Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Hydroxy-1-(4-methoxyphenyl)-3-(2-nitrophenyl)propan-1-one

Xiao-Yang Qiu,[a] Xiao-Niu Fang,[b] Wei-Sheng Liu[c] and Hai-Liang Zhu[d]*

[a]Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, [b]College of Chemistry & Chemical Engineering, JiangXi Province Key Laboratory of Coordination Chemistry, JingGangShan University 343009, Ji'an JiangXi, People's Republic of China, [c]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China, and [d]Institute of Functional Biomolecules, State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: hailiang_zhu@163.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 13.9

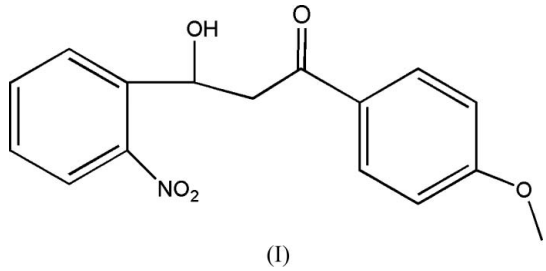
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 May 2006
Accepted 26 May 2006

In the title compound, $C_{16}H_{15}NO_5$, all bond lengths and angles are within normal ranges. The dihedral angle between the two benzene rings is 15.6 (2)°. In the crystal structure, the molecules are linked through weak intermolecular O—H···O hydrogen bonds, forming chains along the *b* axis.

Comment

Recently, we have reported the structures of two chalcone derivatives (Qiu, Liu & Zhu, 2006; Qiu, Yang *et al.*, 2006). As an extension of our work on the structural characterization of chalcone derivatives, the title compound, (I), is reported here.



(I)

The asymmetric unit of (I) (Fig. 1) consists of one molecule of 3-hydroxy-1-(4-methoxyphenyl)-3-(2-nitrophenyl)propan-1-one. In the molecule, all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the two benzene rings is 15.6 (2)°.

In the crystal structure, the molecules are linked through weak intermolecular O—H···O hydrogen bonds, forming chains along the *b* axis (Table 1 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. An aqueous solution of potassium hydroxide

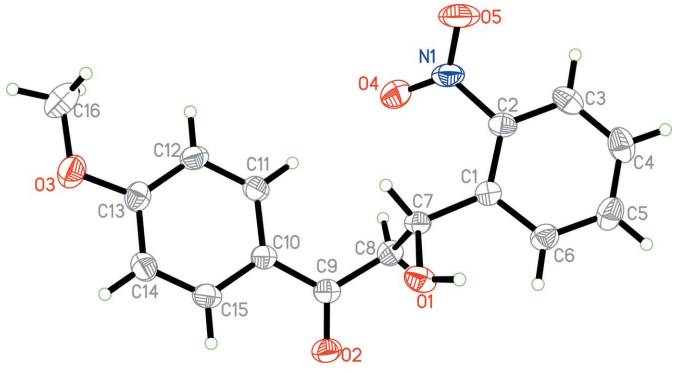


Figure 1
The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme.

(10%, 1 ml) was added, with stirring, overnight to a solution of 2-nitrobenzaldehyde (1 mmol, 0.15 g) and 1-(4-methoxyphenyl)-ethanone (1 mmol, 0.15 g) in ethanol (15 ml) at room temperature. The reaction mixture was then poured into ice and neutralized with hydrochloric acid (5%), yielding a yellow solid. The latter was dissolved in acetone (12 ml) and stirred for about 10 min to give a clear yellow solution. After allowing the solution to stand in air for 12 d, yellow block-shaped crystals were formed at the bottom of the vesssel on slow evaporation of the solvent. These were collected, washed three times with acetone, and dried in a vacuum desiccator using $CaCl_2$. (I) was isolated in 62% yield.

Crystal data

$C_{16}H_{15}NO_5$
M_r = 301.29
Monoclinic, $P2_1/n$
a = 13.5530 (3) Å
b = 7.3761 (2) Å
c = 14.5524 (4) Å
β = 90.172 (1)°
V = 1454.77 (6) Å^3
Z = 4
D_x = 1.376 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, yellow
0.36 × 0.12 × 0.07 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.991
7701 measured reflections
2834 independent reflections
1973 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.03
2834 reflections
204 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.3026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	2.29	2.832 (2)	124

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

The methine H atom, H7, was located in a difference Fourier map and refined with a C—H distance restraint of 1.009 (19) Å. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H and O—H distances of 0.93–0.97 and 0.82 Å, respectively; U_{iso}(H) values were set at 1.2 or 1.5U_{eq}(C) and 1.5U_{eq}(O).

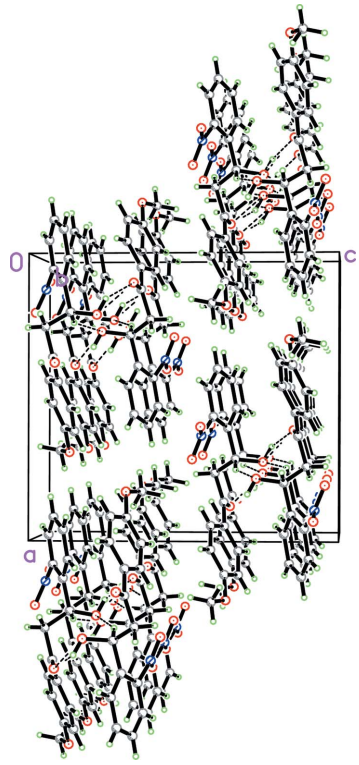


Figure 2
The crystal packing of (I), viewed approximately along the *c* axis. Dashed lines indicate O—H···O hydrogen bonds.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, China, for research grant No. 2006kj158B, and Fuyang Normal College for research grant No. LQ007.

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.
Bruker. (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Qiu, X.-Y., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o1304–o1305.
Qiu, X.-Y., Yang, S.-L., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o1627–o1628.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.