

7-Diethylamino-3-[(2Z)-3-(6-methoxy-2-naphthyl)prop-2-enoyl]-2H-chromen-2-one

H. S. Yathirajan,^a Anil N. Mayekar,^a B. K. Sarojini,^b B. Narayana^c and Michael Bolte^{d*}

^aDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^bDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, ^cDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, India, and ^dInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

Key indicators

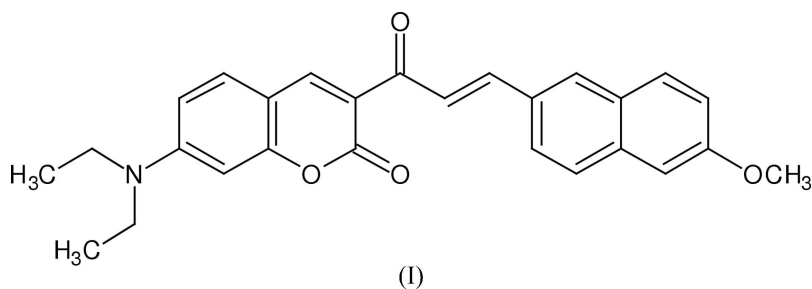
Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.054
 wR factor = 0.151
Data-to-parameter ratio = 14.3

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

The geometric parameters of the title molecule, $\text{C}_{27}\text{H}_{25}\text{NO}_4$, are in the usual ranges. The central $\text{C}=\text{C}$ double bond is *trans* configured, with the two C atoms slightly twisted out of the plane of the naphthyl group. The dihedral angle between the two fused ring systems is 40.90 (4)°.

Comment

Compounds incorporating benzopyrone structural units possess a wide range of biological activities (Pawar & Mulwad, 2004). Coumarins are an important class of molecules because of their applications in synthetic chemistry, medicinal chemistry and photochemistry (Vishnumurthy *et al.*, 1996, 1997, 1999). The coumarin system is the basis of various compounds possessing anticoagulant and anti-inflammatory activities (Lin *et al.*, 2006). The crystal structures of some of these types of compounds have recently been reported in the literature, *viz.* 3-acetyl-7-(diethylamino)coumarin (Hamaker & McCully, 2006), 3-acetyl-6-chloro-2H-chromen-2-one (Chopra *et al.*, 2006) and 7-diethylamino-2-oxo-2H-chromene-3-carboxylic acid (Bardajee *et al.*, 2006). As part of our current research, we have synthesized and determined the crystal structures of some chalcones (Yathirajan, Sarojini *et al.*, 2006; Yathirajan, Narayana *et al.*, 2006; Yathirajan, Vijaya Raj *et al.*, 2006; Yathirajan, Ashalatha *et al.*, 2006; Yathirajan, Sreevidya *et al.*, 2006; Yathirajan *et al.*, 2007). In a continuation of our quest to synthesize new materials which may find uses in the photonics industry, we report here the crystal structure of a new chalcone, (I), containing a benzopyrone unit.



The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). The carbonyl group is twisted by -9.8 (3)° from the plane of the coumarin unit. The torsion angle between the carbonyl group and the C atoms of the double bond is -14.1 (3)°. The torsion angle between the the C atoms of the double bond and the adjacent naphthyl group (C2—C3—C31—C40) is -7.1 (4)°. The two fused ring systems form a dihedral angle of 40.90 (4)°.

Received 25 January 2007
Accepted 29 January 2007

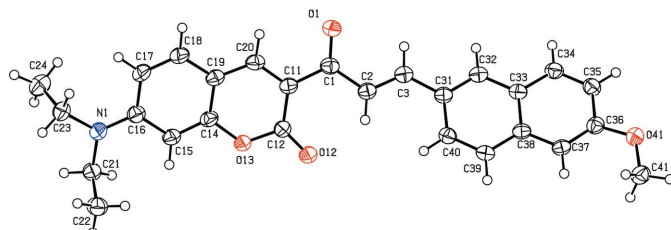


Figure 1
The molecular structure of (I) with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

Experimental

Piperidine (0.5 ml) was added to a thoroughly stirred solution of 7-*N,N*-diethylamino-3-acetylcoumarin (2.59 g, 0.01 mol) and 6-methoxy-2-naphthaldehyde (1.86 g, 0.01 mol) in 25 ml ethanol and the mixture was refluxed for 8 h and cooled. The solid which precipitated was filtered off and recrystallized from an acetone–toluene (1:1) mixture (m.p. 479–481 K). Analysis for $C_{27}H_{25}NO_4$ found (calculated): C 75.78 (75.86), H 5.80 (5.89), N 3.20% (3.28%).

