Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-2-[2-(4-Methylbenzylidene)-hydrazinyl]pyridine

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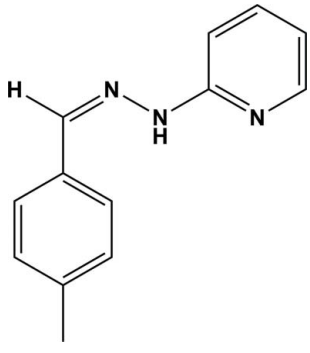
Received 9 December 2010; accepted 14 December 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.154; data-to-parameter ratio = 19.4.

Molecules of the title compound, $C_{13}H_{13}N_3$, are essentially planar (r.m.s. deviation for all non-H atoms = 0.054 Å). The dihedral angle between the two aromatic rings is 6.33 (5)°. In the crystal, pairs of centrosymmetrically related molecules are linked through N—H···N hydrogen bonds, forming N—H···N dimers with graph-set motif $R_2^2(8)$.

Related literature

For the biological activity of hydrazone derivatives, see: Savini *et al.* (2002); Silva *et al.* (2004). For a related structure, see: Yuvaraj *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_{13}N_3$ M_r = 211.26
Monoclinic, $P2_1/c$
a = 5.2385 (8) Å
b = 10.7215 (17) Å
c = 20.590 (3) Å
β = 92.699 (5)°
V = 1155.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.26 × 0.23 × 0.21 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.981, T_{max} = 0.984
10622 measured reflections
2850 independent reflections
1341 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.154
S = 1.00
2850 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N3^{i}	0.86	2.28	3.131 (2)	170

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

HY gratefully acknowledges Yeungnam University for the opportunity to work as a Full-Time Foreign Instructor. SS and DV thank the TBI X-ray Facility, CAS in Crystallography and Biophysics, University of Madras, India, for the data collection and the University Grants Commission (UGC & SAP) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5435).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Savini, L., Chiasserini, L., Gaeta, A. & Pellerano, C. (2002). *Bioorg. Med. Chem.* **10**, 2193–2198.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Silva, G. A., Costa, L. M. M., Brito, F. C. F., Miranda, A. L. P., Barreiro, E. J. & Fraga, C. A. M. (2004). *Bioorg. Med. Chem.* **12**, 3149–3158.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yuvaraj, H., Sundaramoorthy, S., Velmurugan, D. & Kalkhambkar, R. G. (2010). *Acta Cryst.* E**66**, o2733.

supplementary materials

Acta Cryst. (2011). E**67**, o178 [**doi:10.1107/S1600536810052372**]

(*Z*)-2-[2-(4-Methylbenzylidene)hydrazinyl]pyridine

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Comment

The title compound was prepared as part of our continuing interest on the nitrogen based heterocycles (Yuvaraj *et al.*, 2010).

In the title molecule, the C2—C3—C7 and C8—N1—N2 bond angles are 121.65 (2)° and 117.46 (2)°, respectively. The benzene and pyridine form a dihedral angle of 6.33 (5)°.

In the crystal structure,the molecules at (*x*, *y*, *z*) and (1 - *x*,-*y*,-*z*) are linked by N(2)—H(2 A)···N(3) hydrogen bonds, generating a centrosymmetric dimeric ring motif $R_2^2(8)$ (Bernstein *et al.*, 1995). The centroid of the $R_2^2(8)$ motif lies at (1/2,0,0). In addition, there is a weak C—H···N interaction linking the centrosymmetric pair of molecules.

Experimental

A mixture of 2-hydrazinopyridine and *p*-tolualdehyde were refluxed in ethanol with a catalytic quantity of con. HCl or gl. AcOH. After the reaction was over, the contents were cooled down and filtered to form the product. Diffraction quality crystals were obtained upon recrystallization in ethanol.

Refinement

H atoms were positioned geometrically (N—H = 0.86 Å, C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with 1.5U_{eq}(C) for methyl H or 1.2 U_{eq}(C,N) for other H atoms.

