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Pyridine-2-carbaldehyde thiosemicarbazone

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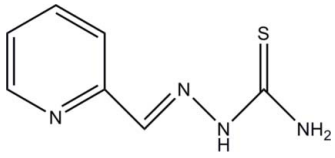
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; R factor = 0.066; wR factor = 0.165; data-to-parameter ratio = 12.8.

The asymmetric unit of the title compound, $C_7H_8N_4S$, contains two independent molecules with slightly different conformations; the dihedral angles between the pyridine ring and mean plane of the thiosemicarbazone unit in the two molecules are 2.88 (5) and 6.30 (5)°. Intermolecular N—H···N and N—H···S hydrogen bonds link the molecules into layers parallel to the *ab* plane.

Related literature

For the properties of thiosemicarbazones, see: Beraldo & Gambino (2004). For the crystal structure of a related compound, see: Gu *et al.* (2008).



Experimental

Crystal data

$C_7H_8N_4S$
M_r = 180.23
Orthorhombic, $Pna2_1$
a = 20.725 (2) Å
b = 4.7857 (6) Å
c = 17.393 (2) Å
V = 1725.1 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 298 (2) K
0.45 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.868, T_{max} = 0.941
7296 measured reflections
2797 independent reflections
1951 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.165
S = 0.96
2797 reflections
218 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}
Absolute structure: Flack (1983), 1218 Friedel pairs
Flack parameter: 0.02 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N8^{i}	0.86	2.18	3.032 (8)	169
N3—H3B···S2^{ii}	0.86	2.57	3.417 (6)	168
N7—H7B···S1^{iii}	0.86	2.60	3.455 (7)	172
N5—H5···N4	0.86	2.36	3.199 (8)	164

Symmetry codes: (i) $x, y+1, z$; (ii) $x-\frac{1}{2}, -y+\frac{5}{2}, z$; (iii) $x+\frac{1}{2}, -y+\frac{5}{2}, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: CV2504).

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supporting information

Acta Cryst. (2009). E**65**, o356 [doi:10.1107/S1600536809001962]

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Li-Hua Song, Xiang Zhang, Kun Jiang and Sheng-Xiang Yang

S1. Comment

Thiosemicarbazones have been known for many years to show a broad spectrum of therapeutic properties against a range of diseases, with antibacterial, antimalarial, antiviral and antitumour activities (Beraldo & Gambino, 2004), In this paper, we present the crystal structure of the title compound, (I).

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in the reported compound (Gu *et al.*, 2008). The mean planes C10/C11/C12/C13/C14/N8 and C9/N6/N5 form a dihedral angle of 2.88 (5)°, while C3/C4/C5/C6/C7/N4 and C2/N2/N1 form a dihedral angle of 6.30 (5)°.

In the crystal, the intermolecular N—H···N and N—H···S hydrogen bonds (Table 1) link the molecules into layers parallel to *ab* plane.

S2. Experimental

Pyridine-2-carbaldehyde (0.5 mmol), thiosemicarbazide (0.5 mmol) and 20 ml ethanol were mixed in 50 ml flask. After stirring 30 min at 373 K, the resulting mixture was recrystalized from ethanol, affording the title compound as a orange crystalline solid. Elemental analysis: calculated for $C_7H_8N_4S$: C 46.65, H 4.47, N 31.09%; found: C46.58, H 4.56, N 31.11%.

S3. Refinement

All H atoms were placed in geometrically idealized positions (N—H 0.86 Å, C—H 0.93 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C,*N*).

