Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Methyl-*N*′-[1-(2-pyridyl)ethylidene]-benzohydrazide

Chun-Bao Tang

Department of Chemistry, Jiaying University, Meizhou 514015, People's Republic of China
Correspondence e-mail: tangchunbao@yahoo.com.cn

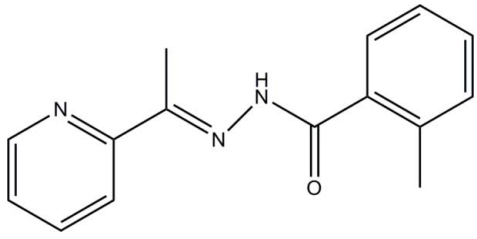
Received 20 December 2010; accepted 25 December 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.158; data-to-parameter ratio = 16.8.

In the title compound, $C_{15}H_{15}N_3O$, the dihedral angle between the pyridine and benzene rings is 36.3 (2)°. In the crystal, molecules are linked through intermolecular N—H···O hydrogen bonds, forming chains along the *b* axis.

Related literature

For general background to hydrazones, see: Rasras *et al.* (2010); Pyta *et al.* (2010); Angelusiu *et al.* (2010). For related structures, see: Fun *et al.* (2008); Singh & Singh (2010); Ahmad *et al.* (2010); Tang (2010). For reference bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{15}N_3O$
M_r = 253.30
Orthorhombic, *Pbcn*
a = 19.296 (3) Å
b = 8.1417 (18) Å
c = 17.294 (3) Å
V = 2716.8 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.986
13661 measured reflections
2966 independent reflections
1539 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.158
S = 1.02
2966 reflections
177 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 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
N1—H1···O1^{i}	0.91 (1)	2.05 (1)	2.937 (2)	165 (3)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Financial support from the Jiaying University research fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5083).

References

Ahmad, T., Zia-ur-Rehman, M., Siddiqui, H. L., Mahmud, S. & Parvez, M. (2010). *Acta Cryst.* E**66**, o976.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Angelusiu, M. V., Barbuceanu, S. F., Draghici, C. & Almajan, G. L. (2010). *Eur. J. Med. Chem.* **45**, 2055–2062.
Bruker (2002). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fun, H.-K., Sujith, K. V., Patil, P. S., Kalluraya, B. & Chantrapromma, S. (2008). *Acta Cryst.* E**64**, o1961–o1962.
Pyta, K., Przybylski, P., Huczynski, A., Hoser, A., Wozniak, K., Schilf, W., Kamienski, B., Grech, E. & Brzezinski, B. (2010). *J. Mol. Struct.* **970**, 147–154.
Rasras, A. J. M., Al-Tel, T. H., Al-Aboudi, A. F. & Al-Qawasmeh, R. A. (2010). *Eur. J. Med. Chem.* **45**, 2307–2313.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, V. P. & Singh, S. (2010). *Acta Cryst.* E**66**, o1172.
Tang, C.-B. (2010). *Acta Cryst.* E**66**, o2482.

supplementary materials

Acta Cryst. (2011). E**67**, o271 [**doi:10.1107/S1600536810054267**]

2-Methyl-*N*'-[1-(2-pyridyl)ethylidene]benzohydrazide

C.-B. Tang

Comment

Hydrazone compounds have received much attention in biological and structural chemistry in the last few years (Rasras *et al.*, 2010; Pyta *et al.*, 2010; Angelusiu *et al.*, 2010; Fun *et al.*, 2008; Singh & Singh, 2010; Ahmad *et al.*, 2010). In the present paper, the author reports the crystal structure of the new title hydrazone compound (Fig. 1).

In the title compound, the dihedral angle between the pyridine and the benzene rings is 36.3 (2)°. The torsion angles C1—C8—N1—N2, C8—N1—N2—C9, and N1—N2—C9—C10 are 7.8 (2), 3.6 (2), and 1.5 (2)°, respectively. Bond lengths in the molecules are normal (Allen *et al.*, 1987) and comparable to those in the similar compound the author reported recently (Tang, 2010).

In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains along the *b* axis (Fig. 2).

