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## *N'*-(2-Methoxybenzylidene)nicotino- hydrazide

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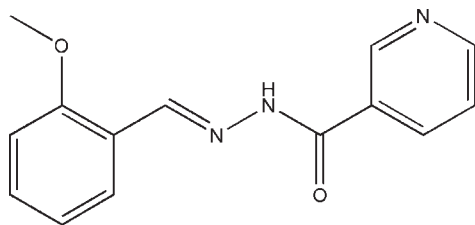
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  
R factor = 0.035;  $wR$  factor = 0.084; data-to-parameter ratio = 8.6.

The title compound,  $\text{C}_{14}\text{H}_{13}\text{N}_3\text{O}_2$ , was prepared by the reaction of 2-methoxybenzaldehyde with nicotinic acid hydrazide in methanol. The dihedral angle between the benzene and pyridine rings is  $5.9$  (3)°. In the crystal structure, molecules are linked by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, leading to the formation of chains along the  $c$  axis; adjacent chains are linked *via*  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds.

### Related literature

For general background to Schiff base compounds, see: Archibald *et al.* (1994); Harada *et al.* (1999); Ogawa *et al.* (1998). For related structures, see: Mohd Lair *et al.* (2009); Sun *et al.* (2009); Wen *et al.* (2009).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{13}\text{N}_3\text{O}_2$   $Z = 4$   
 $M_r = 255.27$  Mo  $K\alpha$  radiation  
 Tetragonal,  $P4_3$   $\mu = 0.09$  mm $^{-1}$   
 $a = 9.3264$  (13) Å  $T = 298$  K  
 $c = 15.594$  (3) Å  $0.20 \times 0.20 \times 0.18$  mm  
 $V = 1356.4$  (4) Å $^3$

#### Data collection

Bruker APEXII CCD area-detector diffractometer 6623 measured reflections  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2004) 1519 independent reflections  
 $T_{\min} = 0.983$ ,  $T_{\max} = 0.985$  1313 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$  H atoms treated by a mixture of independent and constrained refinement  
 $wR(F^2) = 0.084$   $\Delta\rho_{\text{max}} = 0.09$  e Å $^{-3}$   
 $S = 1.06$   $\Delta\rho_{\text{min}} = -0.14$  e Å $^{-3}$   
 1519 reflections  
 176 parameters  
 2 restraints

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N}2-\text{H}2\cdots\text{O}2^{\text{i}}$	0.90 (1)	2.05 (2)	2.897 (2)	157 (3)
$\text{C}4-\text{H}4\cdots\text{O}1^{\text{ii}}$	0.93	2.58	3.469 (3)	160
$\text{C}11-\text{H}11\cdots\text{N}3^{\text{iii}}$	0.93	2.53	3.429 (4)	164
$\text{C}13-\text{H}13\cdots\text{N}1^{\text{i}}$	0.93	2.56	3.487 (3)	176

Symmetry codes: (i)  $-y + 1, x, z - \frac{1}{2}$ ; (ii)  $y + 1, -x + 1, z + \frac{1}{2}$ ; (iii)  $y - 1, -x + 1, z + \frac{1}{2}$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); 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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5028).

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**supplementary materials**

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## *N'*-(2-Methoxybenzylidene)nicotinohydrazide

P. Wang, C. Li and Y.-Q. Su

### Comment

Schiff bases have been received much attention in recent years (Ogawa *et al.*, 1998; Archibald *et al.*, 1994; Harada *et al.*, 1999). As a further investigation of the structures of Schiff base compounds, the title new compound is reported here.

In the title compound, the dihedral angle between the benzene ring and the pyridine ring is 5.9 (3)°. All the bond lengths are comparable with the similar Schiff bases reported previously (Wen *et al.*, 2009; Mohd Lair *et al.*, 2009; Sun *et al.*, 2009).

In the crystal structure, molecules form chains running along the *c* axis through intermolecular N—H···O hydrogen bonds (Table 1 and Fig. 2).

### Experimental

2-Methoxybenzaldehyde (1.0 mmol, 136 mg) and nicotinic acid hydrazide (1.0 mmol, 137 mg) were dissolved in methanol (30 ml). The mixture was stirred at room temperature for 1 h to give a colourless solution. After keeping the solution in air for 3 d, colourless block shaped crystals were formed.