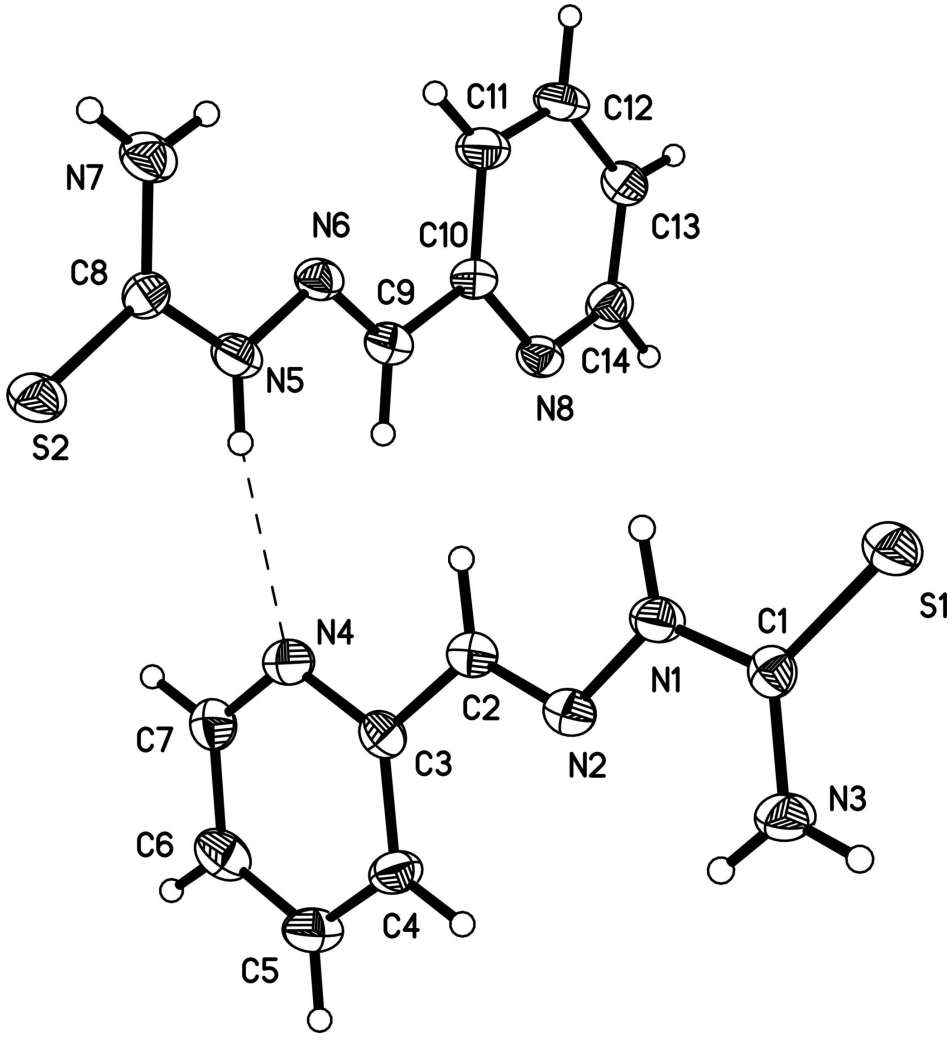

Figure 1

The content of asymmetric unit of the title compound showing the atomic numbering scheme and 30% probability displacement ellipsoids. Dashed line denotes hydrogen bond.

Pyridine-2-carbaldehyde thiosemicarbazone

Crystal data

$C_7H_8N_4S$
$M_r = 180.23$
Orthorhombic, $Pna2_1$
$a = 20.725$ (2) Å
$b = 4.7857$ (6) Å
$c = 17.393$ (2) Å
$V = 1725.1$ (4) Å^3
$Z = 8$
$F(000) = 752$
$D_x = 1.388$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1607 reflections
$\theta = 2.3$–21.6°
$\mu = 0.32$ mm^{-1}
$T = 298$ K
Block, orange
0.45 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.868, T_{max} = 0.941
7296 measured reflections
2797 independent reflections
1951 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −24→20
k = −5→5
l = −20→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.165
S = 0.96
2797 reflections
218 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 6.2026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}
Absolute structure: Flack (1983), 1218 Friedel pairs
Absolute structure parameter: 0.02 (19)

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}
N8	0.6201 (3)	−0.1518 (12)	0.5432 (3)	0.0387 (14)
N1	0.5188 (3)	0.9637 (13)	0.4216 (3)	0.0405 (15)
H1	0.5464	0.9533	0.4584	0.049*
N2	0.5264 (3)	0.8019 (12)	0.3566 (3)	0.0385 (14)
N3	0.4295 (3)	1.1564 (14)	0.3672 (3)	0.0514 (18)
H3A	0.4376	1.0591	0.3267	0.062*
H3B	0.3965	1.2651	0.3682	0.062*
N4	0.6451 (3)	0.3132 (13)	0.2989 (3)	0.0443 (15)
N5	0.7451 (3)	0.5151 (13)	0.4275 (3)	0.0411 (14)
H5	0.7213	0.4881	0.3877	0.049*
N6	0.7334 (3)	0.3664 (12)	0.4937 (3)	0.0371 (14)
N7	0.8267 (3)	0.7425 (15)	0.4879 (4)	0.0493 (17)
H7A	0.8170	0.6506	0.5288	0.059*
H7B	0.8580	0.8603	0.4885	0.059*
S1	0.45768 (9)	1.3182 (4)	0.50951 (10)	0.0483 (5)

