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# 1-Cyclopropylcarbonyl-3-(2-pyridyl)thiourea

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In the title compound, $C_{10}H_{11}N_3OS$, the pyridine ring makes a dihedral angle of 86.8 (3)° with the cyclopropane ring. The amide group and the pyridine are linked by an intermolecular N—H···N hydrogen bond.

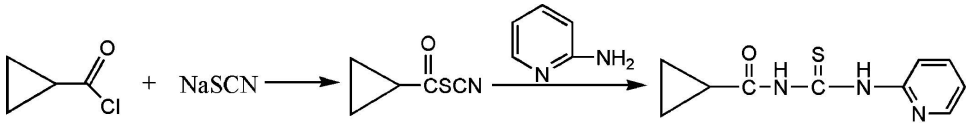
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.038
$wR$ factor = 0.108
Data-to-parameter ratio = 14.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

## Comment

Cyclopropane is a structural unit found in several molecules with biological activity; for example, ciprofloxacin is an excellent bactericide. 1-Aminocyclopropane-1-carboxylic acid (ACC) is known to be the biochemical precursor of the plant hormone ethylene in a process catalysed by the ethylene-forming enzyme (EFE) (Adams *et al.*, 1979). 2,2-Dichloro-3,3-dimethylcyclopropanecarboxylic acid is an effective inducer against the rice blast fungus (Langcake *et al.*, 1983). Thus, it is very important to synthesize new compounds containing cyclopropane, and to study their biological activities. Acyl thiourea derivatives are known to have biological activity; for example, they have been used as bactericides, fungicides and insecticides in many plants (Kamala & Rao, 1989), and a pyridine ring is often used as an active component in pesticide discovery (Elbert *et al.*, 2000). The title compound, (I), contains all three components (cyclopropane, thiourea and pyridine) and may show some insecticidal activity.




(I)

The molecular structure of (I) is shown in Fig. 1. The dihedral angle between the N1-pyridine and C8-cyclopropane rings is 86.8 (3)°. Amide atom N2 and the carbonyl O atom are linked by an intramolecular N—H···O hydrogen bond, forming a six-membered ring. The crystal packing (Fig. 2) is stabilized by van der Waals interactions and intermolecular N—H···N hydrogen bonds which run along the crystallographic [001] direction (Fig. 3 and Table 1).

## Experimental

A solution of cycloprpopanecarbonyl chloride (4.5 mmol, 0.47 g) in anhyrous acetonitrile (3 ml) was added dropwise to a solution of NaSCN (6 mmol, 0.49 g) in anhydrous acetonitrile (10 ml), at room temperature. The reaction mixture was kept at room temperature for 30 min and then at 333 K for 3 h. The solution was cooled, filtered and concentrated to about 4 ml. The residue was added dropwise to a solution of 2-aminopyridine (4.5 mmol, 0.42 g) in anhydrous acetonitrile (8 ml) at room temperature. The reaction mixture was heated

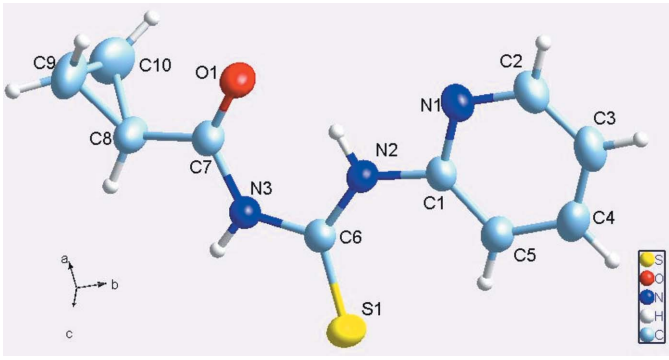



**Figure 1**
View of the asymmetric unit of (I), with displacement ellipsoids drawn at the 40% probability level.

to reflux for 5 h and then was cooled to 278 K overnight to give a solid product. This was recrystallized from acetonitrile and give yellow blocks (m.p. 417–418 K) suitable for an X-ray study. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 12.97 (*s*, 1H, CONHCS), 9.14 (*s*, 1H, CSNH), 8.73 (*d*, 1H, H2), 8.39 (*d*, 1H, H5), 7.74 (*T*, 1H, H3), 7.13 (*T*, 1H, H4), 1.56 (*m*, 1H, H8), 1.18 (*m*, 2H, H10), 1.00 (*m*, 2H, H9). Analysis calculated for $C_{10}H_{11}N_3OS$: C 54.30, H 4.98, N 19.00; found: C 54.52, H 5.02, N 19.13%.

