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3-Cyano-4-[2-(4-methoxyphenyl)ethenyl]-6-methyl-2*H*-1-benzopyran-2-one

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Key indicators

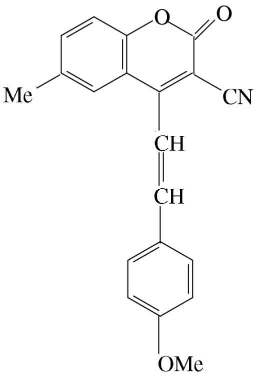
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.144
Data-to-parameter ratio = 8.1

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

Benzopyran derivatives are known to possess various biological activities. In the title compound, $C_{20}H_{15}NO_3$, the benzopyran ring is essentially planar and the dihedral angle between the benzopyran and phenyl rings is 56.5 (1)°. In the crystal, the carbonyl and methoxy O atoms are involved in weak C—H···O-type intermolecular interactions.

Comment

Many derivatives of benzopyran are found to possess medicinal and biological activities like antithrombotic effect, vasodilating effect on coronary vessels, tonic influence on capillary blood vessels, reduction in blood pressure, antispastic and photosensitizing effect (Borowiak & Wolska, 1989). The structure determination of the title compound, (I), was undertaken as part our study on benzopyrans.



(I)

The benzopyran ring is planar, with a maximum deviation of −0.024 (3) Å for C3. The dihedral angle between the phenyl and benzopyran rings is 56.5 (1)°. The alternate single and double bonds between O2 and C10 [O2═C2 1.213 (4), C2—C3 1.449 (5), C3═C4 1.372 (4) and C4—C10 1.443 (4) Å] indicate conjugation (Allen *et al.*, 1987; Alcock & Hough, 1972). The coplanarity of the methoxy carbon with the phenyl ring [C16—C15—O19—C20 1.6 (5)°] results in a close approach between C20 and C16 [2.807 (5) Å] and this causes the widening of C16—C15—O19 [125.3 (3)°] and narrowing of C14—C15—O19 [114.8 (3)°] from 120° (Sheldrick *et al.*, 1980; Koetzle & Williams, 1976; Sakaki *et al.*, 1976). Steric interactions cause the deviation of C4—C10—C5 [123.7 (3)°] and O1—C9—C8 [116.7 (3)°] angles from 120°, a common feature observed in coumarin derivatives (Ramasubbu, 1982; Ramasubbu *et al.*, 1982; Borowiak & Wolska, 1989). In the crystal, weak C—H···O-type intermolecular interactions involving O2 and O19 are observed (Jeffrey & Saenger, 1991).

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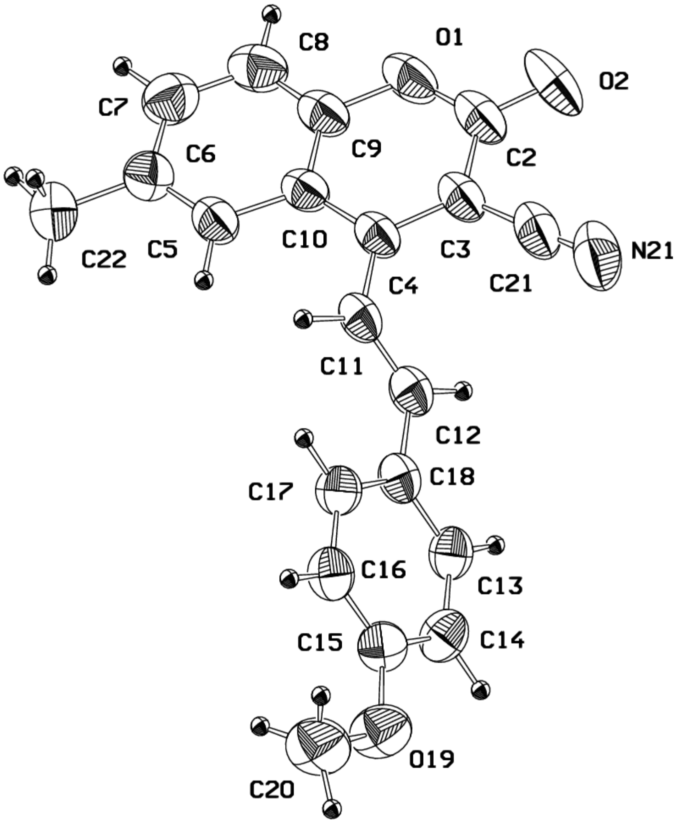

Figure 1
The molecular structure of (I) showing 50% probability displacement ellipsoids.

Experimental

A 3-cyano-4,6-dimethyl-2*H*-1-benzopyran-2-one (0.01 mol) and 4-methoxybenzaldehyde (0.01 mol) mixture was dissolved in chloroform (75–80 ml) and a few drops of piperidine (8–10 drops) were added as a catalyst. The mixture was heated with stirring for 15–16 h. After evaporation, the solid residue was recrystallized from dimethylformamide to give white crystals [m.p. 484 K; yield 56%].

Crystal data

$C_{20}H_{15}NO_3$
$M_r = 317.33$
Orthorhombic, $P2_12_12_1$
$a = 7.8683$ (12) Å
$b = 7.913$ (2) Å
$c = 26.0869$ (11) Å
$V = 1624.1$ (5) Å^3
$Z = 4$
$D_x = 1.298$ Mg m^{-3}

Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 2$–25°
$\mu = 0.71$ mm^{-1}
$T = 293$ (2) K
Needle, white
0.20 × 0.12 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.875$, $T_{\max} = 0.930$
1805 measured reflections
1804 independent reflections
1626 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ not measured
$\theta_{\max} = 69.8°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 31$
3 standard reflections every 60 reflections intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.144$
$S = 1.17$
1804 reflections
222 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 0.2613P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.009$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0079 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O2$^{\rm i}$	0.93	2.67	3.406 (4)	137
C13—H13···O2$^{\rm i}$	0.93	2.55	3.365 (4)	147
C22—H222···O19$^{\rm ii}$	0.96	2.61	3.566 (4)	173

Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $\frac{5}{2} - x, 1 - y, z - \frac{1}{2}$.

All H atoms were fixed using geometrical considerations and their isotropic displacement parameters were refined as two values, one for methyl-H atoms and the other for remaining H atoms. The absolute configuration is indeterminate for the title compound.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP*97 (Zsolnai, 1997); software used to prepare material for publication: *SHELXL*97 and *PARST*95 (Nardelli, 1995).

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