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## Key indicators

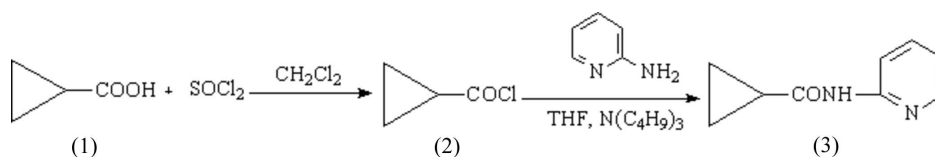
Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.045  
 $wR$  factor = 0.114  
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*N*-(2-Pyridyl)cyclopropanecarboxamideThe title compound,  $\text{C}_9\text{H}_{10}\text{N}_2\text{O}$ , crystallizes with two molecules per asymmetric unit. The crystal packing is stabilized by van der Waals interactions and intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen-bond interactions.

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## Comment

Cyclopropane is a structural unit which has several biological activities; 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). The main active component of cilastatin is (+)-(*S*)-2,2-dimethylcyclopropanecarboxamide (Mu, 1992; Xu *et al.*, 1994). Thus, it is very important to synthesize other new compounds containing cyclopropane, and study their biological activities. The action of thionyl chloride on cyclopropanecarboxylic acid, (1), at room temperature afforded cyclopropanecarbonyl chloride, (2), which when condensed with 2-aminopyridine gave the title compound, (3). This compound was characterized by  $^1\text{H}$  NMR and elemental analysis, and its crystal structure is reported here.



The title compound, (3), crystallizes with two molecules per asymmetric unit (Fig. 1). The dihedral angle between the N1-pyridine and C7-cyclopropane rings is  $77.1(1)^\circ$ , whereas the dihedral angle between the N3-pyridine and C16-cyclo-

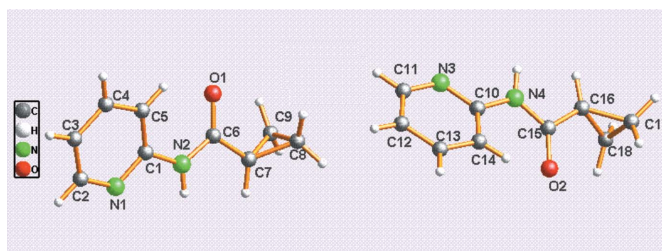
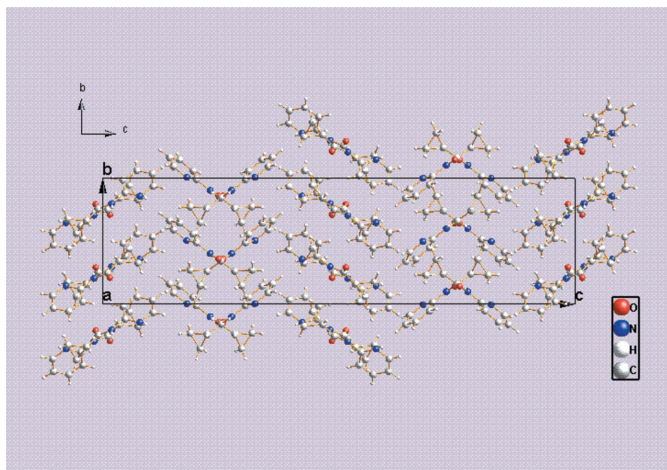
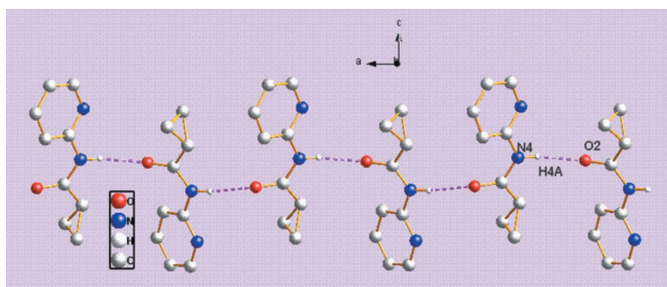


Figure 1

View of the asymmetric unit of (3), with displacement ellipsoids drawn at the 40% probability level.