Experimental

2-Acetylpyridine (0.1 mmol, 12.1 mg) and 2-methylbenzohydrazide (0.1 mmol, 15.0 mg) were dissolved in methanol (20 ml). The mixture was stirred at reflux for 10 min to give a clear colourless solution. Colourless block-shaped crystals of the compound were formed by slow evaporation of the solvent over several days.

Refinement

The amino H atom was located in a difference Fourier map and refined isotropically, with the N—H distances restrained to 0.90 (1) Å [U_{iso}(H) = 0.08 Å^2]. Other H atoms were constrained to ideal geometries and refined as riding, with Csp^2—H = 0.93 Å, and C(methyl)—H = 0.96 Å; U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C$_{methyl}$).

Figures

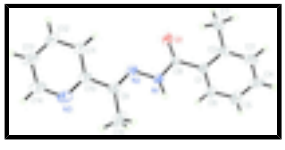


Fig. 1. The molecular structure of the compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

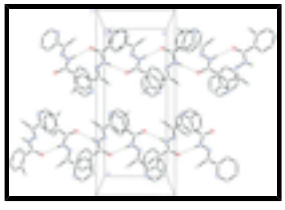


Fig. 2. Molecular packing of the title compound, with hydrogen bonds shown as dashed lines.

2-Methyl-*N*'-[1-(2-pyridyl)ethylidene]benzohydrazide

Crystal data

$C_{15}H_{15}N_3O$	$D_x = 1.239$ Mg m^{-3}
$M_r = 253.30$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbcn*	Cell parameters from 1243 reflections
$a = 19.296$ (3) Å	$\theta = 2.5$–$24.6°$
$b = 8.1417$ (18) Å	$\mu = 0.08$ mm^{-1}
$c = 17.294$ (3) Å	$T = 298$ K
$V = 2716.8$ (9) Å^3	Block, colourless
$Z = 8$	0.20 × 0.20 × 0.18 mm
$F(000) = 1072$	

Data collection

Bruker SMART CCD area-detector diffractometer	2966 independent reflections
Radiation source: fine-focus sealed tube	1539 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.069$
ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -24\rightarrow24$
$T_{min} = 0.984$, $T_{max} = 0.986$	$k = -10\rightarrow10$
13661 measured reflections	$l = -13\rightarrow22$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.056$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.158$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.5475P]$ where $P = (F_o^2 + 2F_c^2)/3$
2966 reflections	$(\Delta/\sigma)_{max} < 0.001$
177 parameters	$\Delta\rho_{max} = 0.17$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.17$ e Å^{-3}

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.

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}
N1	0.26051 (10)	0.9439 (2)	0.05651 (11)	0.0451 (5)
N2	0.28738 (9)	1.0589 (2)	0.00578 (11)	0.0450 (5)
N3	0.43437 (11)	1.1437 (2)	−0.10682 (12)	0.0623 (6)
O1	0.17755 (8)	1.12421 (19)	0.09416 (11)	0.0613 (5)
C1	0.16962 (11)	0.8519 (3)	0.14164 (13)	0.0423 (5)
C2	0.10054 (12)	0.8104 (3)	0.12641 (14)	0.0513 (6)
C3	0.07187 (15)	0.6857 (4)	0.17027 (18)	0.0751 (9)
H3	0.0266	0.6531	0.1602	0.090*
C4	0.10778 (18)	0.6085 (4)	0.22804 (19)	0.0832 (10)
H4	0.0866	0.5263	0.2569	0.100*
C5	0.17470 (16)	0.6520 (3)	0.24329 (16)	0.0689 (8)
H5	0.1990	0.6005	0.2829	0.083*
C6	0.20621 (13)	0.7725 (3)	0.19965 (14)	0.0536 (6)
H6	0.2521	0.8007	0.2092	0.064*
C7	0.05886 (13)	0.8927 (4)	0.06421 (16)	0.0682 (8)
H7A	0.0192	0.8263	0.0520	0.102*
H7B	0.0870	0.9060	0.0188	0.102*
H7C	0.0437	0.9984	0.0820	0.102*
C8	0.20235 (11)	0.9857 (3)	0.09561 (13)	0.0423 (5)
C9	0.34432 (13)	1.0263 (3)	−0.02897 (14)	0.0508 (6)
C10	0.36834 (13)	1.1545 (3)	−0.08374 (13)	0.0499 (6)
C11	0.32524 (14)	1.2794 (3)	−0.10794 (15)	0.0644 (7)
H11	0.2792	1.2825	−0.0921	0.077*
C12	0.35119 (18)	1.3991 (4)	−0.15583 (18)	0.0836 (10)
H12	0.3231	1.4851	−0.1723	0.100*
C13	0.41887 (19)	1.3901 (4)	−0.17897 (18)	0.0831 (10)
H13	0.4377	1.4695	−0.2114	0.100*
C14	0.45800 (16)	1.2616 (4)	−0.15322 (16)	0.0735 (9)
H14	0.5040	1.2561	−0.1690	0.088*
C15	0.38792 (17)	0.8767 (4)	−0.0182 (2)	0.1043 (13)
H15A	0.4022	0.8692	0.0349	0.156*
H15B	0.4281	0.8838	−0.0508	0.156*
H15C	0.3615	0.7810	−0.0317	0.156*
H1	0.2784 (13)	0.8410 (17)	0.0589 (16)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0503 (11)	0.0302 (10)	0.0547 (12)	0.0008 (9)	0.0072 (10)	0.0072 (10)

