Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(+)-*N*-[2-(4-Chlorophenyl)propanoyl]-bornane-10,2-sultam

Wen-Chang Lu, Jun Cao, Chen Cheng, Guang-Ao Yu and Sheng-Hua Liu*

Key Laboratory of Pesticides and Chemical Biology, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China
Correspondence e-mail: chshliu@mail.ccnu.edu.cn

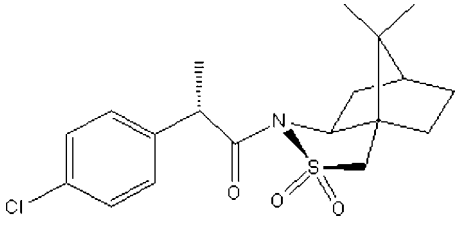
Received 16 November 2007; accepted 21 December 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.180; data-to-parameter ratio = 16.2.

In the molecular structure of the title compound, $C_{19}H_{24}ClNO_3S$, the six-membered ring of the bornane unit shows a boat form, while the five-membered ring of the sultam unit adopts a twist form. Intramolecular C—H···N and C—H···O interactions are observed. In the crystal structure, molecules are connected by intermolecular C—H···O hydrogen bonds into a chain running along the b axis. The crystal was a partial inversion twin with a twin ratio of 0.73 (1):0.27 (1).

Related literature

For related literature, see: Boiadjiev & Lightner (2001); Oppolzer (1989, 1990).



Experimental

Crystal data

$C_{19}H_{24}ClNO_3S$
M_r = 381.90
Monoclinic, $C2$
a = 21.0863 (16) Å
b = 7.7948 (6) Å
c = 12.102 (1) Å
β = 107.433 (1)°
V = 1897.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
5780 measured reflections
3715 independent reflections
3146 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.180
S = 1.10
3715 reflections
229 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1503 Friedel pairs
Flack parameter: 0.27 (1)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···N1	0.96	2.54	3.129 (6)	120
C19—H19···O3	0.93	2.59	3.196 (6)	123
C12—H12···O1	0.98	2.49	3.268 (6)	137
C10—H10A···O3^{i}	0.97	2.36	3.292 (5)	161

Symmetry code: (i) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-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*.

The authors acknowledge financial support from the National Natural Science Foundation of China (grant No. 20572029), the New Century Excellent Talents in Universities (grant No. NCET-04-0743), and the Cultivation Fund of the Key Scientific and Technical Innovation Project, Ministry of Education of China (grant No. 705039).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2250).

References

Boiadjiev, S. E. & Lightner, D. A. (2001). *Tetrahedron Asymm.* **12**, 2551–2564.
Bruker (2001). *SAINT-Plus* (Version 6.45), *SMART* (Version 5.628) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Oppolzer, W. (1989). *Tetrahedron Lett.* **41**, 5603–5606.
Oppolzer, W. (1990). *Pure Appl. Chem.* **62**, 1241–1250.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807067980

supporting information

Acta Cryst. (2008). E**64**, o454 [doi:10.1107/S1600536807067980]

(+)-*N*-[2-(4-Chlorophenyl)propanoyl]bornane-10,2-sultam

Wen-Chang Lu, Jun Cao, Chen Cheng, Guang-Ao Yu and Sheng-Hua Liu

S1. Comment

Pioneering work of Oppolzer (1990) has resulted in the development of bornane[10,2]sultam serve as popular and widely used chiral auxiliaries in asymmetric synthesis. The resulting asymmetric induction using these auxiliaries are high in carbon-carbon bond formation such as alkylation (Oppolzer, 1989), and we have focused our attention on this field. In this paper, we present X-ray crystallographic analysis of the title compound, (I).

In (I), the six-membered ring of sultam shows a boat form (Fig. 1). The planes constructed by C3/C2/C1/C6and C3/C4/C5/C6 form a dihedral angle of 110.71°. The C7/C8/C9 plane makes dihedral angles of 93.92 and 90.93°, respectively, with C3/C2/C1/C6 and C3/C4/C5/C6 planes. Molecules are linked by the intermolecular C—H···O hydrogen bonds into a one-dimensional chain. No direction-specific interactions were observed between the adjacent chains along the *b* axis (Fig. 2).

