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1-(Pyridin-2-yl)thiourea

Maya Tutughamiarso[a] and Michael Bolte[b]*

[a]Institut für Organische Chemie und Chemische Biologie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany, and [b]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

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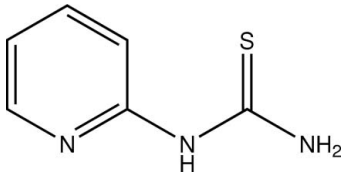
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 13.1.

The title compound, $C_6H_7N_3S$, crystallizes with two essentially planar molecules in the asymmetric unit (r.m.s. deviation for all non-H atoms = 0.055 and 0.006 Å), which are held together by two N—H···S hydrogen bonds. The two molecules are almost identical (r.m.s. deviation for all non-H atoms = 0.066 Å). An intramolecular N—H···N hydrogen bond stabilizes the synperiplanar conformations between the pyridine N atom and the thiocarbonyl C atom, as well as between the pivot C atom of the pyridine ring and the NH_2 group [torsion angles: N—C—N—C = 7.3 (3) and −1.0 (3)°, C—N—C—N = −4.1 (3) and −0.4 (3)°].

Related literature

For related structures, see: Yusof *et al.* (2006) and Liu & Tian (2006).



Experimental

Crystal data

$C_6H_7N_3S$
M_r = 153.21
Monoclinic, $P2_1/c$
a = 14.0116 (13) Å
b = 6.1820 (4) Å
c = 16.8726 (15) Å
β = 97.140 (7)°
V = 1450.2 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 173 (2) K
0.52 × 0.40 × 0.28 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.832, T_{max} = 0.904
11661 measured reflections
2700 independent reflections
2307 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.03
2700 reflections
206 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N61—H61···S62^{i}	0.83 (2)	2.64 (2)	3.4401 (16)	163.3 (19)
N63—H63A···S62′	0.89 (3)	2.55 (2)	3.3383 (16)	148.3 (19)
N63—H63B···N1	0.95 (2)	1.91 (2)	2.664 (2)	134.4 (19)
N61′—H61′···S62	0.87 (2)	2.61 (2)	3.4273 (16)	157.1 (18)
N63′—H63C···N1′	0.86 (2)	2.02 (2)	2.701 (2)	135 (2)
N63′—H63D···S62′^{ii}	0.89 (3)	2.56 (3)	3.4127 (17)	161 (2)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

The authors thank Professor Dr E. Egert for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2476).

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  doi:10.1107/S1600536807057388

supplementary materials

Acta Cryst. (2007). E**63**, o4682 [**doi:10.1107/S1600536807057388**]

1-(Pyridin-2-yl)thiourea

M. Tutughamiarso and M. Bolte

Comment

1-(Pyridin-2-yl)thiourea crystallizes with two essentially planar molecules in the asymmetric unit (r.m.s. deviation for all non-H atoms 0.055 Å and 0.006 Å), which are held together by two N—H···S hydrogen bonds. The two molecules are almost identical (r.m.s. deviation for all non-H atoms 0.066 Å). An intramolecular N—H···N hydrogen bond stabilizes the *syn*-periplanar conformations between the pyridine N atom and the thiocarbonyl C atom, as well as between the C6 atom and the NH_2 group [torsion angle N1—C6—N61—C62: 7.3 (3)°, N1'—C6'—N61'—C62': −1.0 (3)°, C6—N61—C62—N63: −4.1 (3)°, C6'—N61'—C62'—N63': −0.4 (3)°]. The crystal packing shows a network of intermolecular N—H···S hydrogen bonds resulting in corrugated layers.

Experimental

Single crystals of title compound were obtained from recrystallization of the commercially available 1-(pPyridin-2-yl)thiourea from acetonitril at room temperature.

Refinement

All H atoms were initially located by difference Fourier synthesis. Subsequently the positions of those bonded to C atoms were idealized and constrained to ride on their parent atoms with C—H = 0.95Å and fixed individual displacement parameters [U_{iso}(H) = 1.2 U_{eq}(C)]. H atoms bonded to N were refined isotropically.

Figures

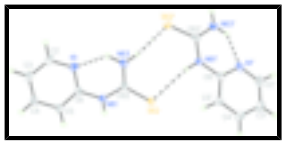

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. Hydrogen bonds shown as dashed lines.