### Refinement

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{C})$ . In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

### Figures

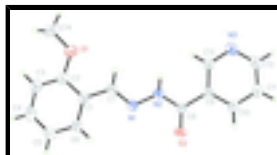


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

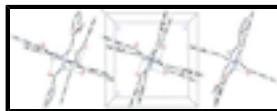


Fig. 2. The crystal packing of the title compound. Intermolecular hydrogen bonds are shown as dashed lines.

## *N*'-(2-Methoxybenzylidene)nicotinohydrazide

### *Crystal data*

$C_{14}H_{13}N_3O_2$	$D_x = 1.250 \text{ Mg m}^{-3}$
$M_r = 255.27$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Tetragonal, $P4_3$	Cell parameters from 2214 reflections
Hall symbol: P 4cw	$\theta = 2.5\text{--}25.3^\circ$
$a = 9.3264 (13) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 15.594 (3) \text{ \AA}$	$T = 298 \text{ K}$
$V = 1356.4 (4) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.20 \times 0.20 \times 0.18 \text{ mm}$
$F(000) = 536$	

### *Data collection*

Bruker APEXII CCD area-detector diffractometer	1519 independent reflections
Radiation source: fine-focus sealed tube graphite	1313 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.028$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$\theta_{\text{max}} = 27.0^\circ$ , $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.983$ , $T_{\text{max}} = 0.985$	$h = -11 \rightarrow 10$
6623 measured reflections	$k = -4 \rightarrow 11$
	$l = -19 \rightarrow 19$

### *Refinement*

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.084$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.084P]$
1519 reflections	where $P = (F_o^2 + 2F_c^2)/3$
176 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
2 restraints	$\Delta\rho_{\text{max}} = 0.09 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$

### *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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.54565 (17)	0.50653 (18)	0.21981 (11)	0.0443 (4)
N2	0.41517 (19)	0.53627 (19)	0.18161 (11)	0.0457 (4)
N3	0.0801 (2)	0.6980 (3)	0.03464 (14)	0.0763 (7)
O1	0.84079 (19)	0.3686 (2)	0.05708 (12)	0.0681 (5)
O2	0.33671 (17)	0.66164 (18)	0.29682 (10)	0.0586 (4)
C1	0.7782 (2)	0.4068 (2)	0.20059 (15)	0.0454 (5)
C2	0.8837 (2)	0.3667 (2)	0.14119 (15)	0.0508 (5)
C3	1.0208 (3)	0.3312 (3)	0.1677 (2)	0.0635 (7)
H3	1.0901	0.3046	0.1279	0.076*
C4	1.0535 (3)	0.3360 (3)	0.2543 (2)	0.0662 (7)
H4	1.1455	0.3123	0.2724	0.079*
C5	0.9519 (3)	0.3753 (3)	0.31421 (19)	0.0621 (6)
H5	0.9751	0.3784	0.3722	0.075*
C6	0.8156 (3)	0.4098 (2)	0.28694 (15)	0.0516 (5)
H6	0.7469	0.4358	0.3273	0.062*
C7	0.6357 (2)	0.4433 (2)	0.17089 (15)	0.0466 (5)
H7	0.6091	0.4202	0.1151	0.056*
C8	0.3205 (2)	0.6206 (2)	0.22245 (13)	0.0420 (5)
C9	0.1932 (2)	0.6646 (2)	0.17108 (14)	0.0428 (5)
C10	0.0723 (3)	0.7159 (3)	0.21159 (16)	0.0623 (7)
H10	0.0690	0.7228	0.2710	0.075*
C11	-0.0433 (3)	0.7567 (4)	0.1626 (2)	0.0797 (9)
H11	-0.1265	0.7907	0.1884	0.096*
C12	-0.0339 (3)	0.7463 (4)	0.07564 (19)	0.0779 (9)
H12	-0.1125	0.7749	0.0432	0.093*
C13	0.1914 (3)	0.6590 (3)	0.08281 (14)	0.0571 (6)
H13	0.2732	0.6259	0.0550	0.069*
C14	0.9423 (4)	0.3294 (4)	-0.0070 (2)	0.0921 (11)
H14A	1.0234	0.3926	-0.0041	0.138*
H14B	0.8987	0.3366	-0.0626	0.138*
H14C	0.9734	0.2325	0.0026	0.138*
H2	0.394 (3)	0.496 (3)	0.1309 (11)	0.080*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0447 (10)	0.0450 (9)	0.0430 (10)	0.0038 (8)	-0.0060 (8)	-0.0027 (8)
N2	0.0473 (10)	0.0510 (10)	0.0387 (10)	0.0048 (8)	-0.0067 (8)	-0.0073 (8)
N3	0.0612 (14)	0.118 (2)	0.0500 (13)	0.0151 (13)	-0.0096 (11)	0.0096 (13)