S2. Experimental

For the preparation of compound (I), 2.4 ml n-BuLi (hexane, 2.5 mol/*L*) was added over 30 min to the THF (25 ml) solution of (+)-*N*-[2-(4-chlorophenyl)-ethanoyl]bornane-10,2-sultam (1.84 g, 5 mmol) at 193 K. After stirring the mixture at 193 K for 1 h, iodomethane 1.6 ml in 4.5 ml HMPA was added and then stirred at 193 K for 3 h. The solution was slowly warming up to room temperature, quenched with water and extracted bt Et_2O to afford a crude product. Single crystals appropriate for data collection were obtained by slow evaporation of a dichloromethane solution at 293 K.

S3. Refinement

All H atoms were constrained to an ideal geometry (C—H = 0.93 - 0.98 Å) and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The ratio of the twin components (major to minor) in crystal selected for diffraction is 0.73 (1):0.27 (1). The absolute configuration of the sultam unit is consistent with the known absolute configuration of (+)-2,10-sultam (Boiadjiev & Lightner, 2001). The major component is (+)-*N*-[(2*S*)-(4-chlorophenyl)-propanoyl] bornane-10,2-sultam, and the minor is (+)-*N*-[(2*R*)-(4-chlorophenyl)-propanoyl] bornane-10,2-sultam. The result was confirmed by HPLC.

