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(*E*)-*N*-(2-Hydroxybenzylidene)-isonicotinohydrazide

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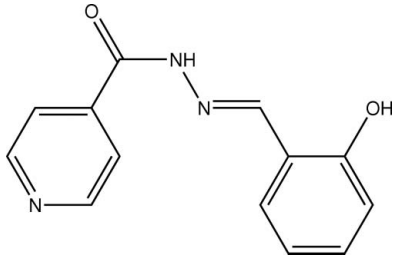
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.104; data-to-parameter ratio = 13.5.

In the molecule of the title compound, $C_{13}H_{11}N_3O_2$, an intramolecular O—H···N hydrogen bond forms a six-membered ring. Intermolecular N—H···N hydrogen bonds connect adjacent molecules to form a zigzag chain parallel to the c axis.

Related literature

For related literature, see: Lee *et al.* (2003); Tang *et al.* (2003). For reference bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{11}N_3O_2$
M_r = 241.25
Monoclinic, $P2_1/c$
a = 8.1467 (12) Å
b = 15.562 (2) Å
c = 10.7457 (12) Å
β = 121.147 (8)°
V = 1165.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.29 × 0.22 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.989
6268 measured reflections
2212 independent reflections
1908 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.104
S = 1.07
2212 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*B*···N3	0.82	1.89	2.6076 (15)	146
N2—H2···N1^{i}	0.86	2.21	3.0530 (15)	165

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2264).

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supplementary materials

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(*E*)-*N*-(2-Hydroxybenzylidene)isonicotinohydrazide

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Comment

The hydrazones fluorescence reagents have good chemical stability and were simply bonded with metal cations (Lee *et al.*, 2003; Tang *et al.*, 2003), therefore the study of complexes characteristic fluorescence response can give support to the cations detection. Here we synthesized the title compound.

The whole molecule is non-planar with a dihedral angle of 21.37 (1)° between the pyridine ring A (N1/C1–C5) and the benzene ring B (C8–C13). There is an intramolecular hydrogen bond O2–H2A···N3, forming a six-numbered ring (Fig. 1). Bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

In the crystal structure, the molecules are connected throughmolecules are N—H···N intermolecular hydrogen bonds (Table 1) forming a zigzag like chain parallel to the *c* axis (Fig. 2)

Experimental

To a solution of Salicylaldehyde (2.1 ml, 0.02 mol) was added dropwise a solution of isoniazide (1.4 g, 0.01 mol) in dry EtOH (30 ml), and the mixture was stirred at 356 K for 2.5 h. After cooling to room temperature, some yellow solid appeared. Then the resulting yellow solid was filtered off, washed with dry EtOH, dried, and recrystallized from dry EtOH. Yellow single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a dry EtOH solution over a period of 5 d.

Refinement

All H atoms attached to C, N and O atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (C), N—H = 0.86 Å and O—H = 0.82 Å with U_{iso}(H) = 1.2U_{eq}(C,*N* or O).

Figures

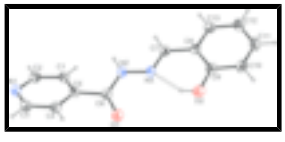

Fig. 1. Molecular view of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed line.

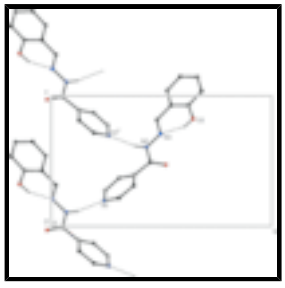

Fig. 2. Partial packing view of compound (I), showing the formation of chains along [010] built from hydrogen bonds shown as dashed lines. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. [symmetry codes: (i) *x*, −*y* + 1/2, *z* + 1/2].