## supplementary materials

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O1	0.0652 (10)	0.0875 (12)	0.0516 (10)	-0.0048 (9)	0.0080 (9)	-0.0131 (9)
O2	0.0685 (10)	0.0673 (10)	0.0399 (8)	0.0156 (8)	-0.0110 (8)	-0.0140 (8)
C1	0.0491 (12)	0.0404 (11)	0.0468 (12)	-0.0005 (9)	0.0015 (9)	-0.0005 (9)
C2	0.0522 (12)	0.0462 (11)	0.0538 (14)	-0.0060 (9)	0.0038 (10)	-0.0048 (10)
C3	0.0490 (13)	0.0615 (14)	0.0799 (18)	-0.0002 (11)	0.0098 (13)	-0.0091 (13)
C4	0.0479 (13)	0.0646 (16)	0.086 (2)	0.0025 (11)	-0.0054 (14)	0.0038 (14)
C5	0.0647 (15)	0.0641 (15)	0.0576 (15)	0.0002 (12)	-0.0114 (13)	0.0085 (12)
C6	0.0554 (13)	0.0517 (12)	0.0478 (13)	0.0016 (10)	0.0009 (10)	0.0040 (10)
C7	0.0519 (12)	0.0485 (11)	0.0395 (10)	0.0022 (9)	-0.0030 (10)	-0.0042 (9)
C8	0.0492 (11)	0.0405 (10)	0.0361 (11)	0.0013 (8)	-0.0022 (9)	-0.0018 (8)
C9	0.0449 (11)	0.0421 (10)	0.0414 (11)	-0.0001 (8)	-0.0009 (9)	-0.0020 (9)
C10	0.0606 (16)	0.0807 (17)	0.0458 (14)	0.0162 (12)	0.0040 (12)	-0.0068 (13)
C11	0.0526 (14)	0.111 (2)	0.076 (2)	0.0233 (14)	0.0058 (14)	-0.0014 (19)
C12	0.0502 (15)	0.114 (2)	0.0692 (19)	0.0146 (14)	-0.0098 (13)	0.0141 (17)
C13	0.0467 (13)	0.0809 (16)	0.0439 (13)	0.0107 (11)	0.0008 (10)	0.0058 (11)
C14	0.080 (2)	0.127 (3)	0.069 (2)	-0.0180 (19)	0.0249 (16)	-0.0256 (19)

### *Geometric parameters (Å, °)*

N1—C7	1.279 (3)	C5—C6	1.379 (3)
N1—N2	1.383 (2)	C5—H5	0.93
N2—C8	1.343 (3)	C6—H6	0.93
N2—H2	0.897 (10)	C7—H7	0.93
N3—C12	1.320 (4)	C8—C9	1.489 (3)
N3—C13	1.332 (3)	C9—C13	1.378 (3)
O1—C2	1.371 (3)	C9—C10	1.378 (3)
O1—C14	1.424 (3)	C10—C11	1.375 (4)
O2—C8	1.231 (2)	C10—H10	0.93
C1—C6	1.391 (3)	C11—C12	1.362 (4)
C1—C2	1.402 (3)	C11—H11	0.93
C1—C7	1.448 (3)	C12—H12	0.93
C2—C3	1.385 (3)	C13—H13	0.93
C3—C4	1.385 (4)	C14—H14A	0.96
C3—H3	0.93	C14—H14B	0.96
C4—C5	1.380 (4)	C14—H14C	0.96
C4—H4	0.93		
C7—N1—N2	114.42 (17)	C1—C7—H7	119.3
C8—N2—N1	119.46 (17)	O2—C8—N2	123.23 (19)
C8—N2—H2	120.9 (19)	O2—C8—C9	121.28 (18)
N1—N2—H2	119.6 (19)	N2—C8—C9	115.49 (17)
C12—N3—C13	116.6 (2)	C13—C9—C10	117.4 (2)
C2—O1—C14	118.3 (2)	C13—C9—C8	122.5 (2)
C6—C1—C2	118.0 (2)	C10—C9—C8	120.1 (2)
C6—C1—C7	122.3 (2)	C11—C10—C9	118.9 (2)
C2—C1—C7	119.7 (2)	C11—C10—H10	120.6
O1—C2—C3	123.9 (2)	C9—C10—H10	120.6
O1—C2—C1	115.1 (2)	C12—C11—C10	118.8 (3)
C3—C2—C1	121.0 (2)	C12—C11—H11	120.6
C4—C3—C2	119.1 (2)	C10—C11—H11	120.6