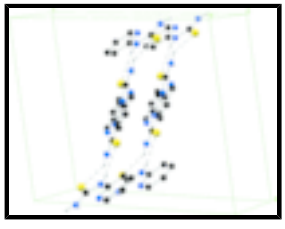

Fig. 2. Partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

1-(Pyridin-2-yl)thiourea

Crystal data

$C_6H_7N_3S$	F_{000} = 640
M_r = 153.21	D_x = 1.403 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 11901 reflections
a = 14.0116 (13) Å	θ = 3.5–25.9º
b = 6.1820 (4) Å	μ = 0.37 mm^{-1}
c = 16.8726 (15) Å	T = 173 (2) K
β = 97.140 (7)º	Block, colourless
V = 1450.2 (2) Å^3	0.52 × 0.40 × 0.28 mm
Z = 8	

Data collection

Stoe IPDS II two-circle diffractometer	2700 independent reflections
Radiation source: fine-focus sealed tube	2307 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.075
T = 173(2) K	θ_{max} = 25.6º
ω scans	θ_{min} = 3.5º
Absorption correction: multi-scan [MULABS (Spek, 2003; Blessing, 1995)]	h = −16→15
T_{min} = 0.832, T_{max} = 0.904	k = −7→7
11661 measured reflections	l = −20→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.3005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.091	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.03	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
2700 reflections	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
206 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.019 (2)
Secondary atom site location: difference Fourier map	

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	0.13558 (11)	0.0118 (2)	0.67619 (8)	0.0223 (3)
C2	0.12387 (15)	−0.1750 (3)	0.71483 (11)	0.0267 (4)
H2	0.1749	−0.2226	0.7533	0.032*
C3	0.04226 (14)	−0.3015 (3)	0.70201 (10)	0.0256 (4)
H3	0.0375	−0.4326	0.7306	0.031*
C4	−0.03333 (14)	−0.2315 (3)	0.64587 (10)	0.0236 (4)
H4	−0.0908	−0.3140	0.6359	0.028*
C5	−0.02313 (13)	−0.0402 (3)	0.60495 (10)	0.0210 (4)
H5	−0.0735	0.0119	0.5668	0.025*
C6	0.06331 (13)	0.0744 (2)	0.62123 (9)	0.0175 (3)
N61	0.07537 (11)	0.2636 (2)	0.57712 (8)	0.0188 (3)
H61	0.0270 (16)	0.303 (3)	0.5476 (12)	0.024 (5)*
C62	0.15552 (12)	0.3890 (3)	0.57543 (9)	0.0169 (3)
S62	0.15173 (3)	0.59971 (7)	0.50991 (2)	0.02136 (15)
N63	0.23412 (11)	0.3401 (3)	0.62421 (9)	0.0239 (3)
H63A	0.2874 (18)	0.420 (4)	0.6260 (13)	0.034 (6)*
H63B	0.2320 (16)	0.220 (3)	0.6586 (13)	0.034 (6)*
N1'	0.40042 (12)	1.2425 (2)	0.49260 (9)	0.0287 (4)
C2'	0.39561 (15)	1.3748 (3)	0.42865 (12)	0.0338 (5)
H2'	0.4304	1.5070	0.4342	0.041*
C3'	0.34342 (15)	1.3303 (3)	0.35574 (11)	0.0333 (5)
H3'	0.3415	1.4296	0.3126	0.040*
C4'	0.29375 (15)	1.1354 (3)	0.34738 (11)	0.0323 (5)
H4'	0.2580	1.0983	0.2977	0.039*
C5'	0.29658 (14)	0.9956 (3)	0.41174 (10)	0.0267 (4)
H5'	0.2626	0.8624	0.4074	0.032*
C6'	0.35137 (12)	1.0571 (3)	0.48370 (10)	0.0212 (4)
N61'	0.35356 (11)	0.9141 (2)	0.54900 (9)	0.0220 (3)
H61'	0.3152 (16)	0.804 (4)	0.5417 (12)	0.027 (5)*
C62'	0.40118 (12)	0.9316 (3)	0.62462 (10)	0.0206 (4)
S62'	0.38933 (3)	0.72820 (7)	0.69093 (3)	0.02639 (16)
N63'	0.45425 (12)	1.1059 (3)	0.64362 (11)	0.0290 (4)
H63C	0.4538 (17)	1.207 (4)	0.6090 (14)	0.035 (6)*