Figures

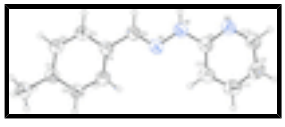

Fig. 1. Perspective view of the molecule showing the displacement ellipsoids drawn at 30% probability level.

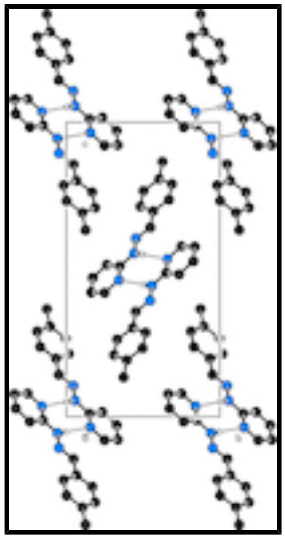

Fig. 2. The crystal packing of the molecules viewed down *a* axis. For clarity, hydrogen atoms which are not involved in hydrogen bonding are omitted

(*Z*)-2-[2-(4-Methylbenzylidene)hydrazinyl]pyridine

Crystal data

$C_{13}H_{13}N_3$	$F(000) = 448$
$M_r = 211.26$	$D_x = 1.215$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 715 reflections
$a = 5.2385$ (8) Å	$\theta = 2.0$–$28.4°$
$b = 10.7215$ (17) Å	$\mu = 0.08$ mm^{-1}
$c = 20.590$ (3) Å	$T = 293$ K
$\beta = 92.699$ (5)°	Block, colourless
$V = 1155.2$ (3) Å^3	0.26 × 0.23 × 0.21 mm
$Z = 4$	

Data collection

Bruker SMART APEXII area-detector diffractometer	2850 independent reflections
Radiation source: fine-focus sealed tube	1341 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.027$
ω and φ scans	$\theta_{max} = 28.4°$, $\theta_{min} = 2.0°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)	$h = -6 \rightarrow 6$
$T_{min} = 0.981$, $T_{max} = 0.984$	$k = -12 \rightarrow 14$
10622 measured reflections	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.154$	$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.0987P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2850 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
147 parameters	$\Delta\rho_{min} = -0.11$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.011 (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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.2431 (4)	0.01692 (17)	0.21369 (9)	0.0756 (5)
H1	−0.2750	0.0866	0.1877	0.091*
C2	−0.3858 (4)	−0.00253 (17)	0.26709 (9)	0.0797 (5)
H2	−0.5119	0.0548	0.2766	0.096*
C3	−0.3465 (3)	−0.10558 (17)	0.30708 (8)	0.0712 (5)
C4	−0.1622 (4)	−0.18826 (18)	0.29040 (9)	0.0852 (6)
H4	−0.1341	−0.2594	0.3156	0.102*
C5	−0.0171 (4)	−0.16896 (18)	0.23728 (9)	0.0874 (6)
H5	0.1077	−0.2269	0.2276	0.105*
C6	−0.0525 (3)	−0.06569 (15)	0.19808 (8)	0.0674 (5)
C7	−0.5002 (4)	−0.1260 (2)	0.36606 (9)	0.0936 (6)
H7A	−0.4823	−0.2110	0.3801	0.140*
H7B	−0.6770	−0.1086	0.3553	0.140*
H7C	−0.4395	−0.0714	0.4003	0.140*
C8	0.1072 (3)	−0.04777 (17)	0.14289 (8)	0.0731 (5)
H8	0.2328	−0.1063	0.1347	0.088*
C9	0.1978 (3)	0.15130 (15)	0.01140 (8)	0.0662 (5)
C10	−0.0022 (4)	0.23520 (18)	0.01634 (9)	0.0813 (5)
H10	−0.1154	0.2281	0.0496	0.098*
C11	−0.0290 (4)	0.32800 (19)	−0.02841 (10)	0.0907 (6)
H11	−0.1607	0.3857	−0.0258	0.109*
C12	0.1387 (4)	0.33637 (19)	−0.07751 (11)	0.0951 (6)

