

N*-[(3*RS*)-3-(4-Chlorophenyl)heptanoyl]bornane-10,2-sultam*Xiu-Fang Cao, Jun Yin, Guang-Ao Yu and Sheng-Hua Liu***

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Correspondence e-mail:
chshliu@mail.ccnu.edu.cn**Key indicators**Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.051
 wR factor = 0.120
Data-to-parameter ratio = 15.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In the title compound, $\text{C}_{23}\text{H}_{32}\text{ClNO}_3\text{S}$, molecules are linked *via* $\text{C}-\text{H} \cdots \text{N/O}$ interactions, forming two-dimensional sheets parallel to the (100) plane.

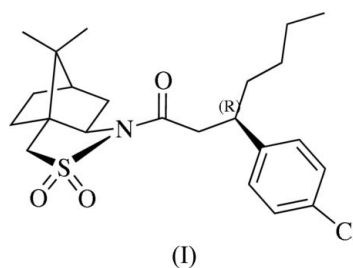
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Comment

The readily available enantiomers of bornane-10,2-sultam serve as efficient, versatile and practical chiral auxiliaries (Oppolzer, 1990), and we have focused our attention on this field. In this paper, we present the X-ray crystallographic analysis of the title compound, (I).

In (I), the six-membered ring of sultam exhibits a boat form (Fig. 1). The $\text{C}9/\text{C}4/\text{C}5/\text{C}6$ and $\text{C}6/\text{C}7/\text{C}8/\text{C}9$ planes form a dihedral angle of 111.1 (1)°. The $\text{C}3/\text{C}6/\text{C}9$ plane forms almost equal dihedral angles with the above planes [124.1 (1) and 124.7 (1)°, respectively]. The molecules are linked *via* $\text{C}-\text{H} \cdots \text{N/O}$ interactions (Table 2) along the b and c axes, forming two-dimensional sheets parallel to the (100) plane (Fig. 2).**Experimental**Compound (I) was synthesized from (–)-sultam and cinnamic chloride (Huang *et al.*, 1999). Crystals suitable for X-ray data collection were obtained by slow evaporation of a dichloromethane solution at 292 K.*Crystal data* $\text{C}_{23}\text{H}_{32}\text{ClNO}_3\text{S}$
 $M_r = 438.01$
Monoclinic, $P2_1$
 $a = 9.2278$ (13) Å
 $b = 9.6269$ (14) Å
 $c = 13.1720$ (19) Å
 $\beta = 99.736$ (2)°
 $V = 1153.3$ (3) Å³
 $Z = 2$ $D_x = 1.261$ Mg m^{−3}
Mo $K\alpha$ radiation
Cell parameters from 1773 reflections
 $\theta = 2.2$ – 21.7 °
 $\mu = 0.28$ mm^{−1}
 $T = 292$ (2) K
Block, colorless
 $0.30 \times 0.20 \times 0.10$ mm*Data collection*Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: none
6334 measured reflections
4179 independent reflections3478 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\text{max}} = 26.0$ °
 $h = -11 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -16 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.120$
 $S = 1.04$
 4179 reflections
 265 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.074P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.18 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983),
 1762 Friedel pairs
 Flack parameter: 0.08 (8)

Table 1

Selected geometric parameters (\AA , $^\circ$).

C8—N1	1.477 (4)	C21—C11	1.748 (4)
C10—S1	1.791 (3)	N1—S1	1.684 (2)
C11—O3	1.196 (3)	O1—S1	1.411 (2)
C11—N1	1.391 (4)	O2—S1	1.417 (2)
C9—C10—S1	107.0 (2)	N1—S1—C10	96.06 (14)
C9—C4—C5—C6	−3.8 (4)	C12—C13—C18—C23	−49.7 (4)
C6—C7—C8—C9	−8.4 (3)	C14—C13—C18—C19	−103.8 (4)
N1—C8—C9—C10	−31.2 (4)	C9—C8—N1—S1	26.1 (3)
C8—C9—C10—S1	23.3 (4)	C8—N1—S1—C10	−11.1 (3)
C11—C12—C13—C14	165.0 (3)	C9—C10—S1—N1	−7.7 (3)
C14—C15—C16—C17	−178.4 (4)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12A \cdots O2	0.97	2.55	3.139 (5)	119
C1—H1A \cdots N1	0.96	2.47	3.141 (4)	126
C20—H20 \cdots O2 ⁱ	0.93	2.48	3.363 (5)	159
C10—H10A \cdots O1 ⁱⁱ	0.97	2.55	3.220 (4)	126

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

All H atoms were constrained to an ideal geometry, with C—H = 0.95–1.00 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The absolute configuration is consistent with the known absolute configuration of (−)-camphor-2,10-sultam (Boiadjiev *et al.*, 2001).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE-Plus* (Bruker, 2001); data reduction: *SAINTE-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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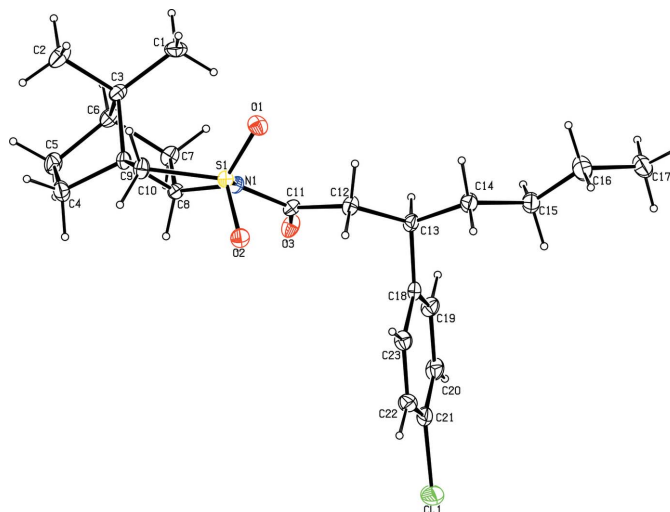


Figure 1

View of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

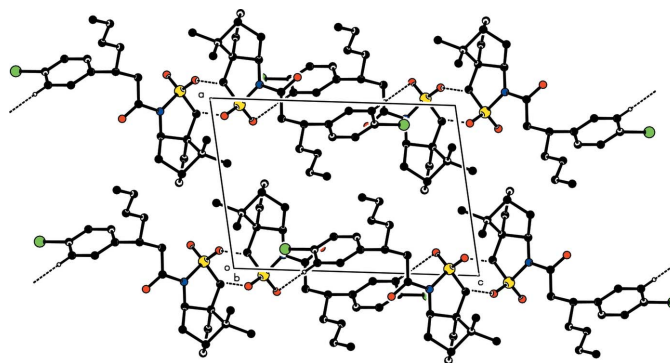


Figure 2

The molecular packing of (I), viewed along the b axis. Dashed lines indicate C—H \cdots O/N interactions. H atoms not involved in these interactions have been omitted for clarity.

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