Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Pyridine-3-carbaldehyde 2-pyridylhydrazone

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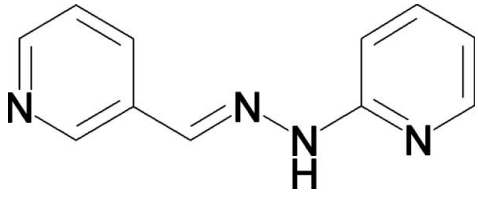
Received 28 March 2007; accepted 11 May 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.047; data-to-parameter ratio = 20.4.

In the crystal structure of the title compound, $C_{11}H_{10}N_4$, molecules form dimers , which form a zigzag pattern in the crystal. The hydrogen-bond network can be described by graph-set notation as $R_2^2(14)$.

Related literature

For related literature, see: Allen *et al.* (1987); Cory *et al.* (1994); Etter (1990); Popp (1989); Seydel *et al.* (1994).



Experimental

Crystal data

$C_{11}H_{10}N_4$
M_r = 198.23
Monoclinic, $P2_1/n$
a = 10.896 (5) Å
b = 4.0270 (17) Å
c = 22.710 (9) Å
β = 94.304 (8)°
V = 993.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293.1 K
0.40 × 0.30 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan Jacobson (1998)
T_{min} = 0.892, T_{max} = 0.992
9025 measured reflections
3614 independent reflections
2273 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.048
S = 0.97
3614 reflections
177 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N3^{i}	1.03 (2)	2.01 (2)	3.0371 (18)	177 (1)

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Molecular Structure Corporation & Rigaku, 2005); program(s) used to solve structure: *SIR88* (Burla *et al.*, 1989); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

This study was supported by the Russian Foundation of Basic Research (No. 06-03-96304).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2161).

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  doi:10.1107/S1600536807023203

supplementary materials

Acta Cryst. (2007). E**63**, o3042 [**doi:10.1107/S1600536807023203**]

Pyridine-3-carbaldehyde 2-pyridylhydrazone

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Comment

2-Pyridylhydrazone (2-pyridinylhydrazone 3-Pyridinecarboxaldehyde, I) belongs to the class of heterocyclic hydrazones, which have an anti-tuberculosis activity (Cory *et al.*, 1994; Seydel *et al.*, 1994). These compounds show some inhibitory activity towards ribonucleotide reductase and anticonvulsant activity as well (Popp, 1989). Crystal structure of (I) has not been solved before. Therefore the aim of the work was to fill this gap. A view of molecule (I) with the atomic numbering is presented in Fig 1. The parameters of the hydrogen bond geometry are shown in Table 1. The bond lengths are within the normal range of such bonds (Allen *et al.*, 1987). The conformational state of the molecule in the crystal structure can be characterized in the following way. The torsion angle N1—C1—C2—C3, which characterizes the orientation of the one pyridine fragment Py1 [N4—C6–C2—C3—C4—C5] with respect to bridge group (C1—N1—N2), is 3.5 (2) °. At other side, he torsion angle C8—C7—N2—N1, which describes the orientation of the second pyridine ring Py2 [N3—C7–C8—C9—C10—C11] with respect to the bridge group, is 0.9 (2) °. The torsion angle C2–C1—N1—N2, which characterize a planarity of bridge group, is 178.86 (13) °. The pyridine fragments are rotated relatively o each other by 8.2 (2)°. The molecular packing architecture is shown in Figs. 2 & 3. The molecules of (I) form dimers by hydrogen bonds N2—H2···N3. The hydrogen-bond network can be described by the graph-set assignment introduced by Etter (1990) as $R_2^2(14)$. The dimers are packed in cups where interact to each other by van-der-Waals forces.

Experimental

The chemical synthesis of the title compound was performed by analogy to procedures described previously (Popp, 1989). Generally, the compound was recrystallized from methanol/water. The 2-Pyridylhydrazone crystal was grown by slow evaporation from methanol solution.