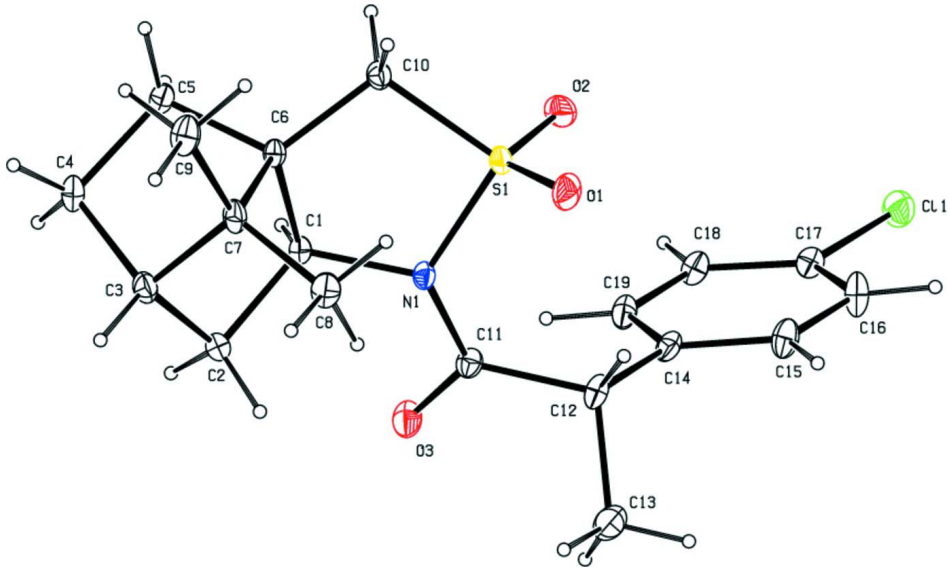


Figure 1

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

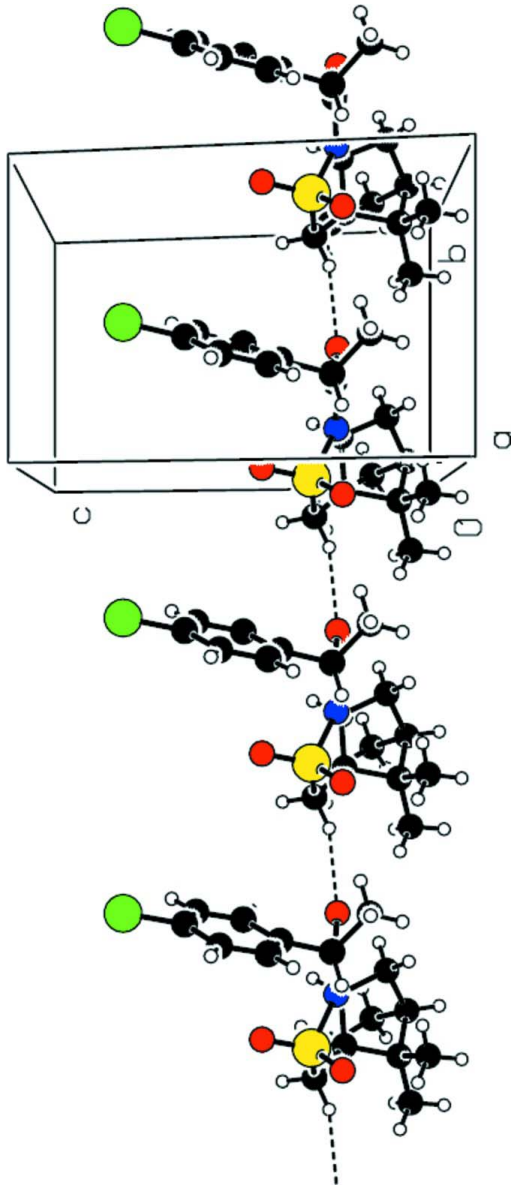


Figure 2

Part of the crystal packing, showing the formation of the one-dimensional chain formed by a C10—H10A···O3 hydrogen bond.

(+)-*N*-[2-(4-Chlorophenyl)propanoyl]bornane-10,2-sultam

Crystal data

$C_{19}H_{24}ClNO_3S$
$M_r = 381.90$
Monoclinic, *C*2
Hall symbol: C 2y
$a = 21.0863\ (16)$ Å
$b = 7.7948\ (6)$ Å
$c = 12.102\ (1)$ Å
$\beta = 107.433\ (1)°$
$V = 1897.8\ (3)$ Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.337$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2555 reflections
$\theta = 2.8–26.0°$
$\mu = 0.33$ mm^{-1}

T = 295 K
Block, colorless

0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
5780 measured reflections
3715 independent reflections

3146 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.0°, θ_{min} = 1.8°
h = −25→26
k = −9→9
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.180
S = 1.10
3715 reflections
229 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1128P)^2 + 0.2113P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 1503 Friedel pairs
Absolute structure parameter: 0.27 (1)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.41765 (17)	0.1484 (5)	0.2515 (3)	0.0363 (8)
H1	0.4074	0.1971	0.3188	0.044*
C2	0.3700 (2)	0.2236 (6)	0.1388 (4)	0.0492 (10)
H2A	0.3436	0.3165	0.1552	0.059*
H2B	0.3942	0.2647	0.0873	0.059*
C3	0.32641 (19)	0.0678 (7)	0.0869 (4)	0.0501 (10)
H3	0.3002	0.0816	0.0056	0.060*
C4	0.28491 (19)	0.0218 (7)	0.1686 (4)	0.0568 (12)
H4A	0.2497	−0.0582	0.1318	0.068*
H4B	0.2655	0.1236	0.1913	0.068*
C5	0.33625 (18)	−0.0616 (6)	0.2743 (4)	0.0463 (10)
H5A	0.3387	−0.0004	0.3453	0.056*
H5B	0.3256	−0.1810	0.2829	0.056*

