Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{(1*R*,3S)-3-[(Dimethylamino)methyl]-2,2-dimethylcyclopropyl}diphenylmethanol

Jiang-Chun Zhong, Min-Gan Wang and Min Wang*

Department of Applied Chemistry, College of Science, China Agricultural University, Beijing 100094, People's Republic of China

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

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.076
Data-to-parameter ratio = 8.0

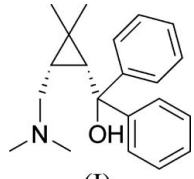
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 26 January 2007
Accepted 26 January 2007

The title compound, $C_{21}H_{27}NO$, crystallizes with two rather similar molecules in the asymmetric unit. Its molecular conformation is stabilized by an intramolecular O—H···N hydrogen bond.

Comment

Cyclopropane occurs as a basic structural motif in a wide range of naturally occurring compounds (Patai & Rappoport, 1987). Recently, Molander *et al.* (2004) used chiral cyclopropane-based ligands in the palladium-catalyzed allylic alkylation of 1,3-diphenylpropenyl acetate with dimethyl malonate. In the light of the above report and our interest in devising new chiral cyclopropane-based ligands, the crystal structure of the title compound, (I), has been determined.



(I)

There are two rather similar molecules in the asymmetric unit of (I), which differ slightly in the orientation of the phenyl rings. The molecular conformation is stabilized by an intramolecular O—H···N hydrogen bond.

Experimental

Compound (I) was prepared according to the method of Zhong *et al.* (2006). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from *n*-hexane.

Crystal data

$C_{21}H_{27}NO$
M_r = 309.44
Monoclinic, $P2_1$
a = 6.2697 (13) Å
b = 16.168 (3) Å
c = 18.260 (4) Å
β = 94.60 (3)°
V = 1845.0 (6) Å^3
Z = 4
D_x = 1.114 Mg m^{-3}
Mo *Kα* radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
Plate, colourless
0.50 × 0.45 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID image-plate diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.967, T_{max} = 0.992
10713 measured reflections
3389 independent reflections
2089 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.076$
$S = 0.99$
3389 reflections
424 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.027P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.074 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—HO1···N1	0.98 (4)	1.88 (4)	2.782 (4)	152 (3)
O2—HO2···N2	0.90 (4)	1.86 (4)	2.716 (4)	157 (3)

H atoms bonded to O were refined freely. The remaining H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined using a riding model, with U_{iso} (H) = $1.2U_{eq}$(C). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *RAPID-AUTO* (Rigaku, 2000); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

Financial support from the National Natural Science Foundation of China (grant No. 20472111) is gratefully acknowledged.

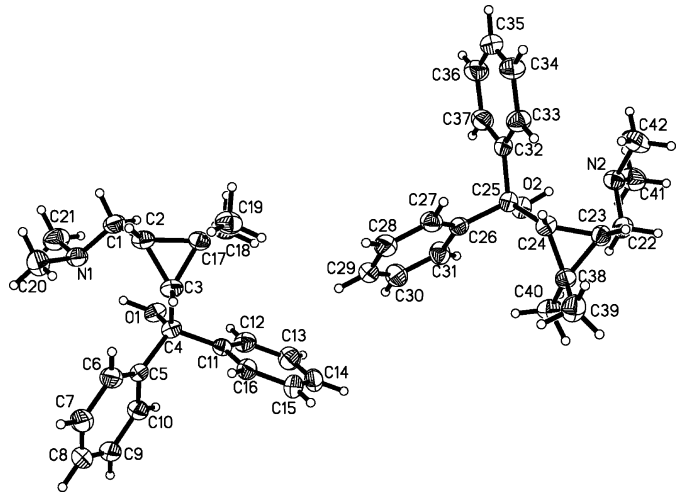


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 30% probability level.

References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Molander, G. A., Burke, J. P. & Carroll, P. J. (2004). *J. Org. Chem.* **69**, 8062–8069.
Patai, S. & Rappoport, Z. (1987). *The Chemistry of the Cyclopropyl Group*, edited by H.-W. Liu, pp. 959–991. New York: John Wiley and Sons.
Rigaku (2000). *RAPID-AUTO* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1991). *SHELXTL*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhong, J. C., Wang, M. A., Guo, H. C., Yin, M. M., Bian, Q. H. & Wang, M. (2006). *Synlett*, pp. 1667–1679.