Figures

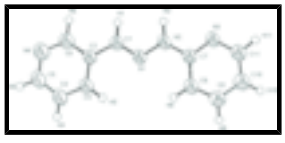

Fig. 1. A view of I with the atomic numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

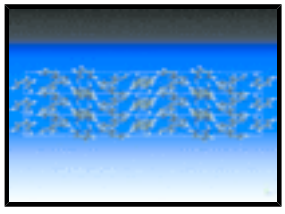

Fig. 2. Projection of crystal lattice molecular packing of (I) along OX axis.

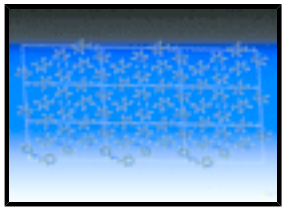

Fig. 3. Projection of crystal lattice molecular packing of (I) along OY axis.

Pyridine-3-carbaldehyde 2-pyridylhydrazone

Crystal data

$C_{11}H_{10}N_4$	F_{000} = 416.00
M_r = 198.23	D_x = 1.325 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 449 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71070 Å
a = 10.896 (5) Å	Cell parameters from 1851 reflections
b = 4.0270 (17) Å	θ = 3.2–30.0º
c = 22.710 (9) Å	μ = 0.09 mm^{-1}
β = 94.304 (8)º	T = 293.1 K
V = 993.6 (7) Å^3	Prism, colorless
Z = 4	0.40 × 0.30 × 0.10 mm

Data collection

Rigaku Saturn diffractometer	θ_{max} = 30.4º
ω scans	h = −14→14
Absorption correction: multi-scan Jacobson (1998)	k = −3→5
T_{min} = 0.892, T_{max} = 0.992	l = −32→31
9025 measured reflections	Standard reflections: ?;
3614 independent reflections	every ? reflections
2273 reflections with $F^2 > 2\sigma(F^2)$	intensity decay: ?
R_{int} = 0.037	

Refinement

Refinement on F	Chebychev polynomial *w*ith 3 parameters (Carruthers & Watkin, 1979) 88.1628 106.9210 44.1569
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max}$ = 0.006
$wR(F^2)$ = 0.048	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
S = 0.97	$\Delta\rho_{min}$ = −0.52 e Å^{-3}
3614 reflections	Extinction correction: Larson (1970) Crystallographic Computing eq. 22
177 parameters	Extinction coefficient: 41 (21)
All H-atom parameters refined	