N2	0.0514 (11)	0.0343 (10)	0.0492 (12)	−0.0062 (9)	0.0018 (10)	0.0042 (9)
N3	0.0678 (14)	0.0579 (14)	0.0611 (14)	−0.0096 (11)	0.0209 (11)	−0.0052 (11)
O1	0.0568 (10)	0.0342 (9)	0.0930 (14)	0.0044 (8)	0.0086 (9)	0.0081 (9)
C1	0.0511 (14)	0.0319 (12)	0.0438 (13)	−0.0001 (10)	0.0069 (11)	−0.0016 (10)
C2	0.0489 (14)	0.0517 (15)	0.0533 (15)	−0.0068 (11)	0.0079 (12)	−0.0033 (12)
C3	0.0606 (17)	0.083 (2)	0.081 (2)	−0.0229 (16)	0.0119 (16)	0.0115 (18)
C4	0.090 (2)	0.078 (2)	0.082 (2)	−0.0174 (18)	0.0242 (19)	0.0276 (18)
C5	0.088 (2)	0.0617 (18)	0.0567 (17)	0.0042 (16)	0.0064 (15)	0.0158 (14)
C6	0.0614 (15)	0.0422 (14)	0.0573 (16)	0.0013 (12)	0.0007 (13)	0.0023 (12)
C7	0.0512 (15)	0.082 (2)	0.0719 (18)	−0.0008 (14)	−0.0049 (14)	0.0016 (16)
C8	0.0439 (13)	0.0300 (12)	0.0531 (14)	−0.0024 (10)	−0.0038 (11)	0.0020 (11)
C9	0.0557 (14)	0.0390 (14)	0.0576 (15)	0.0000 (11)	0.0078 (12)	0.0013 (12)
C10	0.0613 (16)	0.0434 (14)	0.0450 (14)	−0.0095 (12)	0.0070 (12)	−0.0049 (11)
C11	0.0624 (16)	0.0629 (17)	0.0678 (18)	−0.0059 (14)	−0.0004 (14)	0.0220 (15)
C12	0.092 (2)	0.081 (2)	0.078 (2)	−0.0112 (18)	−0.0011 (18)	0.0332 (18)
C13	0.105 (3)	0.081 (2)	0.0635 (19)	−0.032 (2)	0.0128 (18)	0.0146 (17)
C14	0.084 (2)	0.075 (2)	0.0621 (19)	−0.0227 (18)	0.0271 (16)	−0.0054 (17)
C15	0.090 (2)	0.076 (2)	0.147 (3)	0.0296 (18)	0.052 (2)	0.046 (2)

Geometric parameters (Å, °)

