (4)
H1A	0.2033	0.8827	0.9065	0.041*
N2	0.6079 (4)	0.67892 (12)	1.21174 (13)	0.0421 (5)
C1	0.0929 (5)	0.95887 (12)	1.04473 (16)	0.0344 (4)
C2	0.3993 (4)	0.78835 (13)	1.03865 (15)	0.0309 (4)
C3	0.4530 (5)	0.76739 (14)	1.16394 (16)	0.0382 (5)
H3A	0.3784	0.8168	1.2173	0.046*
C4	0.7184 (5)	0.60928 (14)	1.13512 (17)	0.0416 (5)
H4A	0.8238	0.5476	1.1676	0.050*
C5	0.6832 (5)	0.62458 (14)	1.00998 (17)	0.0404 (5)
H5A	0.7667	0.5747	0.9593	0.048*
C6	0.5223 (5)	0.71506 (13)	0.96066 (16)	0.0367 (5)
H6A	0.4964	0.7269	0.8762	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.0796 (11)	0.0451 (9)	0.0339 (8)	0.0183 (7)	0.0064 (7)	−0.0030 (6)
N1	0.0433 (9)	0.0310 (8)	0.0283 (8)	0.0024 (6)	0.0057 (6)	0.0002 (6)
N2	0.0547 (11)	0.0349 (9)	0.0351 (9)	−0.0016 (7)	0.0012 (7)	0.0017 (7)
C1	0.0387 (10)	0.0312 (9)	0.0337 (9)	−0.0020 (7)	0.0065 (7)	−0.0017 (7)
C2	0.0339 (9)	0.0277 (8)	0.0313 (9)	−0.0046 (7)	0.0048 (7)	−0.0007 (7)
C3	0.0501 (12)	0.0311 (9)	0.0335 (10)	−0.0017 (7)	0.0066 (8)	−0.0028 (8)
C4	0.0479 (11)	0.0324 (9)	0.0428 (11)	0.0021 (8)	0.0001 (8)	0.0030 (8)
C5	0.0446 (11)	0.0354 (10)	0.0411 (10)	0.0039 (8)	0.0061 (8)	−0.0042 (8)
C6	0.0416 (11)	0.0380 (10)	0.0305 (9)	0.0014 (8)	0.0050 (7)	−0.0009 (8)

Geometric parameters (Å, º)

O—C1	1.218 (2)	C2—C6	1.392 (2)
N1—C1	1.350 (2)	C3—H3A	0.9300
N1—C2	1.410 (2)	C4—C5	1.374 (3)
N1—H1A	0.8600	C4—H4A	0.9300
N2—C4	1.330 (2)	C5—C6	1.380 (2)
N2—C3	1.344 (2)	C5—H5A	0.9300

C1—C1^{i}	1.541 (3)	C6—H6A	0.9300
C2—C3	1.387 (2)		
C1—N1—C2	127.27 (14)	N2—C3—H3A	118.5
C1—N1—H1A	116.4	C2—C3—H3A	118.5
C2—N1—H1A	116.4	N2—C4—C5	122.78 (17)
C4—N2—C3	118.26 (15)	N2—C4—H4A	118.6
O—C1—N1	126.31 (16)	C5—C4—H4A	118.6
O—C1—C1^{i}	121.25 (19)	C4—C5—C6	119.04 (17)
N1—C1—C1^{i}	112.44 (17)	C4—C5—H5A	120.5
C3—C2—C6	117.65 (16)	C6—C5—H5A	120.5
C3—C2—N1	124.21 (15)	C5—C6—C2	119.30 (16)
C6—C2—N1	118.14 (14)	C5—C6—H6A	120.3
N2—C3—C2	122.94 (16)	C2—C6—H6A	120.3

Symmetry code: (i) $-x, -y+2, -z+2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{ii}	0.86	2.26	3.061 (2)	156

Symmetry code: (ii) $x-1/2, -y+3/2, z-1/2$.