(*E*)-*N*-(2-Hydroxybenzylidene)isonicotinohydrazide

Crystal data

$C_{13}H_{11}N_3O_2$	F_{000} = 504
M_r = 241.25	D_x = 1.374 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2790 reflections
a = 8.1467 (12) Å	θ = 2.6–25.7º
b = 15.562 (2) Å	μ = 0.10 mm^{-1}
c = 10.7457 (12) Å	T = 293 (2) K
β = 121.147 (8)º	Plate, colourless
V = 1165.9 (3) Å^3	0.29 × 0.22 × 0.09 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2212 independent reflections
Radiation source: fine-focus sealed tube	1908 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.014
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 25.7º
T = 293(2) K	θ_{min} = 2.6º
ω scans	h = −9→9
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −18→14
T_{min} = 0.968, T_{max} = 0.989	l = −13→12
6268 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.104	$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.1742P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2212 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
164 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.11674 (17)	0.24122 (7)	0.19619 (12)	0.0453 (3)
N2	0.19855 (16)	0.43183 (7)	0.60543 (11)	0.0418 (3)
H2	0.1578	0.3825	0.6140	0.050*
N3	0.24356 (15)	0.49509 (7)	0.70680 (11)	0.0408 (3)
O1	0.26941 (17)	0.51914 (6)	0.47109 (12)	0.0610 (3)
O2	0.39390 (16)	0.64334 (6)	0.82295 (12)	0.0551 (3)
H2B	0.3605	0.6042	0.7636	0.083*
C1	0.05708 (19)	0.30830 (8)	0.36987 (14)	0.0423 (3)
H1	−0.0065	0.3068	0.4210	0.051*
C2	0.0297 (2)	0.24389 (9)	0.27236 (14)	0.0455 (3)
H2A	−0.0547	0.1997	0.2591	0.055*
C3	0.2340 (2)	0.30658 (9)	0.21573 (15)	0.0467 (3)
H3	0.2949	0.3067	0.1626	0.056*
C4	0.2702 (2)	0.37406 (8)	0.31032 (14)	0.0440 (3)
H4	0.3534	0.4181	0.3202	0.053*
C5	0.18043 (18)	0.37496 (8)	0.39010 (13)	0.0379 (3)
C6	0.22024 (19)	0.44935 (8)	0.49115 (14)	0.0412 (3)
C7	0.22300 (19)	0.47889 (8)	0.81433 (14)	0.0404 (3)
H7	0.1763	0.4256	0.8209	0.048*
C8	0.27183 (17)	0.54288 (8)	0.92658 (13)	0.0373 (3)
C9	0.35359 (18)	0.62208 (8)	0.92655 (14)	0.0409 (3)
C10	0.3940 (2)	0.68162 (9)	1.03475 (16)	0.0537 (4)
H10	0.4457	0.7347	1.0337	0.064*
C11	0.3581 (2)	0.66285 (10)	1.14385 (17)	0.0567 (4)
H11	0.3856	0.7034	1.2156	0.068*
C12	0.2820 (2)	0.58455 (10)	1.14758 (16)	0.0533 (4)
H12	0.2599	0.5717	1.2223	0.064*
C13	0.2388 (2)	0.52549 (9)	1.03945 (15)	0.0459 (3)
H13	0.1865	0.4728	1.0416	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0559 (7)	0.0423 (6)	0.0423 (6)	0.0011 (5)	0.0287 (6)	−0.0024 (5)
N2	0.0562 (7)	0.0343 (6)	0.0381 (6)	−0.0009 (5)	0.0266 (5)	−0.0033 (4)
N3	0.0482 (6)	0.0375 (6)	0.0376 (6)	0.0024 (5)	0.0227 (5)	−0.0026 (4)
O1	0.0929 (8)	0.0444 (6)	0.0648 (7)	−0.0139 (5)	0.0542 (7)	−0.0072 (5)
O2	0.0708 (7)	0.0458 (6)	0.0601 (7)	−0.0115 (5)	0.0420 (6)	−0.0012 (5)
C1	0.0482 (8)	0.0455 (7)	0.0397 (7)	0.0009 (6)	0.0274 (6)	0.0011 (6)
C2	0.0510 (8)	0.0429 (7)	0.0457 (8)	−0.0045 (6)	0.0273 (7)	−0.0016 (6)
C3	0.0601 (9)	0.0456 (8)	0.0487 (8)	0.0028 (6)	0.0382 (7)	0.0016 (6)
C4	0.0551 (8)	0.0388 (7)	0.0466 (8)	−0.0011 (6)	0.0323 (7)	0.0018 (6)
C5	0.0446 (7)	0.0362 (7)	0.0332 (6)	0.0060 (5)	0.0203 (6)	0.0044 (5)
C6	0.0470 (7)	0.0386 (7)	0.0404 (7)	0.0007 (6)	0.0244 (6)	−0.0002 (5)
C7	0.0475 (7)	0.0343 (7)	0.0422 (7)	−0.0008 (5)	0.0253 (6)	−0.0006 (5)
C8	0.0393 (7)	0.0352 (7)	0.0377 (7)	0.0041 (5)	0.0201 (6)	0.0003 (5)
C9	0.0413 (7)	0.0378 (7)	0.0424 (7)	0.0021 (5)	0.0208 (6)	0.0020 (5)
C10	0.0599 (9)	0.0386 (8)	0.0555 (9)	−0.0052 (6)	0.0248 (8)	−0.0075 (6)
C11	0.0647 (10)	0.0520 (9)	0.0476 (8)	0.0064 (7)	0.0250 (8)	−0.0128 (7)
C12	0.0653 (9)	0.0567 (9)	0.0459 (8)	0.0091 (7)	0.0342 (7)	−0.0015 (7)
C13	0.0541 (8)	0.0430 (8)	0.0471 (8)	0.0014 (6)	0.0307 (7)	0.0006 (6)