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement using reflections with $F^2 > 3.0$ sigma(F^2). The weighted *R*-factor(*wR*), goodness of fit (S) and *R*-factor (gt) are based on F, with F set to zero for negative F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.58600 (12)	0.1829 (3)	0.62487 (5)	0.0552 (4)
N2	0.57422 (12)	0.2776 (3)	0.56706 (5)	0.0583 (4)
N3	0.64083 (11)	0.2790 (3)	0.47412 (5)	0.0573 (4)
N4	0.39775 (16)	0.1814 (4)	0.80823 (6)	0.0817 (6)
C1	0.49701 (17)	0.2595 (4)	0.65614 (6)	0.0565 (5)
C2	0.50216 (14)	0.1730 (4)	0.71847 (6)	0.0508 (5)
C3	0.60286 (18)	0.0237 (4)	0.74843 (6)	0.0572 (5)
C4	0.6002 (2)	−0.0391 (4)	0.80754 (8)	0.0679 (6)
C5	0.4975 (2)	0.0415 (5)	0.83536 (9)	0.0752 (7)
C6	0.40282 (18)	0.2461 (5)	0.75060 (8)	0.0685 (6)
C7	0.66146 (14)	0.1757 (4)	0.53006 (6)	0.0501 (5)
C8	0.76185 (16)	−0.0184 (4)	0.54956 (8)	0.0579 (5)
C9	0.84375 (19)	−0.1077 (4)	0.50947 (9)	0.0680 (6)
C10	0.82507 (18)	−0.0028 (4)	0.45175 (8)	0.0669 (6)
C11	0.72443 (17)	0.1861 (4)	0.43666 (8)	0.0614 (6)
H1	0.4229 (13)	0.386 (3)	0.6392 (5)	0.059 (4)*
H2	0.4999 (17)	0.419 (4)	0.5523 (7)	0.101 (6)*
H3	0.6766 (12)	−0.036 (3)	0.7269 (5)	0.058 (4)*
H4	0.6726 (14)	−0.133 (4)	0.8288 (6)	0.075 (5)*
H5	0.4973 (14)	0.002 (4)	0.8809 (7)	0.092 (5)*
H6	0.3308 (14)	0.349 (3)	0.7279 (6)	0.078 (5)*
H8	0.7715 (12)	−0.100 (3)	0.5907 (6)	0.061 (4)*
H9	0.9192 (14)	−0.251 (4)	0.5233 (6)	0.078 (5)*
H10	0.8840 (13)	−0.067 (3)	0.4231 (6)	0.069 (4)*
H11	0.7058 (13)	0.271 (3)	0.3930 (6)	0.071 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0598 (9)	0.0669 (10)	0.0390 (7)	−0.0061 (7)	0.0043 (6)	0.0036 (6)
N2	0.0522 (9)	0.0841 (11)	0.0390 (7)	0.0041 (8)	0.0049 (7)	0.0107 (7)
N3	0.0558 (8)	0.0752 (10)	0.0411 (7)	−0.0023 (7)	0.0056 (6)	0.0025 (7)
N4	0.0849 (12)	0.1059 (13)	0.0575 (10)	−0.0055 (10)	0.0267 (9)	0.0024 (9)
C1	0.0503 (11)	0.0746 (14)	0.0447 (10)	0.0025 (10)	0.0046 (8)	0.0070 (9)
C2	0.0500 (10)	0.0583 (11)	0.0445 (8)	−0.0014 (8)	0.0070 (8)	0.0002 (8)
C3	0.0602 (11)	0.0648 (12)	0.0472 (10)	−0.0018 (10)	0.0072 (9)	0.0035 (9)
C4	0.0756 (14)	0.0746 (13)	0.0529 (12)	−0.0008 (11)	−0.0003 (11)	0.0077 (10)

C5	0.0966 (17)	0.0823 (15)	0.0478 (11)	−0.0209 (13)	0.0121 (12)	0.0046 (11)
C6	0.0600 (12)	0.0914 (16)	0.0552 (11)	0.0032 (11)	0.0129 (10)	0.0052 (11)
C7	0.0486 (10)	0.0576 (11)	0.0445 (9)	−0.0085 (9)	0.0056 (8)	−0.0009 (8)
C8	0.0608 (12)	0.0626 (12)	0.0499 (10)	−0.0022 (9)	0.0026 (9)	0.0042 (10)
C9	0.0669 (13)	0.0690 (14)	0.0688 (13)	0.0071 (10)	0.0104 (10)	0.0033 (10)
C10	0.0723 (14)	0.0683 (13)	0.0626 (11)	0.0054 (11)	0.0224 (10)	−0.0035 (10)
C11	0.0668 (12)	0.0700 (13)	0.0483 (10)	−0.0022 (10)	0.0107 (9)	−0.0009 (9)

Geometric parameters (Å, °)

