Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

3-Hydroxy-3-(6-methoxynaphthalen-2-yl)-1-phenylprop-2-en-1-one

Chun-Yang Zheng,[a,b] Ling Fan[a,b] and Dun-Jia Wang[a]*

[a]Hubei Key Laboratory of Bioanalytical Techniques, Department of Chemistry and Environmental Engineering, Hubei Normal University, Huangshi 435002, People's Republic of China, and [b]College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: dunjiawang@163.com

Received 4 December 2006
Accepted 11 December 2006

Key indicators

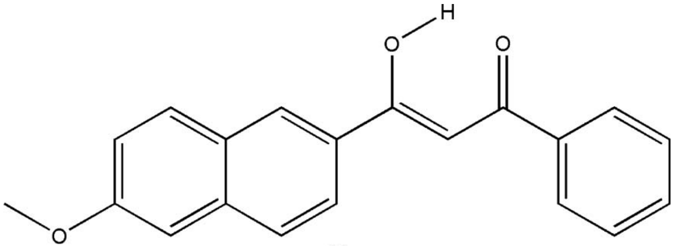
Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.004 Å
R factor = 0.068
wR factor = 0.138
Data-to-parameter ratio = 15.1

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

The title compound, $C_{20}H_{16}O_3$, is in the enol form, stabilized by an intramolecular O—H···O hydrogen bond.

Comment

1,3-Diketones are widely used as effective chelating reagents for a very large number of metallic systems (Malandrino *et al.*, 1998; Melby *et al.*, 1964; Wu *et al.*, 2002; Yuan *et al.*, 1998), The structures of 1,3-diketones have also received increasing attention in the study of tautomerism (Vila *et al.*, 1991).



(I)

The title compound (I) (Fig. 1), is in the enol form stabilized by an intramolecular hydrogen bond between O3 and O2 (Table 1). The geometric data are in agreement with reported literature values (Bertolasi *et al.*, 1991; Gilli *et al.*, 2004; Vila *et al.*, 1991; Wang *et al.*, 2006).

Experimental

1-(2-Methoxynaphthalen-6-yl)ethanone (6.00 g, 0.03 mol), ethyl benzoate (5.25 g, 0.035 mol), $NaNH_2$ (1.56 g, 0.04 mol) and benzene (50 ml) were placed into a three-necked, round-bottom flask. The mixture was heated with stirring to 323 K and maintained at that temperature for 6 h under a blanket of nitrogen. The reaction mixture was then cooled to room temperature, acidified with dilute hydrochloric acid, and stirring was continued until all solids had dissolved. The benzene layer was separated and washed with saturated

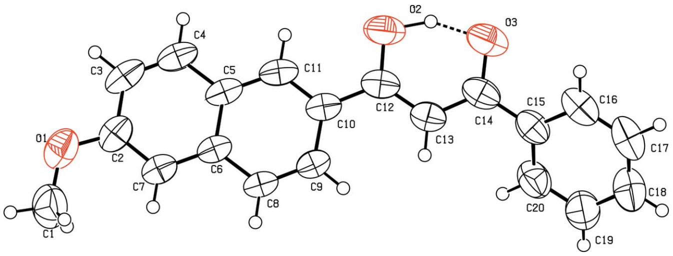


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates the intramolecular hydrogen bond.

doi:10.1107/S1600536806053797

$NaHCO_3$ solution, dried over anhydrous Na_2SO_4 and removed by evaporation. The residual oil solidified on standing and was recrystallized from an ethanol solution to give the title compound (I) (yield 5.68 g, 62.3%, m.p. 416 K). Crystals suitable for X-ray diffraction were grown by slow evaporation of a CH_2Cl_2–EtOH (1:2) solution at room temperature. IR (KBr, ν cm^{-1}): 1628 (C$=$O), 1541 (C$=$C), 2975 (C—H, alkyl); calculated for $C_{20}H_{16}O_3$: C 78.93, H 5.30%; found: C 78.89, H 5.28%.

Crystal data

$C_{20}H_{16}O_3$
$M_r = 304.33$
Orthorhombic, *Pbca*
$a = 11.213$ (2) Å
$b = 8.1919$ (16) Å
$c = 33.739$ (6) Å
$V = 3099.1$ (10) Å^3
$Z = 8$
$D_x = 1.304$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 297$ (2) K
Plate, yellow
0.23 × 0.20 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.977$, $T_{\max} = 0.986$
23289 measured reflections
3202 independent reflections
2279 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
$\theta_{\max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.138$
$S = 1.16$
3202 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.8925P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.11$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C12—O2	1.302 (3)	C13—C14	1.394 (3)
C12—C13	1.389 (3)	C14—O3	1.291 (3)
O2—C12—C13	120.1 (2)	O3—C14—C13	120.3 (3)
C12—C13—C14	121.9 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H3*A*···O3	1.13 (3)	1.43 (4)	2.486 (3)	152 (3)

H atoms were included in the riding model approximation with C—H = 0.93 to 0.97 Å and with $U_{\rm iso}$(H) = 1.2 (1.5 for methyl) times $U_{\rm eq}$(C). The H atom of the hydroxyl group was located in a difference Fourier map and its position was refined freely, with $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(O).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); 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, 2001); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Hubei Normal University and the Natural Science Foundation of the Educational Commission of Hubei Province (No. J200522002 and No. Z200622001) for financial support.

References

Bertolasi, V., Cilli, P., Ferretti, V. & Gilli, G. (1991). *J. Am. Chem. Soc.* **113**, 4917–4925.
Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Gilli, P., Bertolasi, V., Pretto, L., Ferretti, V. & Gilli, G. (2004). *J. Am. Chem. Soc.* **126**, 3845–3855.
Malandrino, G., Benelli, C., Castelli, F. & Fragala, I. L. (1998). *Chem. Mater.* **10**, 3434–3444.
Melby, L. R., Rose, N. J., Abranmson, E. & Caris, J. C. (1964). *J. Am. Chem. Soc.* **86**, 5117–5125.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Vila, A. J., Lagier, C. M. & Olivieri, A. C. (1991). *J. Phys. Chem.* **95**, 5069–5073.
Wang, D.-J., Zheng, C.-Y. & Fan, L. (2006). *Acta Cryst.* E**62**, o3681–o3682.
Wu, F. B., Han, S. Q., Zhang, C. & He, Y. F. (2002). *Anal. Chem.* **74**, 5882–5889.
Yuan, J. L. & Matsumoto, K. (1998). *Anal. Chem.* **70**, 596–601.