organic papers

1-Acetyl-5-(2,6-dichlorophenyl)-3-(2-naphthyl)-2-pyrazoline

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Key indicators

Single-crystal X-ray study
$T = 294$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.109
Data-to-parameter ratio = 16.1

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

In the title compound, $C_{21}H_{16}Cl_2N_2O$, the pendant benzene ring and the naphthalene ring system make dihedral angles of 82.9 (3) and 6.7 (3)°, respectively, with the central pyrazoline ring.

Comment

The title compound, (I) (Fig. 1), was prepared and structurally characterized as part of our ongoing studies (Lu *et al.*, 2006) of pyrazoline derivatives.


(I)
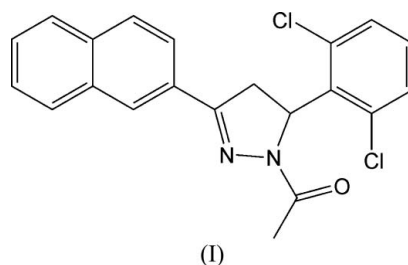
The pendant C1–C6 benzene ring and the C10–C19 naphthalene ring system make dihedral angles of 82.9 (3) and 6.7 (3)°, respectively, with the N1/N2/C7/C8/C9 pyrazoline ring. The C1- and C10-containing ring systems are inclined to each other at an angle of 80.6 (3)°. The molecule of (I) is chiral; in the arbitrarily chosen asymmetric unit, atom C7 has an *R* configuration, but crystal symmetry generates a racemic mixture.

In the crystal structure of (I), molecules are linked by weak C—H···O interactions (Table 1 and Fig. 2) into inversion-generated dimeric pairs.

Experimental

A mixture of 3-(2,6-dichlorophenyl)-1-(2-naphthyl)prop-2-en-1-one (5.0 mmol), hydrazine hydrate (25.0 mmol) and acetic acid (30 ml)
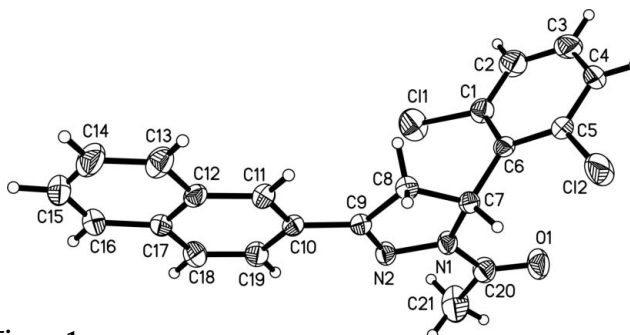
Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

was heated at reflux for 5 h, then poured on to crushed ice. The resulting precipitate was separated by filtration, washed with water, and crystallized from trichloromethane–methanol (1:1) to obtain the title compound. The title compound (40 mg) was dissolved in a mixture of trichloromethane (10 ml) and methanol (10 ml) and the solution was kept at room temperature for 10 d. Natural evaporation of the solution gave colourless crystals of (I) suitable for X-ray analysis (m.p. 513–514 K).

Crystal data

$C_{21}H_{16}Cl_2N_2O$	$Z = 4$
$M_r = 383.26$	$D_x = 1.357$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 10.749$ (2) Å	$\mu = 0.36$ mm^{-1}
$b = 12.763$ (3) Å	$T = 294$ (2) K
$c = 14.629$ (3) Å	Block, colorless
$\beta = 110.798$ (3)°	$0.26 \times 0.24 \times 0.20$ mm
$V = 1876.1$ (7) Å^3	

Data collection

Bruker SMART CCD diffractometer	10324 measured reflections
	3817 independent reflections
ω scans	2170 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	$R_{int} = 0.054$
	$\theta_{max} = 26.4°$
$T_{min} = 0.913$, $T_{max} = 0.932$	

Refinement

|	
Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.4418P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.02$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
3817 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
237 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.0404 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^i	0.93	2.57	3.359 (4)	143

Symmetry code: (i) $-x + 1, -y, -z$.

All H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).
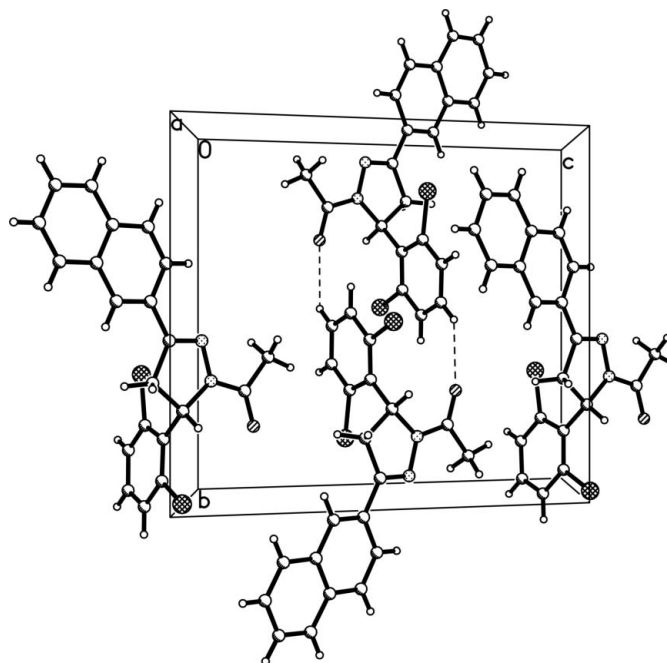
Figure 2
Part of the crystal structure of (I), showing C—H···O interactions as dashed lines.

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, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SMART* (Version 5.01), *SAINT* (Version 5.01), *SADABS* and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Lu, Z.-K., Yu, J.-F. & Huang, P.-M. (2006). *Acta Cryst.* E**62**, o5755–o5756.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.