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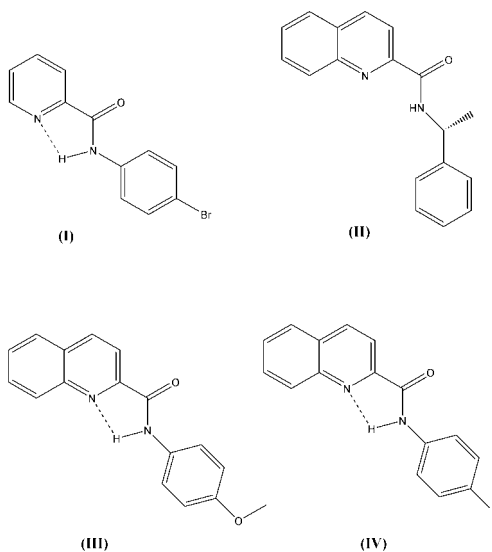
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## Key indicators

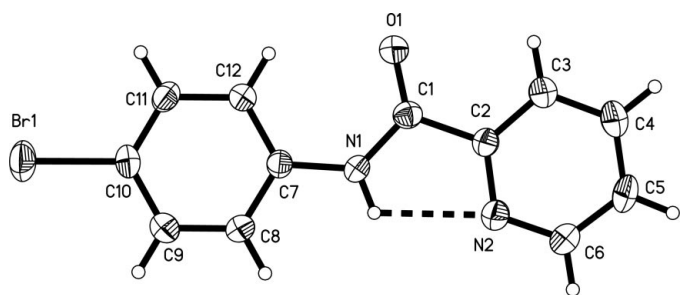
Single-crystal X-ray study  
T = 294 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
R factor = 0.041  
wR factor = 0.080  
Data-to-parameter ratio = 17.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**N-(4-Bromophenyl)pyridine-2-carboxamide**In the title compound,  $\text{C}_{12}\text{H}_9\text{BrN}_2\text{O}$ , (I), the pyridyl and bromophenyl rings are almost coplanar. There is an intramolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bond between the pyridine N atom and the amide N atom [ $\text{N}\cdots\text{N} = 2.657(3) \text{ \AA}$  and  $\text{N}-\text{H}\cdots\text{N} = 112.6^\circ$ ].

## Comment

It has been shown that the previously reported ligands (II), (III) and (IV) (Yang *et al.*, 2001; Qi *et al.*, 2003*a,b*) easily form  $\text{Ru}^{\text{III}}$  complexes *via* the coordination of the pyridine and amide N atoms. However, these  $\text{Ru}^{\text{III}}$  complexes are difficult to crystallize and this may be due to the steric effect of the bulky quinolyl ring. Therefore, ligand (I), with less steric hindrance of the pyridine ring, was prepared. We expect that it will be easier to form metal complexes of this ligand and to grow single crystals of these complexes for X-ray analysis.The pyridyl and bromophenyl rings of (I) are almost coplanar, forming a dihedral angle of  $2.4(1)^\circ$ . The amide group is rotated out of the bromophenyl and pyridyl ring planes, with dihedral angles of  $1.5(1)$  and  $1.2(1)^\circ$ , respectively. There is an intramolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bond between the pyridine N and amide N atoms (see Table 1). The title compound has been found to be an acaricide for control of plant pest mites (Lettau *et al.*, 1982).

## Experimental

The title compound was synthesized from 2-pyridinecarboxylic acid and 4-bromoaniline according to the procedure of Ray *et al.* (1997). The crystal used for data collection was obtained by slow evaporation from a saturated ethanol/water solution at room temperature.Received 28 January 2003  
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**Figure 1**  
The molecular structure of (I), showing ellipsoids at the 30% probability level.

#### Crystal data

$C_{12}H_9BrN_2O$	$Z = 2$
$M_r = 277.12$	$D_x = 1.662 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 6.2634 (11) \text{ \AA}$	Cell parameters from 1232 reflections
$b = 8.2355 (15) \text{ \AA}$	$\theta = 1\text{--}27.5^\circ$
$c = 10.9828 (18) \text{ \AA}$	$\mu = 3.69 \text{ mm}^{-1}$
$\alpha = 88.282 (4)^\circ$	$T = 294 (2) \text{ K}$
$\beta = 87.215 (4)^\circ$	Prism, yellow
$\gamma = 78.268 (3)^\circ$	$0.26 \times 0.24 \times 0.18 \text{ mm}$
$V = 553.91 (17) \text{ \AA}^3$	

#### Data collection

Bruker SMART CCD area-detector diffractometer	2508 independent reflections
$\varphi$ and $\omega$ scans	1399 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.018$
$T_{\text{min}} = 0.447$ , $T_{\text{max}} = 0.557$	$\theta_{\text{max}} = 27.5^\circ$
3649 measured reflections	$h = -8 \rightarrow 8$
	$k = -10 \rightarrow 9$
	$l = -11 \rightarrow 14$

#### Refinement

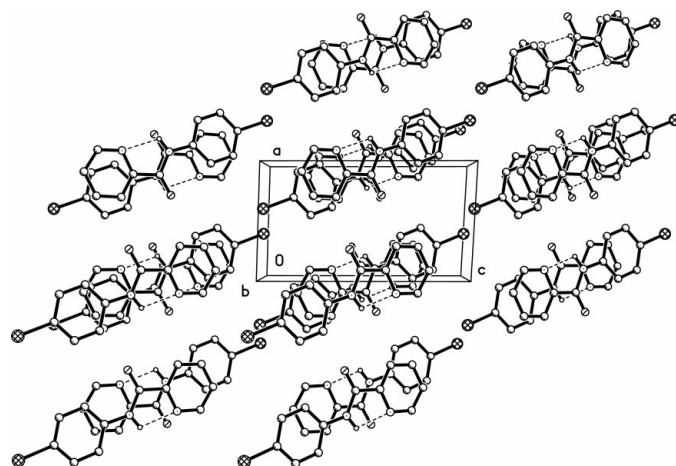
Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
$wR(F^2) = 0.080$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2508 reflections	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
145 parameters	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$

**Table 1**

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$N1\text{--}H1A\cdots N2$	0.86	2.20	2.657 (3)	113

All H atoms were included in calculated positions, with C—H distances of 0.93  $\text{\AA}$  and an N—H distance of 0.86  $\text{\AA}$ . They were then



**Figure 2**

The molecular packing, viewed along the  $b$  axis.

included in the refinement in riding-motion approximation, with  $U_{\text{iso}} = 1.2U_{\text{eq}}$  of the carrier atom.

Data collection: SMART (Siemens, 1995); cell refinement: SMART; data reduction: SAINT (Siemens, 1995) and SHELXTL-NT (Siemens, 1995); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-NT; software used to prepare material for publication: SHELXTL-NT.

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