Crystal data

$C_{27}H_{25}NO_4$
 $M_r = 427.48$
Monoclinic, $P2_1/c$
 $a = 20.8426$ (13) Å
 $b = 7.9413$ (8) Å
 $c = 13.5838$ (9) Å
 $\beta = 107.246$ (5)°
 $V = 2147.3$ (3) Å³

$Z = 4$
 $D_x = 1.322$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 173$ (2) K
Thick plate, red
 $0.23 \times 0.17 \times 0.09$ mm

Data collection

Stoe IPDS II two-circle
diffractometer
 ω scans
Absorption correction: none
12741 measured reflections

4162 independent reflections
3162 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.057$
 $\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.151$
 $S = 1.09$
4162 reflections
292 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.8794P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.25$ e Å⁻³
 $\Delta\rho_{min} = -0.23$ e Å⁻³

H atoms were found in a difference map, but they were subsequently refined using a riding model, with C–H = 0.95–0.99 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(\text{methyl C})$. The methyl groups were allowed to rotate but not to tip.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

ANM thanks the University of Mysore for permission to carry out the research work. One of the authors (BKS) thanks AICTE, Government of India, for financial assistance through the Career Award for Young Teacher's Scheme.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bardajee, G. R., Winnik, M. A. & Lough, A. J. (2006). *Acta Cryst. E62*, o3076–o3078.
- Chopra, D., Venugopal, K. N., Jayashree, B. S. & Row, T. N. G. (2006). *Acta Cryst. E62*, o2310–o2312.
- Hamaker, C. G. & McCully, C. S. (2006). *Acta Cryst. E62*, o2072–o2074.
- Lin, C. M., Huang, S. T., Lee, F. W., Kuo, H. S. & Lin, M. H. (2006). *Bioorg. Med. Chem. Lett.* **16**, 4402–, 4409.
- Pawar, R. B. & Mulwad, V. V. (2004). *Chem. Heterocycl. Compd.* **440**, 257–264.
- Sheldrick, G. M. (1990). *Acta Cryst. A46*, 467–473.
- Sheldrick, G. M. (1997). *SHELXL97*. Univ. of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
- Vishnumurthy, K., Guru Row, T. N. & Venkatesan, K. (1996). *J. Chem. Soc. Perkin Trans. 2*, pp. 1475–1478.
- Vishnumurthy, K., Guru Row, T. N. & Venkatesan, K. (1997). *J. Chem. Soc. Perkin Trans. 2*, pp. 615–619.
- Vishnumurthy, K., Guru Row, T. N. & Venkatesan, K. (1999). *Tetrahedron Lett.* **55**, 4095–4108.
- Yathirajan, H. S., Ashalatha, B., Narayana, B., Bindya, S. & Bolte, M. (2006). *Acta Cryst. E62*, o4551–o4553.
- Yathirajan, H. S., Bindya, S., Mithun, A., Narayana, B. & Bolte, M. (2007). *Acta Cryst. E63*, o61–o62.
- Yathirajan, H. S., Narayana, B., Ashalatha, B., Sarojini, B. K. & Bolte, M. (2006). *Acta Cryst. E62*, o4440–o4441.
- Yathirajan, H. S., Sarojini, B. K., Bindya, S., Narayana, B. & Bolte, M. (2006). *Acta Cryst. E62*, o4046–o4047.
- Yathirajan, H. S., Sreevidya, T. V., Narayana, B., Sarojini, B. K. & Bolte, M. (2006). *Acta Cryst. E62*, o5923–o5924.
- Yathirajan, H. S., Vijaya Raj, K. K., Narayana, B., Sarojini, B. K. & Bolte, M. (2006). *Acta Cryst. E62*, o4444–o4445.