**Figure 2**  
The molecular packing of (3), viewed along the *a* axis. H atoms bonded to C atoms have been omitted for clarity.



**Figure 3**  
View of the hydrogen bonding (dashed lines) in (3).

propane rings is  $73.89 (122)^\circ$ . For the similar compound 3-[(*E*)-2-chloro-3,3,3-trifluoroprop-1-enyl]-2,2-dimethyl-*N*-(3-pyridyl)cyclopropanecarboxamide acetone hemisolvate, (4) (Liu *et al.*, 2006), the dihedral angle between the pyridine and cyclopropane rings is  $73.0 (3)^\circ$ .

The crystal packing (Fig. 2) is stabilized by van der Waals interactions and intermolecular N—H $\cdots$ O hydrogen bonding, forming infinite chains (Fig. 3 and Table 1). Whereas, in (3), the hydrogen bonding involves amide NH groups and carbonyl O atoms, in (4) the hydrogen bonding involves amide NH groups and pyridine N atoms.

## Experimental

To a solution of (1) (2 mmol, 0.17 g) in dichloromethane (10 ml) was added dropwise a solution of thionyl chloride (8 mmol, 0.6 ml) in dichloromethane (2 ml) at room temperature. The reaction mixture was kept at this temperature for 1 h. The solution was concentrated to give cyclopropanecarbonyl chloride, (2). To a solution of 2-aminopyridine (2 mmol, 0.19 g) in tetrahydrofuran (10 ml), was added triethylamine (3 mmol, 0.4 ml); cyclopropanecarbonyl chloride, (2), in tetrahydrofuran (5 ml) was then added dropwise at 273 K. The reaction mixture was kept at room temperature for 2–3 h, then filtered and concentrated. The residue was separated by silica-gel chromatography (eluant petroleum ether–AcOEt 3:1) to afford the

title compound, (3). Colourless single crystals were grown from a solution of AcOEt–cyclohexane (1:4).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.37 (*d*, 1H, H2), 8.21 (*d*, 1H, H5), 7.87 (*T*, 1H, H3), 7.13 (*T*, 1H, H4), 1.74 (*m*, 1H, H7), 1.13 (*m*, 2H, H9), 0.96 (*m*, 2H, H8). Analysis calculated for  $\text{C}_9\text{H}_{10}\text{N}_2\text{O}$ : C 66.70, H 6.19, N 17.24; found: C 66.67, H 6.17, N 17.28%.

## Crystal data

$\text{C}_9\text{H}_{10}\text{N}_2\text{O}$	$Z = 16$
$M_r = 162.19$	$D_x = 1.255 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 9.475 (4) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 9.844 (4) \text{ \AA}$	$T = 294 (2) \text{ K}$
$c = 36.821 (15) \text{ \AA}$	Block, colorless
$V = 3434 (2) \text{ \AA}^3$	$0.35 \times 0.32 \times 0.28 \text{ mm}$

## Data collection

Bruker APEX-II CCD area-detector diffractometer	17436 measured reflections
$\varphi$ and $\omega$ scans	3019 independent reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	1512 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.970$ , $T_{\max} = 0.983$	$R_{\text{int}} = 0.069$
	$\theta_{\max} = 25.0^\circ$

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.02$	$\Delta\rho_{\max} = 0.15 \text{ e \AA}^{-3}$
3019 reflections	$\Delta\rho_{\min} = -0.13 \text{ e \AA}^{-3}$
218 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0045 (6)

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2A $\cdots$ O1 <sup>i</sup>	0.86	2.00	2.836 (2)	165
N4—H4A $\cdots$ O2 <sup>ii</sup>	0.86	2.12	2.972 (2)	172

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

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.98  $\text{\AA}$  and N—H = 0.86  $\text{\AA}$ . For all H atoms,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

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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