N1—N2	1.3640 (16)	C8—C9	1.370 (2)
N1—C1	1.282 (2)	C9—C10	1.378 (2)
N2—C7	1.378 (2)	C10—C11	1.357 (2)
N3—C7	1.3396 (19)	N2—H2	1.026 (18)
N3—C11	1.345 (2)	C1—H1	1.007 (14)
N4—C5	1.334 (2)	C3—H3	1.001 (14)
N4—C6	1.340 (2)	C4—H4	0.971 (15)
C1—C2	1.455 (2)	C5—H5	1.048 (17)
C2—C3	1.384 (2)	C6—H6	0.996 (15)
C2—C6	1.382 (2)	C8—H8	0.988 (14)
C3—C4	1.368 (2)	C9—H9	1.034 (16)
C4—C5	1.364 (3)	C10—H10	0.981 (15)
C7—C8	1.390 (2)	C11—H11	1.054 (14)
N2—N1—C1	116.45 (13)	C7—N2—H2	122.0 (9)
N1—N2—C7	118.97 (13)	N1—C1—H1	122.0 (8)
C7—N3—C11	116.11 (13)	C2—C1—H1	117.6 (8)
C5—N4—C6	116.20 (18)	C2—C3—H3	120.0 (7)
N1—C1—C2	120.39 (15)	C4—C3—H3	120.8 (7)
C1—C2—C3	123.61 (15)	C3—C4—H4	118.9 (9)
C1—C2—C6	119.24 (15)	C5—C4—H4	121.8 (9)
C3—C2—C6	117.15 (15)	N4—C5—H5	117.3 (8)
C2—C3—C4	119.20 (17)	C4—C5—H5	119.0 (8)
C3—C4—C5	119.28 (19)	N4—C6—H6	119.8 (9)
N4—C5—C4	123.69 (18)	C2—C6—H6	115.7 (9)
N4—C6—C2	124.47 (17)	C7—C8—H8	120.8 (8)
N2—C7—N3	114.31 (13)	C9—C8—H8	120.9 (8)
N2—C7—C8	122.40 (14)	C8—C9—H9	119.2 (8)
N3—C7—C8	123.29 (15)	C10—C9—H9	121.1 (8)
C7—C8—C9	118.19 (16)	C9—C10—H10	119.5 (8)
C8—C9—C10	119.65 (18)	C11—C10—H10	122.4 (8)
C9—C10—C11	118.10 (18)	N3—C11—H11	114.5 (8)
N3—C11—C10	124.66 (16)	C10—C11—H11	120.9 (8)
N1—N2—H2	119.0 (9)		
N2—N1—C1—C2	−179.10 (14)	C1—C2—C3—C4	178.10 (17)
C1—N1—N2—C7	−174.09 (15)	C1—C2—C6—N4	−179.27 (17)
N1—N2—C7—N3	179.33 (13)	C3—C2—C6—N4	−0.2 (2)
N1—N2—C7—C8	−0.5 (2)	C6—C2—C3—C4	−1.0 (2)
C7—N3—C11—C10	0.5 (2)	C2—C3—C4—C5	1.2 (2)
C11—N3—C7—N2	179.64 (14)	C3—C4—C5—N4	−0.2 (3)

C11—N3—C7—C8	−0.5 (2)	N2—C7—C8—C9	179.95 (14)
C5—N4—C6—C2	1.1 (2)	N3—C7—C8—C9	0.1 (2)
C6—N4—C5—C4	−0.8 (3)	C7—C8—C9—C10	0.4 (2)
N1—C1—C2—C3	3.7 (2)	C8—C9—C10—C11	−0.4 (2)
N1—C1—C2—C6	−177.31 (16)	C9—C10—C11—N3	−0.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N3^{i}	1.026 (18)	2.012 (18)	3.0371 (18)	176.5 (13)