C4—C3—H3	120.4	N3—C12—C11	124.0 (3)
C2—C3—H3	120.4	N3—C12—H12	118.0
C5—C4—C3	121.1 (2)	C11—C12—H12	118.0
C5—C4—H4	119.4	N3—C13—C9	124.3 (2)
C3—C4—H4	119.4	N3—C13—H13	117.9
C6—C5—C4	119.1 (3)	C9—C13—H13	117.9
C6—C5—H5	120.4	O1—C14—H14A	109.5
C4—C5—H5	120.4	O1—C14—H14B	109.5
C5—C6—C1	121.7 (2)	H14A—C14—H14B	109.5
C5—C6—H6	119.2	O1—C14—H14C	109.5
C1—C6—H6	119.2	H14A—C14—H14C	109.5
N1—C7—C1	121.4 (2)	H14B—C14—H14C	109.5
N1—C7—H7	119.3		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2 $\cdots$ O2 <sup>i</sup>	0.90 (1)	2.05 (2)	2.897 (2)	157 (3)
C4—H4 $\cdots$ O1 <sup>ii</sup>	0.93	2.58	3.469 (3)	160
C11—H11 $\cdots$ N3 <sup>iii</sup>	0.93	2.53	3.429 (4)	164
C13—H13 $\cdots$ N1 <sup>i</sup>	0.93	2.56	3.487 (3)	176

Symmetry codes: (i)  $-y+1, x, z-1/4$ ; (ii)  $y+1, -x+1, z+1/4$ ; (iii)  $y-1, -x+1, z+1/4$ .

Fig. 1

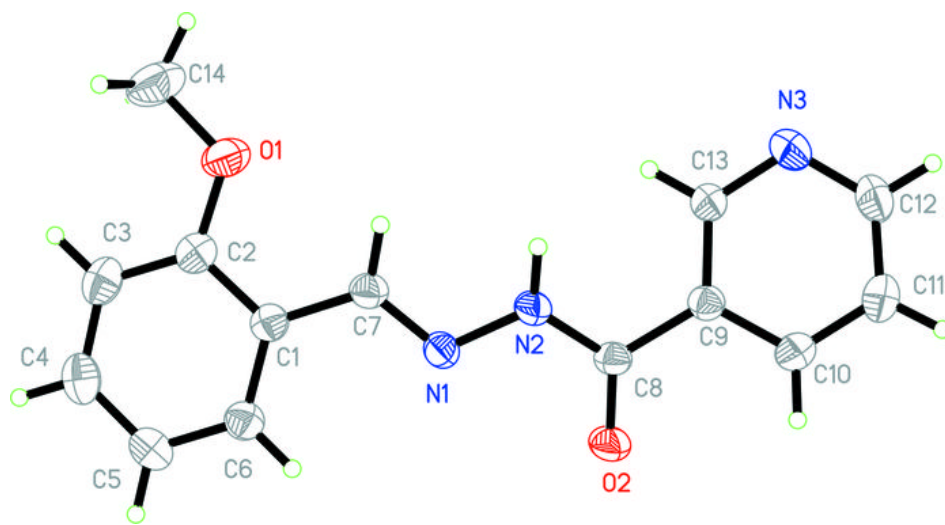




Fig. 2

