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An asymmetric epoxidate: [3-(4-chlorophenyl)oxiran-2-yl](5-naphthyl)methanone

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Key indicators

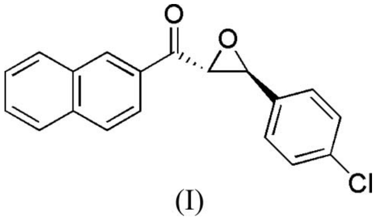
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.095
Data-to-parameter ratio = 14.2

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

The title compound, $C_{19}H_{13}ClO_2$, exists as the *trans* isomer. Both chiral centres at the oxirane C atoms are in the *R* configuration.

Comment

Epoxides are valuable intermediates in the preparation of oxygen-containing natural and synthetic compounds (Beller *et al.*, 1998; Jorgensen *et al.*, 1989; Rao *et al.*, 1991). Enantiopure oxiranes are utilized in organic syntheses because they can be transformed into 1,2-difunctionalized derivatives by nucleophilic ring-opening reactions (Gorzynski-Smith, 1984; Rao *et al.*, 1983). Given their tremendous importance in synthesis, there has been considerable interest in the development of asymmetric methods to prepare epoxides (Enders *et al.*, 1996, 1997; Elston *et al.*, 1997; Nemoto, Ohshima & Shibasaki, 2001; Nemoto, Ohshima, Yamaguchi *et al.*, 2001). In the course of our studies, we obtained single crystals of the title compound, (I) (Fig. 1), and report here its crystal structure.



(I)

A perspective view of (I) with the atom-labelling scheme is shown in Fig. 1. The molecule is the *trans* isomer. The chiral centres at C12 and C13 have *R* configurations.

No conventional hydrogen bonds were observed in the crystal structure, although there is a C—H···O contact, where the C12···O1^i distance is 3.094 (4) Å and the angle at H12 is 105° [symmetry code: (i) $2 - x$, $-\frac{1}{2} + y$, $1 - z$].

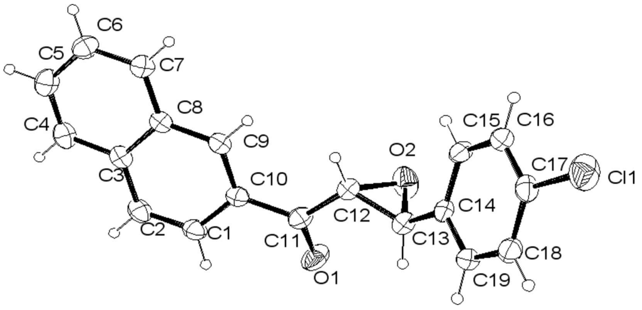


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-labelling scheme.

Experimental

The title compound was synthesized by the Darzens reaction of 2-bromo-1-(naphthalen-5-yl)ethanone and 4-chlorobenzaldehyde in water, in accordance with the literature (Tanaka & Shiraishi, 2001). Crystals suitable for X-ray structural analysis were grown by slow evaporation of an ethanol solution of the compound at room temperature.

Crystal data

$C_{19}H_{13}ClO_2$
$M_r = 308.74$
Monoclinic, $P2_1$
$a = 6.0842$ (13) Å
$b = 8.3402$ (18) Å
$c = 14.593$ (3) Å
$\beta = 96.849$ (4)°
$V = 735.2$ (3) Å^3
$Z = 2$

$D_x = 1.395$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1425 reflections
$\theta = 2.8$–23.5°
$\mu = 0.26$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.642$, $T_{\max} = 1.000$
4167 measured reflections

2822 independent reflections
2119 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 26.5$°
$h = -6 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -18 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.095$
$S = 1.08$
2822 reflections
199 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.0885P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Absolute structure: Flack (1983), with 1198 Friedel pairs
Flack parameter: −0.05 (8)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker, 1998); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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o730 Zhang *et al.* • $C_{19}H_{13}ClO_2$ *Acta Cryst.* (2006). E**62**, o729–o730