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

Fig. 1

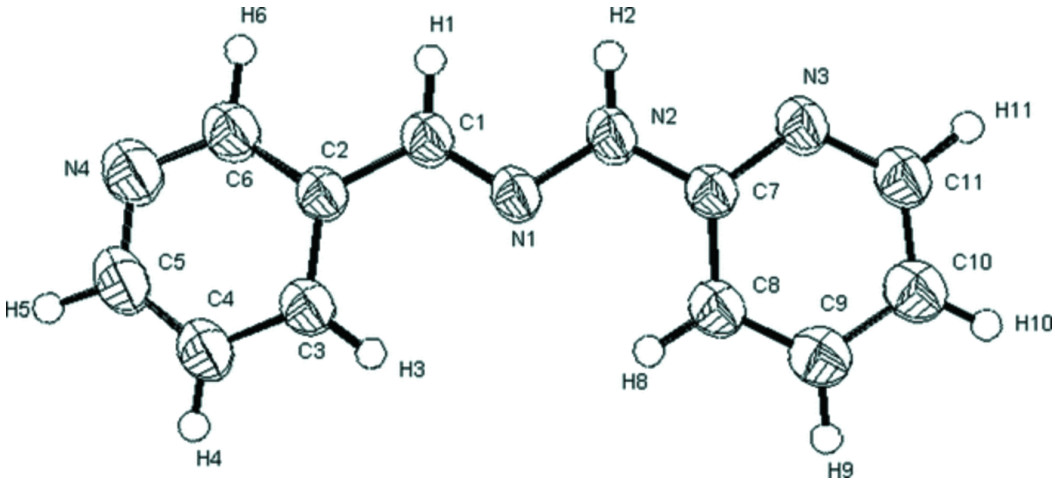
H6
H1
H2
N3
H11
C1
N2
N4
C6
C2
C7
C11
N1
C5
C10
C8
C4
C9
H5
H10
C3
H3
H8
H4
H9

Fig. 2

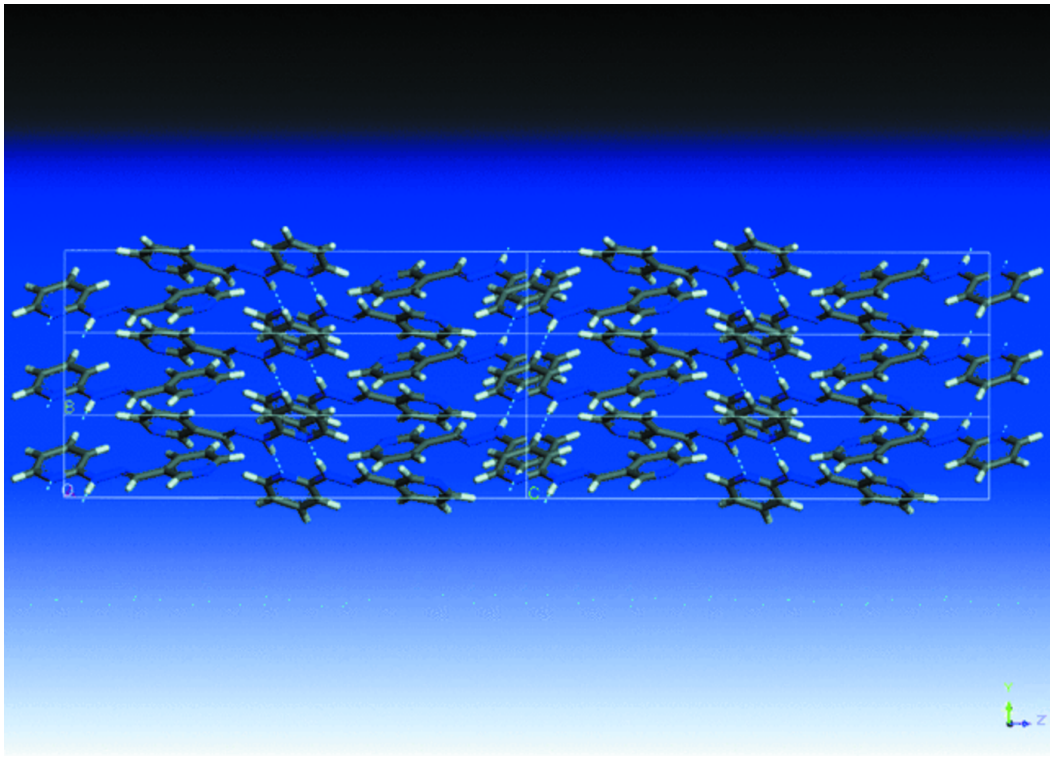

Fig. 3