S2	0.80649 (9)	0.8767 (4)	0.34251 (11)	0.0480 (5)
C1	0.4677 (3)	1.1390 (15)	0.4274 (4)	0.0352 (16)
C2	0.5761 (3)	0.6438 (14)	0.3561 (4)	0.0383 (17)
H2	0.6046	0.6495	0.3975	0.046*
C3	0.5892 (3)	0.4557 (14)	0.2926 (4)	0.0362 (16)
C4	0.5478 (3)	0.4143 (16)	0.2310 (4)	0.0438 (18)
H4	0.5097	0.5157	0.2272	0.053*
C5	0.5637 (4)	0.2228 (17)	0.1758 (5)	0.054 (2)
H5A	0.5367	0.1944	0.1338	0.064*
C6	0.6199 (4)	0.0727 (17)	0.1829 (5)	0.054 (2)
H6	0.6310	−0.0623	0.1468	0.065*
C7	0.6591 (4)	0.1270 (17)	0.2447 (4)	0.049 (2)
H7	0.6976	0.0283	0.2488	0.058*
C8	0.7935 (3)	0.7027 (15)	0.4244 (4)	0.0365 (17)
C9	0.6886 (3)	0.1868 (15)	0.4895 (4)	0.0383 (18)
H9	0.6667	0.1636	0.4432	0.046*
C10	0.6706 (3)	0.0160 (14)	0.5554 (4)	0.0351 (16)
C11	0.7028 (4)	0.0259 (17)	0.6248 (4)	0.049 (2)
H11	0.7375	0.1461	0.6317	0.058*
C12	0.6825 (4)	−0.1454 (17)	0.6836 (5)	0.053 (2)
H12	0.7030	−0.1408	0.7311	0.063*
C13	0.6313 (3)	−0.3245 (16)	0.6709 (4)	0.0471 (19)
H13	0.6166	−0.4438	0.7093	0.057*
C14	0.6029 (3)	−0.3205 (17)	0.6003 (5)	0.047 (2)
H14	0.5691	−0.4445	0.5914	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N8	0.044 (3)	0.040 (3)	0.033 (3)	0.004 (3)	−0.004 (3)	0.003 (3)
N1	0.044 (3)	0.044 (4)	0.033 (3)	0.003 (3)	−0.006 (3)	−0.004 (3)
N2	0.043 (3)	0.039 (3)	0.034 (4)	−0.002 (3)	−0.003 (3)	−0.001 (3)
N3	0.049 (4)	0.064 (4)	0.041 (4)	0.013 (3)	−0.013 (3)	−0.018 (3)
N4	0.043 (3)	0.050 (4)	0.040 (4)	0.002 (3)	−0.005 (3)	−0.002 (3)
N5	0.048 (4)	0.047 (4)	0.029 (3)	0.001 (3)	−0.002 (3)	−0.003 (3)
N6	0.042 (3)	0.037 (3)	0.032 (4)	−0.001 (3)	−0.003 (2)	−0.007 (3)
N7	0.053 (3)	0.057 (4)	0.038 (4)	0.014 (3)	−0.003 (3)	−0.013 (3)
S1	0.0529 (10)	0.0535 (11)	0.0384 (11)	0.0042 (10)	−0.0040 (9)	−0.0095 (10)
S2	0.0506 (10)	0.0558 (11)	0.0377 (10)	0.0049 (10)	−0.0046 (9)	−0.0140 (10)
C1	0.035 (4)	0.034 (4)	0.037 (4)	−0.006 (3)	0.003 (3)	0.001 (3)
C2	0.040 (4)	0.040 (4)	0.034 (4)	0.000 (3)	−0.003 (3)	0.001 (3)
C3	0.043 (4)	0.033 (4)	0.033 (4)	0.001 (3)	0.003 (3)	−0.001 (3)
C4	0.040 (4)	0.050 (5)	0.041 (4)	0.010 (4)	−0.010 (3)	−0.003 (4)
C5	0.058 (5)	0.061 (5)	0.042 (5)	0.000 (5)	−0.014 (4)	−0.004 (4)
C6	0.070 (5)	0.056 (5)	0.038 (5)	0.003 (4)	0.002 (4)	−0.008 (4)
C7	0.044 (4)	0.058 (5)	0.044 (5)	0.008 (4)	0.005 (4)	−0.002 (4)
C8	0.034 (4)	0.037 (4)	0.038 (4)	−0.010 (3)	0.000 (3)	−0.004 (3)
C9	0.043 (4)	0.039 (4)	0.033 (4)	0.001 (3)	−0.003 (3)	−0.002 (3)