H12	0.1231	0.3990	−0.1087	0.114*
C13	0.3290 (4)	0.2497 (2)	−0.07891 (10)	0.0895 (6)
H13	0.4430	0.2554	−0.1121	0.107*
N1	0.0784 (3)	0.04629 (14)	0.10557 (6)	0.0720 (4)
N2	0.2388 (3)	0.05650 (13)	0.05528 (6)	0.0749 (4)
H2A	0.3623	0.0046	0.0513	0.090*
N3	0.3633 (3)	0.15655 (13)	−0.03568 (7)	0.0742 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0777 (12)	0.0642 (10)	0.0860 (12)	0.0007 (9)	0.0162 (9)	0.0076 (9)
C2	0.0744 (12)	0.0739 (12)	0.0927 (12)	0.0054 (10)	0.0244 (10)	0.0042 (10)
C3	0.0665 (11)	0.0751 (11)	0.0727 (10)	−0.0031 (9)	0.0112 (8)	0.0009 (9)
C4	0.0932 (14)	0.0836 (13)	0.0798 (12)	0.0151 (11)	0.0158 (10)	0.0178 (10)
C5	0.0928 (14)	0.0874 (13)	0.0837 (12)	0.0246 (11)	0.0219 (11)	0.0115 (10)
C6	0.0682 (11)	0.0661 (10)	0.0687 (10)	−0.0004 (9)	0.0094 (8)	−0.0022 (8)
C7	0.0926 (14)	0.1023 (15)	0.0878 (13)	0.0005 (12)	0.0244 (11)	0.0100 (11)
C8	0.0754 (12)	0.0720 (11)	0.0729 (10)	0.0023 (9)	0.0137 (9)	−0.0022 (9)
C9	0.0638 (11)	0.0657 (11)	0.0693 (10)	−0.0110 (9)	0.0067 (8)	−0.0058 (8)
C10	0.0767 (12)	0.0795 (12)	0.0884 (12)	0.0016 (11)	0.0117 (10)	−0.0051 (11)
C11	0.0797 (14)	0.0773 (13)	0.1152 (16)	0.0026 (10)	0.0057 (12)	0.0009 (12)
C12	0.0857 (15)	0.0804 (13)	0.1190 (16)	−0.0064 (12)	0.0035 (13)	0.0221 (12)
C13	0.0778 (13)	0.0941 (14)	0.0976 (14)	−0.0129 (12)	0.0151 (10)	0.0157 (12)
N1	0.0709 (9)	0.0764 (10)	0.0699 (8)	−0.0061 (7)	0.0162 (7)	−0.0064 (8)
N2	0.0737 (10)	0.0783 (10)	0.0741 (9)	0.0027 (8)	0.0191 (7)	0.0002 (8)
N3	0.0671 (9)	0.0762 (10)	0.0801 (9)	−0.0092 (7)	0.0115 (8)	0.0036 (8)

Geometric parameters (Å, °)

C1—C2	1.374 (2)	C8—N1	1.273 (2)
C1—C6	1.383 (2)	C8—H8	0.9300
C1—H1	0.9300	C9—N3	1.332 (2)
C2—C3	1.387 (2)	C9—N2	1.370 (2)
C2—H2	0.9300	C9—C10	1.388 (2)
C3—C4	1.366 (2)	C10—C11	1.359 (2)
C3—C7	1.504 (2)	C10—H10	0.9300
C4—C5	1.377 (3)	C11—C12	1.373 (3)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.378 (2)	C12—C13	1.364 (3)
C5—H5	0.9300	C12—H12	0.9300
C6—C8	1.455 (2)	C13—N3	1.344 (2)
C7—H7A	0.9600	C13—H13	0.9300
C7—H7B	0.9600	N1—N2	1.3680 (17)
C7—H7C	0.9600	N2—H2A	0.8600
C2—C1—C6	120.95 (17)	N1—C8—C6	121.34 (17)
C2—C1—H1	119.5	N1—C8—H8	119.3
C6—C1—H1	119.5	C6—C8—H8	119.3

