N,N'-Bis(pyridin-2-yl)benzene-1,4-dicarboxamide

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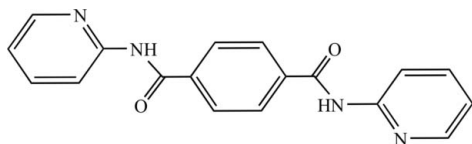Correspondence e-mail: jdchen@cycu.edu.tw

Molecules of the title compound, $C_{18}H_{14}N_4O_2$, are located around an inversion center and connected into chains in the crystal via intermolecular N—H$\cdots$N hydrogen bonds generating an $R_2^2(8)$ motif.

Related literature

For N,N'-bis(pyridinyl) derivatives of 1,4-benzenedicarboxamide and their metal complexes, see: Tsai et al. (2010).

Experimental

Crystal data

$C_{18}H_{14}N_4O_2$	γ = 73.695 (6)°
M_r = 318.33	V = 369.72 (4) Å^3
Triclinic, $P\bar{1}$	Z = 1
a = 5.7895 (4) Å	Mo $K\alpha$ radiation
b = 7.8315 (6) Å	μ = 0.10 mm^{-1}
c = 8.4460 (5) Å	T = 298 K
α = 82.906 (6)°	0.60 × 0.60 × 0.56 mm
β = 74.083 (5)°	

Data collection

Siemens P4 diffractometer	1521 reflections with $I > 2\sigma(I)$
Absorption correction: ψ scan (XSCANS; Siemens, 1995)	R_{int} = 0.013
T_{min} = 0.831, T_{max} = 0.851	3 standard reflections every 97 reflections
1962 measured reflections	intensity decay: none
1787 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	110 parameters
$wR(F^2)$ = 0.112	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
1787 reflections	$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1A$\cdots$N2^i	0.86	2.34	3.1679 (15)	163

Symmetry code: (i) $-x + 1, -y, -z + 1$.

Data collection: XSCANS (Siemens, 1995); cell refinement: XSCANS; data reduction: XSCANS 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.

References

Sheldrick, G. M. (2008). Acta Cryst. A**64**, 112–122.
Siemens (1995). XSCANS. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tsai, T.-P., Huang, Y.-T., Ray, U., Chang, Y.-J., Cheng, P.-C., Wu, C.-J., Chen, J.-D. & Wang, J. C. (2010). Polyhedron, pp. 3081–3088.

supporting information

N,*N*′-Bis(pyridin-2-yl)benzene-1,4-dicarboxamide

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S1. Comment

Several Cu(II), Cd(II) and Hg(II) complexes containg *N*,*N*′-bis(2/3-aryl)-1,4-benzenedicarboxamide ligands have been reported, which show one-dimensional and two-dimensional structures (Tsai, *et al.*, 2010). Within this project the crystal structure of the title compound was determined.

  In its crystal structure intermolecular N—H···N hydrogen bonds are found (Tab. 1) and the molecule is located on a center of inversion (Fig. 1).

S2. Experimental

The title compound was prepared according to a published procedure (Tsai, *et al.*, 2010). Block crystals suitable for X-ray crystallography were obtained by slow evaporization of the solvent from a solution of the title compound in methanol.

S3. Refinement

All the hydrogen atoms were placed into idealized positions and refined in the riding atom approximation with C—H = 0.93 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2 U_{eq}(C, N).
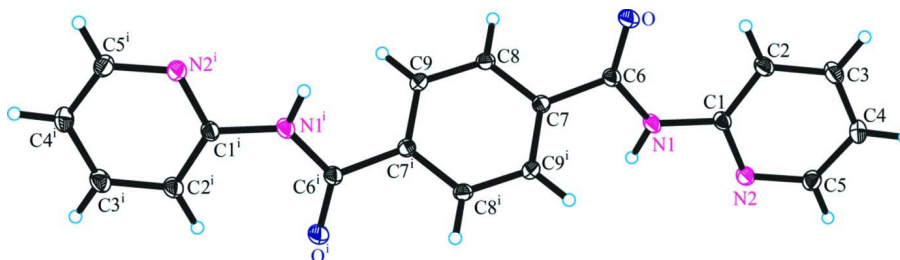
Figure 1

Crystal structure of the title compound with atom labeling and displacement ellipsoids drawn at the 30% probability level. Symmetry code: (i) =-*x* + 2,-*y*,-*z*.

N,*N*′-Bis(pyridin-2-yl)benzene-1,4-dicarboxamide

Crystal data

$C_{18}H_{14}N_4O_2$	$\alpha = 82.906\ (6)°$
$M_r = 318.33$	$\beta = 74.083\ (5)°$
Triclinic, $P\overline{1}$	$\gamma = 73.695\ (6)°$
Hall symbol: -P 1	$V = 369.72\ (4)$ Å^3
$a = 5.7895\ (4)$ Å	$Z = 1$
$b = 7.8315\ (6)$ Å	$F(000) = 166$
$c = 8.8460\ (5)$ Å	$D_x = 1.430$ Mg m^{-3}

Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 50 reflections
θ = 4.8–15.0°
μ = 0.10 mm⁻¹

T = 298 K
Block, pale yellow
0.60 × 0.60 × 0.56 mm

Data collection

Bruker P4
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: *ψ* scan
  (*XSCANS*; Siemens, 1995)
T_{min} = 0.831, T_{max} = 0.851
1962 measured reflections

1787 independent reflections
1521 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 28.0°, θ_{min} = 2.4°
h = 0→7
k = −9→10
l = −11→11
3 standard reflections every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.06
1787 reflections
110 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
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.1049P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å⁻³
$\Delta\rho_{min}$ = −0.19 e Å⁻³
Extinction correction: *SHELXL97* (Sheldrick,
  2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.193 (17)

Special details

Experimental. 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.