N1—C8	1.354 (3)	C6—H6	0.9300
N1—N2	1.384 (2)	C7—H7A	0.9600
N1—H1	0.907 (10)	C7—H7B	0.9600
N2—C9	1.280 (3)	C7—H7C	0.9600
N3—C14	1.332 (3)	C9—C10	1.484 (3)
N3—C10	1.338 (3)	C9—C15	1.492 (3)
O1—C8	1.225 (2)	C10—C11	1.379 (3)
C1—C6	1.386 (3)	C11—C12	1.374 (4)
C1—C2	1.400 (3)	C11—H11	0.9300
C1—C8	1.490 (3)	C12—C13	1.368 (4)
C2—C3	1.383 (3)	C12—H12	0.9300
C2—C7	1.501 (3)	C13—C14	1.365 (4)
C3—C4	1.369 (4)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.365 (4)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.379 (3)	C15—H15C	0.9600
C5—H5	0.9300		
C8—N1—N2	117.17 (17)	H7B—C7—H7C	109.5
C8—N1—H1	121.7 (17)	O1—C8—N1	123.0 (2)
N2—N1—H1	120.7 (18)	O1—C8—C1	121.2 (2)
C9—N2—N1	118.60 (19)	N1—C8—C1	115.71 (19)
C14—N3—C10	117.3 (2)	N2—C9—C10	114.9 (2)
C6—C1—C2	120.6 (2)	N2—C9—C15	126.5 (2)
C6—C1—C8	120.8 (2)	C10—C9—C15	118.5 (2)
C2—C1—C8	118.7 (2)	N3—C10—C11	122.2 (2)
C3—C2—C1	117.1 (2)	N3—C10—C9	116.2 (2)
C3—C2—C7	120.4 (2)	C11—C10—C9	121.6 (2)

C1—C2—C7	122.5 (2)	C12—C11—C10	119.1 (3)
C4—C3—C2	122.3 (3)	C12—C11—H11	120.4
C4—C3—H3	118.8	C10—C11—H11	120.4
C2—C3—H3	118.8	C13—C12—C11	119.1 (3)
C5—C4—C3	120.1 (3)	C13—C12—H12	120.4
C5—C4—H4	120.0	C11—C12—H12	120.4
C3—C4—H4	120.0	C14—C13—C12	118.3 (3)
C4—C5—C6	119.7 (3)	C14—C13—H13	120.9
C4—C5—H5	120.1	C12—C13—H13	120.9
C6—C5—H5	120.1	N3—C14—C13	124.0 (3)
C5—C6—C1	120.2 (2)	N3—C14—H14	118.0
C5—C6—H6	119.9	C13—C14—H14	118.0
C1—C6—H6	119.9	C9—C15—H15A	109.5
C2—C7—H7A	109.5	C9—C15—H15B	109.5
C2—C7—H7B	109.5	H15A—C15—H15B	109.5
H7A—C7—H7B	109.5	C9—C15—H15C	109.5
C2—C7—H7C	109.5	H15A—C15—H15C	109.5
H7A—C7—H7C	109.5	H15B—C15—H15C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.91 (1)	2.05 (1)	2.937 (2)	165 (3)

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

Fig. 1

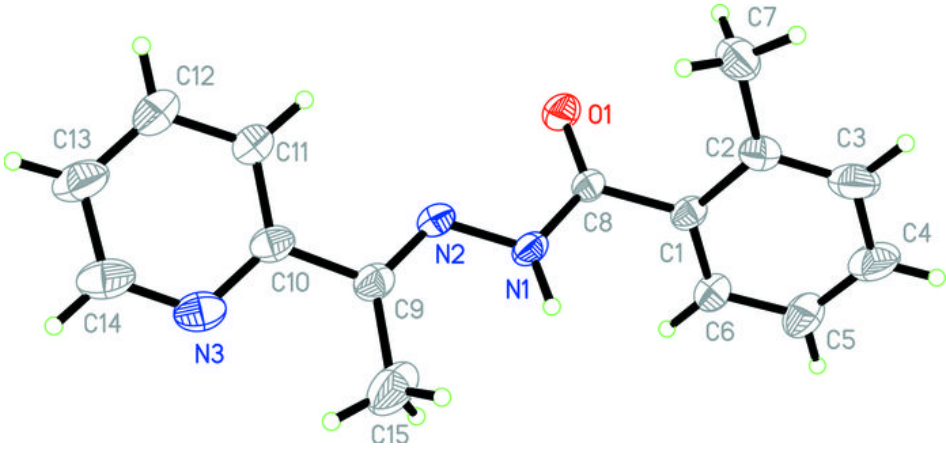


Fig. 2