Geometric parameters (Å, °)

N1—C2	1.3323 (17)	C4—C5	1.3853 (18)
N1—C3	1.3357 (18)	C4—H4	0.9300
N2—C6	1.3558 (17)	C5—C6	1.5034 (18)
N2—N3	1.3699 (15)	C7—C8	1.4521 (17)
N2—H2	0.8600	C7—H7	0.9300
N3—C7	1.2756 (16)	C8—C13	1.3978 (18)
O1—C6	1.2148 (16)	C8—C9	1.4009 (18)
O2—C9	1.3546 (16)	C9—C10	1.3867 (19)
O2—H2B	0.8200	C10—C11	1.378 (2)
C1—C5	1.3809 (19)	C10—H10	0.9300
C1—C2	1.3822 (18)	C11—C12	1.377 (2)
C1—H1	0.9300	C11—H11	0.9300
C2—H2A	0.9300	C12—C13	1.3770 (19)
C3—C4	1.3830 (19)	C12—H12	0.9300
C3—H3	0.9300	C13—H13	0.9300
C2—N1—C3	116.40 (11)	N2—C6—C5	114.76 (11)
C6—N2—N3	117.97 (11)	N3—C7—C8	120.60 (12)
C6—N2—H2	121.0	N3—C7—H7	119.7
N3—N2—H2	121.0	C8—C7—H7	119.7
C7—N3—N2	118.14 (11)	C13—C8—C9	118.38 (12)
C9—O2—H2B	109.5	C13—C8—C7	119.66 (12)
C5—C1—C2	118.88 (12)	C9—C8—C7	121.95 (11)
C5—C1—H1	120.6	O2—C9—C10	118.20 (12)

C2—C1—H1	120.6	O2—C9—C8	122.17 (12)
N1—C2—C1	124.04 (12)	C10—C9—C8	119.63 (13)
N1—C2—H2A	118.0	C11—C10—C9	120.58 (14)
C1—C2—H2A	118.0	C11—C10—H10	119.7
N1—C3—C4	123.84 (12)	C9—C10—H10	119.7
N1—C3—H3	118.1	C12—C11—C10	120.61 (13)
C4—C3—H3	118.1	C12—C11—H11	119.7
C3—C4—C5	118.84 (12)	C10—C11—H11	119.7
C3—C4—H4	120.6	C13—C12—C11	119.22 (14)
C5—C4—H4	120.6	C13—C12—H12	120.4
C1—C5—C4	117.98 (12)	C11—C12—H12	120.4
C1—C5—C6	124.03 (11)	C12—C13—C8	121.55 (13)
C4—C5—C6	117.97 (12)	C12—C13—H13	119.2
O1—C6—N2	123.36 (12)	C8—C13—H13	119.2
O1—C6—C5	121.87 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2B···N3	0.82	1.89	2.6076 (15)	146
N2—H2···N1^{i}	0.86	2.21	3.0530 (15)	165

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

Fig. 1

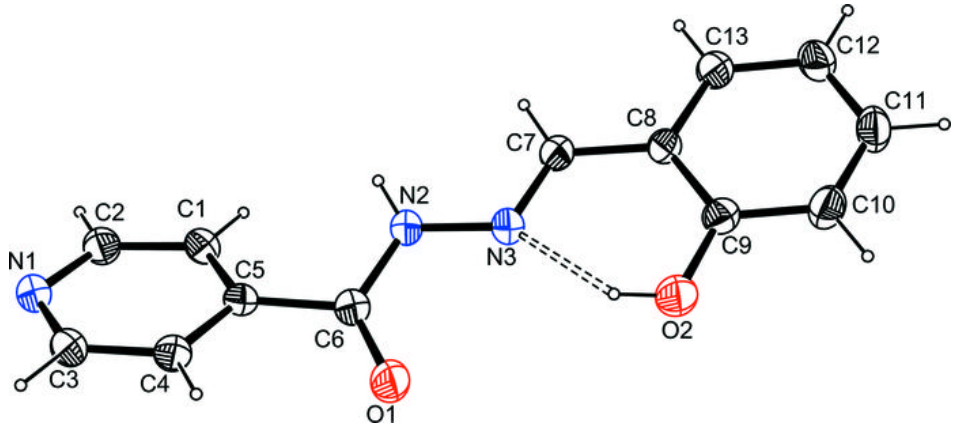

Fig. 2