H63D	0.485 (2)	1.118 (4)	0.6931 (16)	0.046 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0221 (8)	0.0209 (7)	0.0232 (7)	0.0018 (6)	0.0004 (6)	0.0045 (6)
C2	0.0319 (10)	0.0243 (9)	0.0239 (9)	0.0054 (8)	0.0037 (7)	0.0066 (7)
C3	0.0371 (11)	0.0168 (8)	0.0251 (9)	0.0022 (8)	0.0121 (8)	0.0025 (7)
C4	0.0315 (10)	0.0180 (8)	0.0227 (9)	−0.0058 (7)	0.0081 (7)	−0.0030 (6)
C5	0.0245 (9)	0.0188 (8)	0.0193 (8)	−0.0015 (7)	0.0010 (7)	−0.0018 (6)
C6	0.0216 (9)	0.0150 (8)	0.0162 (7)	0.0006 (7)	0.0037 (6)	−0.0015 (6)
N61	0.0175 (8)	0.0182 (7)	0.0193 (7)	−0.0014 (6)	−0.0032 (6)	0.0032 (5)
C62	0.0174 (8)	0.0173 (8)	0.0162 (7)	−0.0003 (6)	0.0025 (6)	−0.0026 (6)
S62	0.0198 (2)	0.0209 (2)	0.0225 (2)	−0.00443 (16)	−0.00109 (17)	0.00586 (15)
N63	0.0179 (8)	0.0251 (8)	0.0271 (8)	−0.0034 (7)	−0.0033 (6)	0.0059 (6)
N1'	0.0265 (9)	0.0281 (8)	0.0306 (8)	−0.0096 (7)	0.0003 (7)	0.0047 (6)
C2'	0.0342 (12)	0.0292 (10)	0.0387 (11)	−0.0077 (9)	0.0071 (9)	0.0089 (8)
C3'	0.0351 (11)	0.0375 (11)	0.0286 (10)	−0.0005 (9)	0.0093 (8)	0.0122 (8)
C4'	0.0351 (11)	0.0404 (11)	0.0207 (9)	−0.0017 (9)	0.0006 (8)	0.0043 (8)
C5'	0.0269 (10)	0.0306 (10)	0.0221 (9)	−0.0069 (8)	0.0008 (7)	0.0022 (7)
C6'	0.0161 (9)	0.0249 (9)	0.0225 (9)	−0.0026 (7)	0.0019 (7)	0.0019 (7)
N61'	0.0216 (8)	0.0226 (8)	0.0204 (7)	−0.0082 (6)	−0.0035 (6)	0.0023 (6)
C62'	0.0146 (8)	0.0248 (9)	0.0213 (8)	0.0007 (7)	−0.0014 (6)	−0.0012 (6)
S62'	0.0258 (3)	0.0291 (3)	0.0218 (2)	−0.00563 (19)	−0.00690 (18)	0.00572 (17)
N63'	0.0285 (9)	0.0294 (9)	0.0261 (8)	−0.0099 (7)	−0.0089 (7)	0.0028 (7)

Geometric parameters (Å, °)

N1—C6	1.342 (2)	N1'—C6'	1.335 (2)
N1—C2	1.346 (2)	N1'—C2'	1.349 (2)
C2—C3	1.380 (3)	C2'—C3'	1.379 (3)
C2—H2	0.9500	C2'—H2'	0.9500
C3—C4	1.399 (3)	C3'—C4'	1.390 (3)
C3—H3	0.9500	C3'—H3'	0.9500
C4—C5	1.386 (2)	C4'—C5'	1.385 (3)
C4—H4	0.9500	C4'—H4'	0.9500
C5—C6	1.401 (2)	C5'—C6'	1.406 (2)
C5—H5	0.9500	C5'—H5'	0.9500
C6—N61	1.408 (2)	C6'—N61'	1.410 (2)
N61—C62	1.368 (2)	N61'—C62'	1.369 (2)
N61—H61	0.83 (2)	N61'—H61'	0.87 (2)
C62—N63	1.325 (2)	C62'—N63'	1.326 (2)
C62—S62	1.7051 (16)	C62'—S62'	1.7047 (18)
N63—H63A	0.89 (3)	N63'—H63C	0.86 (2)
N63—H63B	0.95 (2)	N63'—H63D	0.89 (3)
C6—N1—C2	117.08 (15)	C6'—N1'—C2'	117.17 (16)
N1—C2—C3	123.97 (17)	N1'—C2'—C3'	124.12 (18)
N1—C2—H2	118.0	N1'—C2'—H2'	117.9