C10	0.039 (4)	0.034 (4)	0.033 (4)	0.000 (3)	−0.005 (3)	0.001 (3)
C11	0.050 (4)	0.056 (5)	0.040 (5)	0.008 (4)	−0.011 (3)	−0.006 (4)
C12	0.060 (5)	0.067 (6)	0.031 (4)	−0.006 (4)	−0.011 (4)	−0.006 (4)
C13	0.048 (4)	0.052 (5)	0.042 (5)	0.001 (4)	0.000 (3)	−0.013 (4)
C14	0.041 (4)	0.050 (5)	0.050 (5)	0.003 (4)	−0.002 (3)	0.003 (4)

Geometric parameters (Å, º)

N8—C14	1.328 (9)	C2—C3	1.450 (9)
N8—C10	1.336 (8)	C2—H2	0.9300
N1—C1	1.354 (8)	C3—C4	1.388 (9)
N1—N2	1.380 (8)	C4—C5	1.367 (10)
N1—H1	0.8600	C4—H4	0.9300
N2—C2	1.278 (8)	C5—C6	1.373 (10)
N3—C1	1.316 (9)	C5—H5A	0.9300
N3—H3A	0.8600	C6—C7	1.372 (10)
N3—H3B	0.8600	C6—H6	0.9300
N4—C7	1.330 (9)	C7—H7	0.9300
N4—C3	1.348 (8)	C9—C10	1.458 (10)
N5—C8	1.347 (8)	C9—H9	0.9300
N5—N6	1.375 (8)	C10—C11	1.379 (9)
N5—H5	0.8600	C11—C12	1.376 (11)
N6—C9	1.267 (9)	C11—H11	0.9300
N7—C8	1.314 (9)	C12—C13	1.382 (10)
N7—H7A	0.8600	C12—H12	0.9300
N7—H7B	0.8600	C13—C14	1.362 (10)
S1—C1	1.679 (7)	C13—H13	0.9300
S2—C8	1.671 (8)	C14—H14	0.9300
C14—N8—C10	117.2 (6)	C4—C5—H5A	120.3
C1—N1—N2	119.9 (6)	C6—C5—H5A	120.3
C1—N1—H1	120.1	C7—C6—C5	118.3 (7)
N2—N1—H1	120.1	C7—C6—H6	120.8
C2—N2—N1	115.5 (6)	C5—C6—H6	120.8
C1—N3—H3A	120.0	N4—C7—C6	123.5 (7)
C1—N3—H3B	120.0	N4—C7—H7	118.2
H3A—N3—H3B	120.0	C6—C7—H7	118.2
C7—N4—C3	118.0 (6)	N7—C8—N5	116.9 (7)
C8—N5—N6	120.7 (6)	N7—C8—S2	124.0 (6)
C8—N5—H5	119.7	N5—C8—S2	119.1 (5)
N6—N5—H5	119.7	N6—C9—C10	121.4 (7)
C9—N6—N5	115.6 (6)	N6—C9—H9	119.3
C8—N7—H7A	120.0	C10—C9—H9	119.3
C8—N7—H7B	120.0	N8—C10—C11	122.6 (7)
H7A—N7—H7B	120.0	N8—C10—C9	114.3 (6)
N3—C1—N1	116.8 (6)	C11—C10—C9	123.1 (7)
N3—C1—S1	124.8 (6)	C12—C11—C10	118.8 (7)
N1—C1—S1	118.5 (5)	C12—C11—H11	120.6

N2—C2—C3	121.5 (6)	C10—C11—H11	120.6
N2—C2—H2	119.2	C11—C12—C13	119.0 (7)
C3—C2—H2	119.2	C11—C12—H12	120.5
N4—C3—C4	121.4 (6)	C13—C12—H12	120.5
N4—C3—C2	114.4 (6)	C14—C13—C12	117.8 (8)
C4—C3—C2	124.2 (6)	C14—C13—H13	121.1
C5—C4—C3	119.3 (7)	C12—C13—H13	121.1
C5—C4—H4	120.4	N8—C14—C13	124.5 (8)
C3—C4—H4	120.4	N8—C14—H14	117.8
C4—C5—C6	119.5 (7)	C13—C14—H14	117.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N8^{i}	0.86	2.18	3.032 (8)	169
N3—H3*B*···S2^{ii}	0.86	2.57	3.417 (6)	168
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Symmetry codes: (i) x, y+1, z; (ii) x−1/2, −y+5/2, z; (iii) x+1/2, −y+5/2, z.