Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(Dibenzoylamino)pyridine

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.086
Data-to-parameter ratio = 8.2

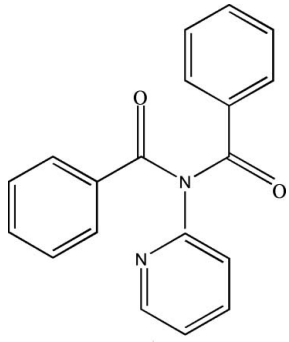
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 16 March 2006
Accepted 8 April 2006

The title compound, $C_{19}H_{14}N_2O_2$, is a highly effective nematicide. No inter- or intramolecular hydrogen bonds are observed in the crystal structure.

Comment

The title compound, (I), was synthesized and tested *in vitro* and *in vivo* on *Meloidogyne incognita* at 10 mg ml^{-1} concentration. The compound reduced nematode infestation of cowpea plants significantly and improved their growth. Treatment by soil drench was more effective than by foliar spray (Roy *et al.*, 1993). In the present paper, we report the crystal structure of (I).



(I)

The title compound crystallizes in the orthorhombic space group $P2_12_12_1$, with one molecule in the asymmetric unit (Fig. 1). The N1—C15—C16—C17 torsion angle is 179.63 (17)° and the N1—C8—C9—C10 torsion angle is 149.54 (17)°. The O1—C7—N1—C8 torsion angle is −18.6 (2)° and the O2—C8—N1—C7 torsion angle is 138.92 (17)°. No inter- or intramolecular hydrogen bonds are observed.

Experimental

Compound (I) was prepared from 2-aminopyridine (2.45 g) and benzoyl chloride (2 ml) in tetrahydrofuran (50 ml) solution at 313 K by stirring for 12 h. The melting point is 441.2 K (Protiva *et al.*, 1950). Colourless block-shaped single crystals suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{19}H_{14}N_2O_2$
M_r = 302.32
Orthorhombic, $P2_12_12_1$
a = 9.0343 (18) Å
b = 9.2051 (18) Å
c = 19.152 (4) Å
V = 1592.7 (5) Å^3
Z = 4
D_x = 1.261 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
Block, colourless
0.42 × 0.41 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	13101 measured reflections
φ or ω scans	1708 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1580 reflections with $I > 2\sigma(I)$
$T_{min} = 0.966$, $T_{max} = 0.982$	$R_{int} = 0.028$
	$\theta_{max} = 25.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.0123P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.086$	$\Delta\rho_{max} = 0.10$ e Å^{-3}
$S = 1.16$	$\Delta\rho_{min} = -0.11$ e Å^{-3}
1708 reflections	Extinction correction: *SHELXL97*
209 parameters	Extinction coefficient: 0.016 (3)
H-atom parameters constrained	

H atoms were placed in calculated positions and constrained to ride on their parent atoms with distances C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the SRCICT of Tianjin University for financial support.

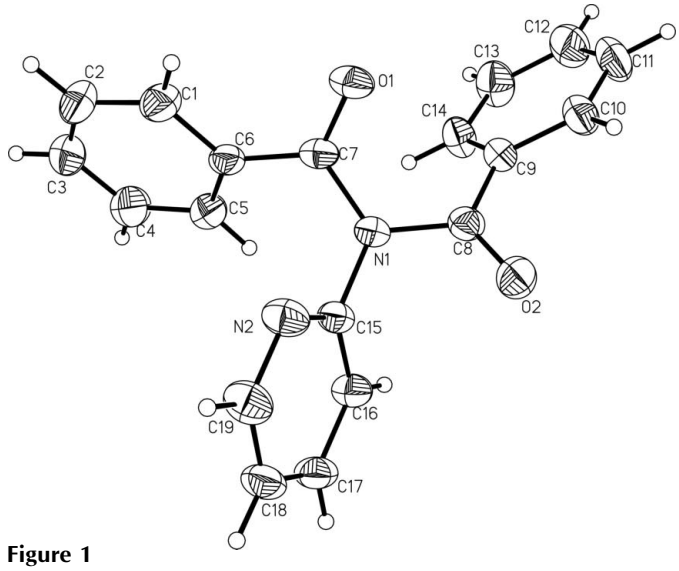


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

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