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3-Cyano-6-methyl-4-(2-naphthylethenyl)-1-benzopyran-2-one

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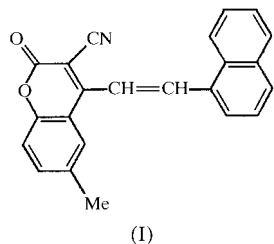
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In the title compound, C₂₃H₁₅NO₂, the naphthyl unit is planar and the benzopyran unit is nearly planar. These two moieties are inclined at an angle of 9.10 (6)° with respect to one another.

Comment

Many derivatives of benzopyrans are found to possess medicinal and biological activities (Malhotra *et al.*, 1997). In order to study the activity of the title compound, (I), an X-ray structure analysis was undertaken. The naphthyl unit is planar with a maximum deviation of −0.037 (2) Å for the C21 atom. The benzopyran unit is nearly planar; torsion angles: O1—C2—C3—C4 −8.9 (3), C2—C3—C4—C10 7.8 (3), C3—C4—C10—C9 −1.1 (3), C4—C10—C9—O1 −4.5 (3), C10—C9—O1—C2 −3.4 (3) and C9—O1—C2—C3 3.0 (3)°. The dihedral angle between the benzopyran and naphthyl rings is 9.10 (6)°. As a result, there is conjugation which is evident from the alternate single and double bonds: O10=C2 1.202 (3), C2—C3 1.456 (3), C3=C4 1.370 (3), C4—C14 1.464 (3), C14=C15 1.333 (3), C15—C23 1.464 (3), C23=C22 1.367 (3), C22—C21 1.411 (3), C21=C20 1.357 (4) and C20—C25 1.400 (4) Å. No unusual bond lengths or angles were observed (Allen *et al.*, 1987).



Experimental

A mixture of 3-cyano-4,6-dimethyl-1-benzopyran-2-one (0.01 mol) and 1-naphthaldehyde (0.01 mol) was dissolved in chloroform

(140 ml) and a few drops of piperidine were added as a catalyst. The mixture was heated with stirring for 13–14 h. After evaporation, the solid residue obtained was recrystallized from dimethylformamide to give dark-yellow crystals (m.p. 514 K; yield 49%).

Crystal data

C₂₃H₁₅NO₂
M_r = 337.36
Monoclinic, P2₁/c
a = 7.814 (5) Å
b = 11.561 (3) Å
c = 18.580 (7) Å
β = 101.96 (4)°
V = 1642.0 (13) Å³
Z = 4

D_x = 1.365 Mg m^{−3}
Mo Kα radiation
Cell parameters from 25 reflections
θ = 2–25°
μ = 0.087 mm^{−1}
T = 293 (2) K
Rectangular, dark yellow
0.15 × 0.12 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.974, T_{max} = 0.994
3103 measured reflections
2878 independent reflections
2095 reflections with I > 2σ(I)

R_{int} = 0.024
θ_{max} = 25°
h = 0 → 9
k = 0 → 13
l = −22 → 21
3 standard reflections every 100 reflections
frequency: 150 min
intensity decay: none

Refinement

Refinement on F²
R[F² > 2σ(F²)] = 0.042
wR(F²) = 0.144
S = 0.831
2878 reflections
238 parameters
H-atom parameters constrained

w = 1/[σ²(F_o²) + (0.0935P)² + 0.9948P]
where P = (F_o² + 2F_c²)/3
(Δ/σ)_{max} = 0.003
Δρ_{max} = 0.17 e Å^{−3}
Δρ_{min} = −0.19 e Å^{−3}

Table 1

Selected geometric parameters (Å, °).

O1—C2	1.352 (3)	C9—C8	1.374 (3)
O1—C9	1.378 (3)	C3—C4	1.370 (3)
C10—C9	1.397 (3)	C3—C2	1.456 (3)
C10—C5	1.399 (3)	O10—C2	1.202 (3)
C10—C4	1.446 (3)	C12—N12	1.139 (3)
C2—O1—C9—C8	−177.5 (2)	C9—O1—C2—C3	3.0 (3)
C2—O1—C9—C10	3.4 (3)	C4—C3—C2—O1	−8.9 (3)
C5—C10—C9—C8	−2.1 (3)	C10—C5—C6—C13	−178.4 (2)
C4—C10—C9—O1	−4.5 (3)	C8—C7—C6—C5	−1.7 (3)
C9—C10—C4—C3	−1.1 (3)		

The title structure was solved by *DIRDIF* methods taking naphthalene coordinates from *DIRDIF ORBASE* (*DIRDIF96*; Beurskens *et al.*, 1996). All H atoms were located from difference Fourier maps and were included in the structure-factor calculations with isotropic displacement parameters equal to 1.1U_{eq} of the carrier atom, but the parameters were not refined (Sheldrick, 1997). The geometrical calculations were performed using *PARST* (Nardelli, 1996).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *DIRDIF96* (Beurskens *et al.*, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

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