C1—C2—C3	121.63 (17)	N3—C9—N2	115.09 (16)
C1—C2—H2	119.2	N3—C9—C10	123.05 (17)
C3—C2—H2	119.2	N2—C9—C10	121.86 (17)
C4—C3—C2	117.02 (16)	C11—C10—C9	118.63 (18)
C4—C3—C7	121.33 (17)	C11—C10—H10	120.7
C2—C3—C7	121.65 (17)	C9—C10—H10	120.7
C3—C4—C5	121.69 (18)	C10—C11—C12	119.8 (2)
C3—C4—H4	119.2	C10—C11—H11	120.1
C5—C4—H4	119.2	C12—C11—H11	120.1
C4—C5—C6	121.46 (18)	C13—C12—C11	117.68 (19)
C4—C5—H5	119.3	C13—C12—H12	121.2
C6—C5—H5	119.3	C11—C12—H12	121.2
C5—C6—C1	117.22 (16)	N3—C13—C12	124.55 (19)
C5—C6—C8	119.79 (16)	N3—C13—H13	117.7
C1—C6—C8	122.99 (16)	C12—C13—H13	117.7
C3—C7—H7A	109.5	C8—N1—N2	117.46 (15)
C3—C7—H7B	109.5	N1—N2—C9	118.41 (15)
H7A—C7—H7B	109.5	N1—N2—H2A	120.8
C3—C7—H7C	109.5	C9—N2—H2A	120.8
H7A—C7—H7C	109.5	C9—N3—C13	116.24 (17)
H7B—C7—H7C	109.5		
C6—C1—C2—C3	−0.5 (3)	N3—C9—C10—C11	−0.8 (3)
C1—C2—C3—C4	−1.1 (3)	N2—C9—C10—C11	179.07 (15)
C1—C2—C3—C7	179.13 (16)	C9—C10—C11—C12	0.6 (3)
C2—C3—C4—C5	1.6 (3)	C10—C11—C12—C13	−0.3 (3)
C7—C3—C4—C5	−178.62 (18)	C11—C12—C13—N3	0.2 (3)
C3—C4—C5—C6	−0.6 (3)	C6—C8—N1—N2	179.29 (13)
C4—C5—C6—C1	−1.0 (3)	C8—N1—N2—C9	174.71 (14)
C4—C5—C6—C8	179.16 (17)	N3—C9—N2—N1	179.08 (13)
C2—C1—C6—C5	1.5 (3)	C10—C9—N2—N1	−0.8 (2)
C2—C1—C6—C8	−178.67 (16)	N2—C9—N3—C13	−179.22 (14)
C5—C6—C8—N1	179.65 (16)	C10—C9—N3—C13	0.7 (2)
C1—C6—C8—N1	−0.2 (3)	C12—C13—N3—C9	−0.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···N3^{i}	0.86	2.28	3.131 (2)	170

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

Fig. 1

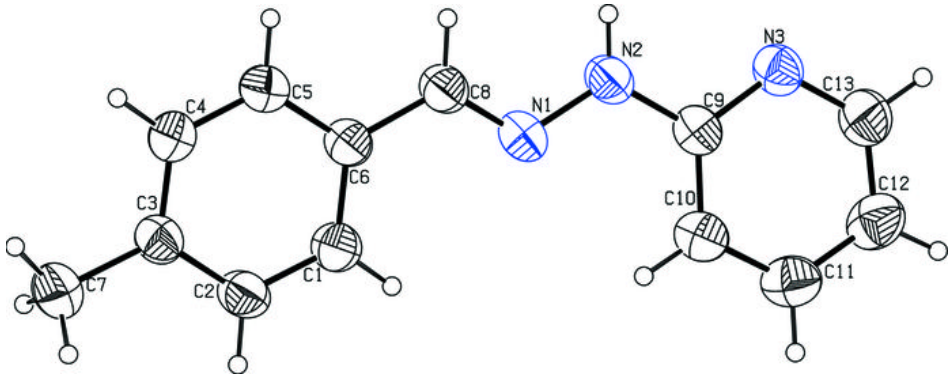

Fig. 2