Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Hydroxy-5-nitrobenzyl alcohol

Gang Lei,* Huan-Xia Zhang and Shao-Jin Gu

Department of Chemistry, China West Normal University, Nanchong 637002, People's Republic of China

Correspondence e-mail: leigang307@yahoo.com.cn

Received 25 July 2006
Accepted 29 August 2006

Key indicators

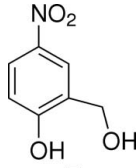
Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.144
Data-to-parameter ratio = 12.6

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

The title compound, $C_7H_7NO_4$, crystallizes with two molecules in the asymmetric unit. The nitro groups are twisted slightly out of the planes of the benzene rings by 8.5 (2) and 4.4 (2)°. The crystal packing is stabilized by O—H···O and C—H···O hydrogen bonds.

Comment

The title compound, (I), is an intermediate used in the synthesis of a new acyclic molecular receptor that binds quaternary ammonium salts (Jeong *et al.*, 1998).



(I)

Bond lengths and angles in (I) are normal for a compound of this type. Compound (I) crystallizes in the monoclinic space group $P2_1/c$ with Z' = 2. The nitro groups of the two independent molecules show a slightly different twist from the

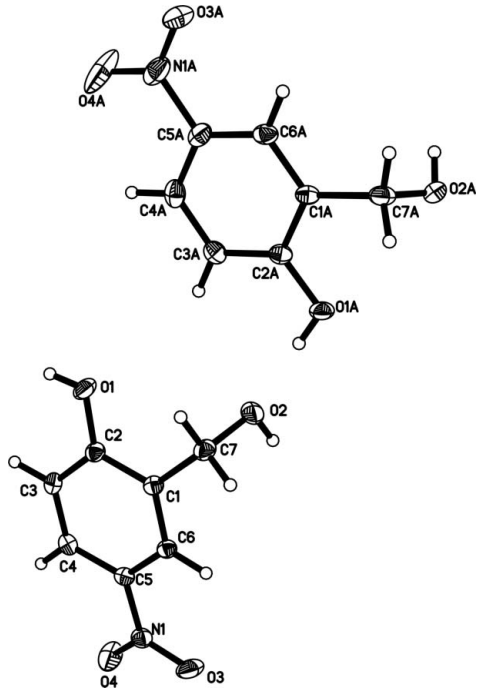


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

planes of the benzene rings [8.5 (2) and 4.4 (2)°] (Fig. 1). The crystal packing is stabilized by O—H···O and C—H···O hydrogen bonds (Table 1 and Fig. 2).

Experimental

Compound (I) was prepared according to the procedure of Arenz & Giannis (2001). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from dichloromethane.

Crystal data

$C_7H_7NO_4$
M_r = 169.14
Monoclinic, $P2_1/c$
a = 7.2099 (3) Å
b = 9.6277 (4) Å
c = 21.5374 (8) Å
β = 98.091 (1)°
V = 1480.13 (10) Å^3
Z = 8
D_x = 1.518 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 153 (2) K
Block, colourless
0.63 × 0.33 × 0.32 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
11817 measured reflections
2750 independent reflections
2583 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.00
2750 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.081P)^2 + 1.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.011 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O2A^{i}	0.84	1.82	2.647 (2)	167
O2—H2O···O4^{ii}	0.84	2.04	2.864 (2)	168
O1A—H1OA···O2	0.84	1.81	2.6467 (19)	178
O2A—H2OA···O3^{iii}	0.84	2.14	2.927 (2)	156
C7A—H7AB···O1A^{iv}	0.99	2.55	3.404 (2)	145
C6A—H6A···O4A^{v}	0.95	2.52	3.363 (3)	148
C7—H7B···O3A^{vi}	0.99	2.42	3.320 (3)	151

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $-x+1, -y+2, -z+1$; (v) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (vi) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

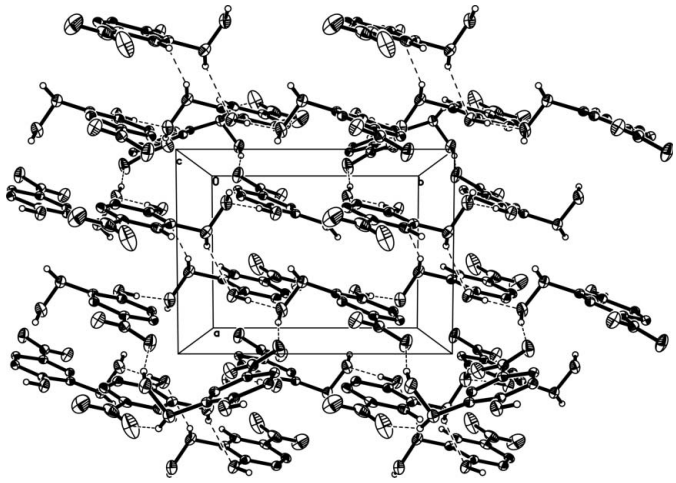


Figure 2
The crystal packing for (I), with displacement ellipsoids at the 30% probability level, viewed along the c axis. Dashed lines depict the intermolecular hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

All H atoms were placed in calculated positions and included in the final cycles of refinement using a riding model. with O—H = 0.84 Å and C—H = 0.95 or 0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(C,O).

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank the Centre for Testing and Analysis, Cheng Du Branch, Chinese Academy of Sciences, for analytical support.

References

Arenz, C. & Giannis, A. (2001). *Eur. J. Org. Chem.* **1**, 137–140.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Jeong, K. S., Hahn, K. M. & Cho, Y. L. (1998). *Tetrahedron Lett.* **39**, 3779–3782.
Rigaku/MSC (2004). *RAPID-AUTO*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.