

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

8-Methyl-5-methylene-2-oxotricyclo-[5.3.1.1^{3,9}]dodecan-endo-8-olIsa Y. H. Chan,^a Roger Bishop,^a Donald C. Craig,^a Marcia L. Scudder^{a*} and Weimin Yue^b^aSchool of Chemistry, University of New South Wales, Sydney 2052, Australia, and^bSchool of Pharmacy, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, People's Republic of China

Correspondence e-mail: m.scudder@unsw.edu.au

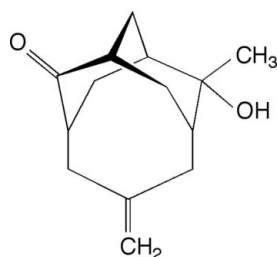
Received 7 April 2008; accepted 8 April 2008

Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.049; wR factor = 0.053; data-to-parameter ratio = 14.3.

The title compound, $\text{C}_{14}\text{H}_{20}\text{O}_2$, crystallizes with homochiral chains of molecules hydrogen bonded together along the b axis. Adjacent chains in the ab plane contain molecules of the same chirality, leading to a chiral segregation of the molecules into layers.

Related literature

For related literature, see: Yue *et al.* (2002, 2006, 2007, 1997, 2000).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{20}\text{O}_2$
 $M_r = 220.3$
 Monoclinic, $P2_1/c$
 $a = 7.554$ (3) Å
 $b = 13.196$ (3) Å
 $c = 12.597$ (5) Å
 $\beta = 108.16$ (2)°

$V = 1193.2$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 294$ K
 $0.25 \times 0.20 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4
 diffractometer
 Absorption correction: none
 2247 measured reflections
 2079 independent reflections

1296 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$
 1 standard reflection
 frequency: 30 min
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.052$
 $S = 1.27$
 2079 reflections

145 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1O1}\cdots\text{O2}^i$	1.00	1.87	2.867 (4)	180

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: local program; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *RAELS* (Rae, 2000); molecular graphics: *ORTEPII* (Johnson, 1976) and *CrystalMaker* (Palmer, 2005); software used to prepare material for publication: local programs.

This research was supported by the Australian Research Council and the Shanghai Pujiang Program (WY).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2391).

References

- Altomare, A., Casciarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
 Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
 Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
 Palmer, D. (2005). *CrystalMaker*. CrystalMaker Software Ltd, Yarnton, Oxfordshire, England. <http://www.CrystalMaker.co.uk>.
 Rae, A. D. (2000). *RAELS*. Australian National University, Canberra, Australia.
 Yue, W., Bishop, R., Craig, D. C. & Scudder, M. L. (2000). *Tetrahedron*, **56**, 6667–6673.
 Yue, W., Bishop, R., Craig, D. C. & Scudder, M. L. (2002). *CrystEngComm*, **4**, 591–595.
 Yue, W., Bishop, R., Craig, D. C. & Scudder, M. L. (2007). *Acta Cryst.* **E63**, o4689.
 Yue, W., Bishop, R., Scudder, M. L. & Craig, D. C. (1997). *J. Chem. Soc. Perkin Trans. 1*, pp. 2937–2946.
 Yue, W., Nakano, K., Bishop, R., Craig, D. C., Harris, K. D. M. & Scudder, M. L. (2006). *CrystEngComm*, **8**, 250–256.