*Crystal data*

$C_{10}H_{11}N_3OS$
$M_r$ = 221.28
Monoclinic, $P2_1/c$
$a$ = 8.457 (3) Å
$b$ = 12.178 (4) Å
$c$ = 10.998 (4) Å
$\beta$ = 96.958 (4)°
$V$ = 1124.4 (7) Å$^3$
$Z$ = 4
$D_x$ = 1.307 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 293 (2) K
Block, colorless
0.34 × 0.32 × 0.21 mm

*Data collection*

Bruker APEX-II CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.970, $T_{max}$ = 0.983
5822 measured reflections
1984 independent reflections
1390 reflections with $I > \sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
$S$ = 1.01
1984 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.2411P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0045 (6)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2′···O1 | 0.86 | 1.92 | 2.655 (2) | 142 |
| N3—H3′···N1$^{i}$ | 0.86 | 2.15 | 2.997 (2) | 171 |

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

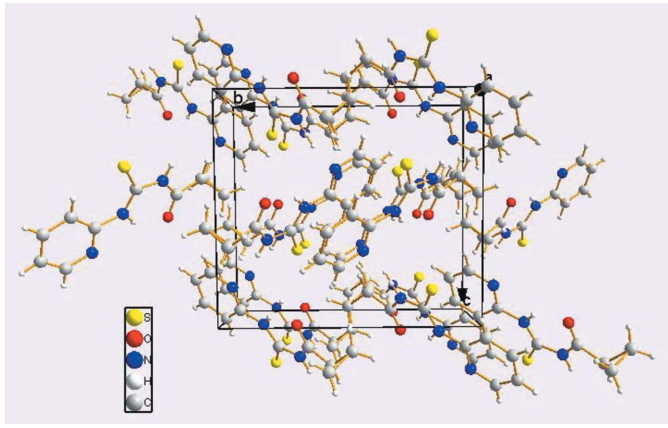



**Figure 2**
The molecular packing of (I), viewed along the *a* axis.

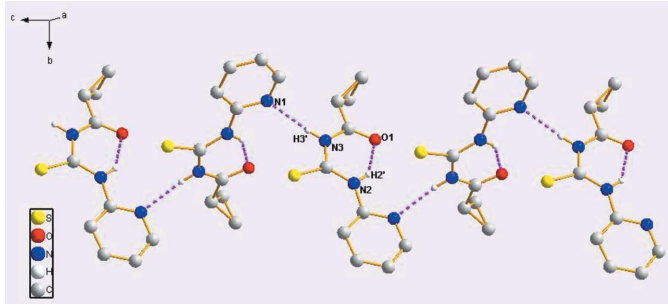



**Figure 3**
View of the hydrogen bonding (dashed lines) in (I). H atoms bonded to C atoms have been omitted for clarity.

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å and N—H = 0.86 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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## References

Adams, D. O. & Yang, S. F. (1979). *Proc. Natl Acad. Sci.* **76**, 170–174.
Bruker (1997). *SAINT*, *SADABS* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Elbert, A., Erdelen, C., Kuhnhold, J., Nauen, R., Schmidt, H. W. & Hattori, Y. (2000). *BCPC Conf. Pests Dis.* **1**, 21–26.
Kamala, K. & Rao, P. J. (1989). *Synth. Commun.* **19**, 2621–2625.
Langcake, P., Cartwright, D. W. & Ride, J. P. (1983). *The Dichlorocyclopropanes and Other Fungicides with Indirect Mode of Action.* In *Systemische Verbindungen und antifungale Verbindungen*, edited by H. Lyr & C. Polter, pp. 199–210. Berlin: Akademie-Verlag.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.