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	1.1101 (2)	0.21659 (16)	0.30550 (13)	0.0497 (3)
N1	0.7461 (2)	0.13586 (16)	0.41052 (13)	0.0369 (3)
H1A	0.6695	0.0611	0.3982	0.044*
N2	0.4263 (2)	0.20173 (15)	0.63054 (13)	0.0353 (3)
C1	0.6435 (2)	0.23152 (17)	0.54787 (14)	0.0316 (3)
C2	0.7512 (3)	0.35023 (19)	0.59089 (16)	0.0393 (3)

H2B	0.9066	0.3632	0.5336	0.047*
C3	0.6200 (3)	0.4479 (2)	0.72110 (18)	0.0434 (4)
H3A	0.6853	0.5296	0.7523	0.052*
C4	0.3907 (3)	0.42384 (19)	0.80528 (17)	0.0422 (3)
H4A	0.2982	0.4900	0.8924	0.051*
C5	0.3035 (3)	0.29915 (19)	0.75631 (16)	0.0381 (3)
H5A	0.1507	0.2816	0.8138	0.046*
C6	0.9524 (2)	0.14708 (17)	0.29436 (15)	0.0322 (3)
C7	0.9716 (2)	0.06764 (16)	0.14401 (14)	0.0290 (3)
C8	1.2030 (2)	−0.03051 (17)	0.06322 (14)	0.0314 (3)
H8A	1.3391	−0.0509	0.1057	0.038*
C9	1.2324 (2)	−0.09833 (17)	−0.08032 (15)	0.0321 (3)
H9A	1.3876	−0.1641	−0.1340	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.0418 (6)	0.0697 (7)	0.0464 (6)	−0.0318 (5)	−0.0005 (5)	−0.0194 (5)
N1	0.0417 (6)	0.0460 (6)	0.0291 (5)	−0.0261 (5)	−0.0008 (5)	−0.0092 (5)
N2	0.0366 (6)	0.0411 (6)	0.0302 (5)	−0.0166 (5)	−0.0041 (4)	−0.0045 (4)
C1	0.0368 (6)	0.0353 (6)	0.0256 (6)	−0.0148 (5)	−0.0065 (5)	−0.0023 (5)
C2	0.0426 (7)	0.0445 (8)	0.0364 (7)	−0.0224 (6)	−0.0055 (6)	−0.0067 (6)
C3	0.0532 (9)	0.0383 (7)	0.0443 (8)	−0.0182 (6)	−0.0115 (7)	−0.0100 (6)
C4	0.0491 (8)	0.0360 (7)	0.0382 (7)	−0.0074 (6)	−0.0055 (6)	−0.0110 (5)
C5	0.0360 (7)	0.0401 (7)	0.0353 (7)	−0.0101 (6)	−0.0029 (5)	−0.0041 (5)
C6	0.0332 (6)	0.0359 (6)	0.0298 (6)	−0.0144 (5)	−0.0052 (5)	−0.0039 (5)
C7	0.0300 (6)	0.0323 (6)	0.0259 (6)	−0.0139 (5)	−0.0030 (4)	−0.0015 (4)
C8	0.0267 (6)	0.0384 (7)	0.0308 (6)	−0.0119 (5)	−0.0068 (5)	−0.0011 (5)
C9	0.0263 (6)	0.0359 (6)	0.0320 (6)	−0.0084 (5)	−0.0020 (5)	−0.0057 (5)

Geometric parameters (Å, º)

O—C6	1.2169 (16)	C4—C5	1.377 (2)
N1—C6	1.3614 (16)	C4—H4A	0.9300
N1—C1	1.4034 (16)	C5—H5A	0.9300
N1—H1A	0.8600	C6—C7	1.5009 (17)
N2—C1	1.3375 (17)	C7—C8	1.3888 (17)
N2—C5	1.3403 (17)	C7—C9^i	1.3936 (17)
C1—C2	1.3932 (18)	C8—C9	1.3860 (17)
C2—C3	1.378 (2)	C8—H8A	0.9300
C2—H2B	0.9300	C9—C7^i	1.3936 (17)
C3—C4	1.384 (2)	C9—H9A	0.9300
C3—H3A	0.9300		
C6—N1—C1	127.85 (11)	N2—C5—C4	123.77 (13)
C6—N1—H1A	116.1	N2—C5—H5A	118.1
C1—N1—H1A	116.1	C4—C5—H5A	118.1
C1—N2—C5	117.11 (11)	O—C6—N1	124.94 (12)

N2—C1—C2	123.38 (12)	O—C6—C7	120.89 (11)
N2—C1—N1	112.88 (11)	N1—C6—C7	114.16 (11)
C2—C1—N1	123.70 (12)	C8—C7—C9^i	119.81 (11)
C3—C2—C1	117.84 (13)	C8—C7—C6	118.37 (11)
C3—C2—H2B	121.1	C9^i—C7—C6	121.72 (11)
C1—C2—H2B	121.1	C9—C8—C7	120.42 (12)
C2—C3—C4	119.75 (13)	C9—C8—H8A	119.8
C2—C3—H3A	120.1	C7—C8—H8A	119.8
C4—C3—H3A	120.1	C8—C9—C7^i	119.77 (11)
C5—C4—C3	118.06 (13)	C8—C9—H9A	120.1
C5—C4—H4A	121.0	C7^i—C9—H9A	120.1
C3—C4—H4A	121.0		

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

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*A*⋯N2^{ii}	0.86	2.34	3.1679 (15)	163

Symmetry code: (ii) −*x*+1, −*y*, −*z*+1.