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(4*S*,5*S*)-2-Benzyloxy-4-methyl-5-(4-tolylthiocarbonyl)-oxazoline

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Key indicators

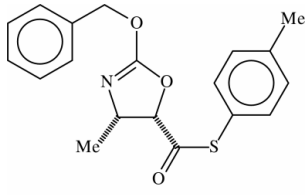
Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.003 Å
R factor = 0.030
wR factor = 0.079
Data-to-parameter ratio = 15.4

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

The five-membered ring in the title compound, $C_{19}H_{19}NO_3S$, is almost planar. The *cis* configuration of the ring substituents and the absolute configuration determination confirm the proposed mechanism of the stereospecific synthesis.

Comment

The title compound, (I), was synthesized as part of a study of the stereocontrolled synthesis of *anti*-α-hydroxy-β-amino acid derivatives (Ambroise *et al.*, 2002). The crystal structure of (I) was determined in order to confirm the relative stereochemistry of the substituents on the heterocyclic ring; this was found to be *cis*.



(I)

The central five-membered ring is almost planar (Fig. 1), with a root-mean-square deviation of 0.026 Å for the component atoms. The geometry (Table 1) is very similar to that observed for the only other reported structure of a comparable oxazoline (Seki & Matsumoto, 1999), which also has the *cis* configuration.

There are no notable intermolecular interactions.

Experimental

The synthesis of the title compound is described by Ambroise *et al.* (2002).

Crystal data

$C_{19}H_{19}NO_3S$
M_r = 341.41
Monoclinic, $P2_1$
a = 11.9010 (9) Å
b = 5.7705 (4) Å
c = 13.7964 (10) Å
β = 109.043 (2)°
V = 895.61 (11) Å^3
Z = 2
D_x = 1.266 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6005 reflections
θ = 2.7–28.7°
μ = 0.20 mm^{-1}
T = 160 (2) K
Rectangular block, colourless
0.52 × 0.40 × 0.34 mm

Data collection

Siemens SMART 1K CCD diffractometer
ω rotation with narrow frames
Absorption correction: multi-scan (*XPREP* in *SHELXTL*; Sheldrick, 1994)
T_{min} = 0.750, T_{max} = 0.928
6725 measured reflections
3382 independent reflections
3203 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.7°
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 7$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.0826P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.030$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.079$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
3382 reflections	Absolute structure: Flack (1983), 1056 Friedel pairs
219 parameters	Flack parameter = −0.08 (6)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.361 (2)	C1—O3	1.3292 (17)
O1—C3	1.4424 (16)	N1—C2	1.4760 (19)
C1—N1	1.258 (2)	C2—C3	1.569 (2)
C1—O1—C3	104.94 (11)	C1—N1—C2	105.93 (14)
O1—C1—N1	120.79 (13)	N1—C2—C3	103.97 (11)
O1—C1—O3	109.94 (13)	O1—C3—C2	103.94 (11)
N1—C1—O3	129.27 (15)		
C3—O1—C1—N1	5.39 (18)	C1—O1—C3—C2	−6.31 (14)
O1—C1—N1—C2	−1.42 (18)	N1—C2—C3—O1	5.71 (14)
C1—N1—C2—C3	−2.87 (15)		

H atoms were placed geometrically and refined with a riding model (including free rotation about C—methyl bonds), and with U_{iso} constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom.

Data collection: *SMART* (Siemens, 1995); cell refinement: local programs; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

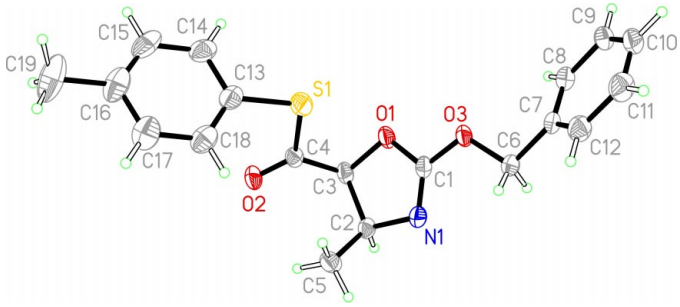


Figure 1
The molecular structure of (I), with atom labels and 50% probability ellipsoids for non-H atoms.

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