C3—C2—H2	118.0	C3'—C2'—H2'	117.9
C2—C3—C4	118.29 (16)	C2'—C3'—C4'	117.84 (17)
C2—C3—H3	120.9	C2'—C3'—H3'	121.1
C4—C3—H3	120.9	C4'—C3'—H3'	121.1
C5—C4—C3	119.01 (17)	C5'—C4'—C3'	119.77 (18)
C5—C4—H4	120.5	C5'—C4'—H4'	120.1
C3—C4—H4	120.5	C3'—C4'—H4'	120.1
C4—C5—C6	118.31 (16)	C4'—C5'—C6'	117.90 (17)
C4—C5—H5	120.8	C4'—C5'—H5'	121.1
C6—C5—H5	120.8	C6'—C5'—H5'	121.1
N1—C6—C5	123.31 (15)	N1'—C6'—C5'	123.19 (16)
N1—C6—N61	118.37 (15)	N1'—C6'—N61'	119.29 (15)
C5—C6—N61	118.32 (15)	C5'—C6'—N61'	117.52 (15)
C62—N61—C6	129.40 (15)	C62'—N61'—C6'	129.79 (15)
C62—N61—H61	115.7 (15)	C62'—N61'—H61'	114.5 (14)
C6—N61—H61	114.9 (15)	C6'—N61'—H61'	115.4 (14)
N63—C62—N61	118.61 (15)	N63'—C62'—N61'	118.90 (16)
N63—C62—S62	122.24 (13)	N63'—C62'—S62'	122.56 (14)
N61—C62—S62	119.14 (12)	N61'—C62'—S62'	118.55 (13)
C62—N63—H63A	121.6 (14)	C62'—N63'—H63C	118.2 (15)
C62—N63—H63B	118.2 (14)	C62'—N63'—H63D	118.9 (16)
H63A—N63—H63B	120.2 (19)	H63C—N63'—H63D	123 (2)
C6—N1—C2—C3	−1.0 (3)	C6'—N1'—C2'—C3'	0.2 (3)
N1—C2—C3—C4	−0.4 (3)	N1'—C2'—C3'—C4'	−0.9 (3)
C2—C3—C4—C5	0.6 (3)	C2'—C3'—C4'—C5'	1.1 (3)
C3—C4—C5—C6	0.6 (2)	C3'—C4'—C5'—C6'	−0.7 (3)
C2—N1—C6—C5	2.3 (2)	C2'—N1'—C6'—C5'	0.3 (3)
C2—N1—C6—N61	−176.99 (15)	C2'—N1'—C6'—N61'	−179.53 (17)
C4—C5—C6—N1	−2.1 (3)	C4'—C5'—C6'—N1'	−0.1 (3)
C4—C5—C6—N61	177.19 (15)	C4'—C5'—C6'—N61'	179.78 (17)
N1—C6—N61—C62	7.3 (3)	N1'—C6'—N61'—C62'	−1.0 (3)
C5—C6—N61—C62	−172.06 (16)	C5'—C6'—N61'—C62'	179.15 (18)
C6—N61—C62—N63	−4.1 (3)	C6'—N61'—C62'—N63'	0.4 (3)
C6—N61—C62—S62	174.97 (13)	C6'—N61'—C62'—S62'	−179.88 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N61—H61···S62^{i}	0.83 (2)	2.64 (2)	3.4401 (16)	163.3 (19)
N63—H63A···S62'	0.89 (3)	2.55 (2)	3.3383 (16)	148.3 (19)
N63—H63B···N1	0.95 (2)	1.91 (2)	2.664 (2)	134.4 (19)
N61'—H61'···S62	0.87 (2)	2.61 (2)	3.4273 (16)	157.1 (18)
N63'—H63C···N1'	0.86 (2)	2.02 (2)	2.701 (2)	135 (2)
N63'—H63D···S62'^{ii}	0.89 (3)	2.56 (3)	3.4127 (17)	161 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1

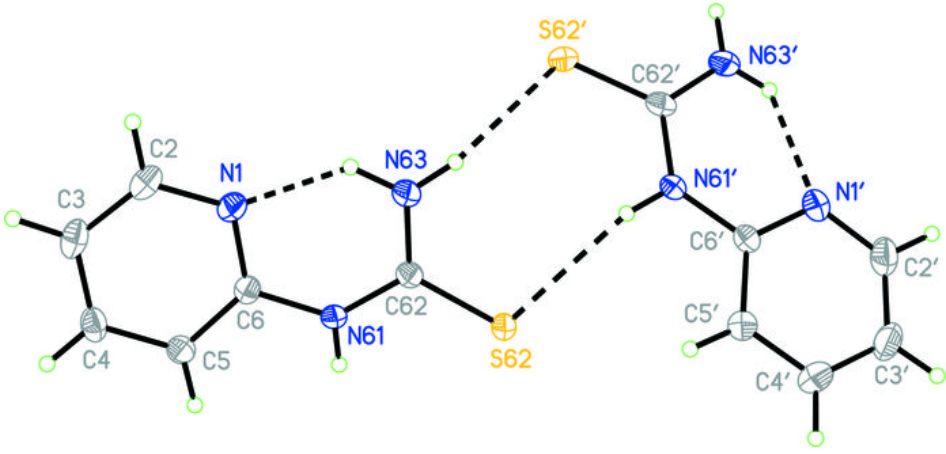

Fig. 2