C6	0.40133 (17)	−0.0439 (5)	0.2421 (3)	0.0364 (8)
C7	0.37733 (19)	−0.0803 (6)	0.1092 (3)	0.0486 (10)
C8	0.4297 (2)	−0.0585 (7)	0.0450 (4)	0.0582 (13)
H8A	0.4640	−0.1429	0.0721	0.087*
H8B	0.4488	0.0542	0.0595	0.087*
H8C	0.4090	−0.0731	−0.0367	0.087*
C9	0.3474 (3)	−0.2582 (7)	0.0795 (5)	0.0661 (14)
H9A	0.3291	−0.2688	−0.0030	0.099*
H9B	0.3128	−0.2747	0.1150	0.099*
H9C	0.3813	−0.3433	0.1076	0.099*
C10	0.46138 (18)	−0.1414 (5)	0.3168 (4)	0.0421 (9)
H10A	0.4653	−0.2514	0.2819	0.051*
H10B	0.4570	−0.1614	0.3933	0.051*
C11	0.5168 (2)	0.3268 (5)	0.2714 (4)	0.0438 (9)
C12	0.59037 (19)	0.3421 (6)	0.2804 (4)	0.0511 (11)
H12	0.6053	0.2315	0.2587	0.061*
C13	0.5985 (3)	0.4787 (9)	0.1933 (5)	0.0770 (15)
H13A	0.5714	0.4486	0.1168	0.115*
H13B	0.6443	0.4837	0.1947	0.115*
H13C	0.5851	0.5886	0.2142	0.115*
C14	0.63302 (19)	0.3854 (6)	0.4024 (4)	0.0475 (10)
C15	0.7005 (2)	0.3585 (7)	0.4306 (5)	0.0612 (13)
H15	0.7185	0.3183	0.3741	0.073*
C16	0.7427 (2)	0.3902 (9)	0.5418 (5)	0.0722 (16)
H16	0.7879	0.3674	0.5602	0.087*
C17	0.7166 (2)	0.4547 (6)	0.6224 (4)	0.0513 (11)
C18	0.6501 (2)	0.4816 (7)	0.5981 (4)	0.0541 (10)
H18	0.6327	0.5210	0.6555	0.065*
C19	0.6085 (2)	0.4500 (6)	0.4877 (4)	0.0525 (11)
H19	0.5633	0.4726	0.4706	0.063*
Cl1	0.76886 (6)	0.4977 (2)	0.76187 (10)	0.0713 (4)
N1	0.48941 (14)	0.1662 (4)	0.2660 (3)	0.0379 (7)
O1	0.57014 (16)	−0.0733 (5)	0.2551 (4)	0.0704 (10)
O2	0.56815 (15)	0.0226 (5)	0.4436 (3)	0.0658 (9)
O3	0.48162 (16)	0.4517 (4)	0.2627 (3)	0.0652 (9)
S1	0.53270 (4)	−0.01249 (12)	0.32646 (8)	0.0425 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0282 (16)	0.043 (2)	0.0375 (19)	0.0012 (14)	0.0089 (15)	−0.0034 (15)
C2	0.036 (2)	0.055 (3)	0.054 (2)	0.0044 (18)	0.0085 (19)	0.0126 (19)
C3	0.035 (2)	0.070 (3)	0.040 (2)	0.0050 (19)	0.0048 (16)	0.0042 (19)
C4	0.0293 (17)	0.074 (3)	0.064 (3)	−0.0003 (19)	0.0094 (18)	−0.005 (2)
C5	0.0349 (19)	0.054 (3)	0.050 (2)	−0.0066 (16)	0.0133 (17)	−0.0024 (18)
C6	0.0295 (16)	0.042 (2)	0.0350 (17)	−0.0029 (14)	0.0053 (13)	−0.0059 (15)
C7	0.0311 (18)	0.068 (3)	0.040 (2)	−0.0032 (18)	0.0003 (16)	−0.0083 (19)
C8	0.050 (2)	0.086 (4)	0.039 (2)	−0.003 (2)	0.0138 (17)	−0.007 (2)

C9	0.050 (3)	0.078 (4)	0.062 (3)	−0.019 (2)	0.006 (2)	−0.027 (3)
C10	0.0339 (18)	0.042 (2)	0.046 (2)	−0.0011 (16)	0.0052 (16)	−0.0013 (17)
C11	0.040 (2)	0.040 (2)	0.050 (2)	−0.0063 (16)	0.0127 (17)	−0.0082 (17)
C12	0.0341 (19)	0.058 (3)	0.064 (3)	−0.0119 (18)	0.0193 (19)	−0.014 (2)
C13	0.065 (3)	0.094 (4)	0.074 (3)	−0.021 (3)	0.024 (3)	0.007 (4)
C14	0.040 (2)	0.039 (2)	0.069 (3)	−0.0104 (16)	0.023 (2)	−0.0057 (19)
C15	0.044 (2)	0.073 (3)	0.075 (3)	−0.001 (2)	0.029 (2)	−0.020 (3)
C16	0.032 (2)	0.099 (4)	0.082 (4)	0.000 (2)	0.011 (2)	−0.023 (3)
C17	0.045 (2)	0.053 (3)	0.056 (2)	−0.0047 (19)	0.0165 (19)	−0.002 (2)
C18	0.045 (2)	0.063 (3)	0.060 (2)	−0.009 (2)	0.0233 (18)	−0.009 (2)
C19	0.0355 (19)	0.049 (3)	0.075 (3)	−0.0019 (17)	0.0184 (19)	−0.009 (2)
Cl1	0.0574 (6)	0.0895 (9)	0.0600 (7)	−0.0096 (7)	0.0069 (5)	0.0001 (7)
N1	0.0274 (14)	0.0417 (17)	0.0414 (17)	−0.0041 (13)	0.0053 (13)	−0.0031 (13)
O1	0.0474 (17)	0.065 (2)	0.110 (3)	0.0134 (15)	0.0403 (19)	0.0048 (19)
O2	0.0575 (18)	0.068 (2)	0.0543 (17)	−0.0164 (16)	−0.0104 (14)	0.0087 (16)
O3	0.0473 (16)	0.0416 (19)	0.103 (3)	−0.0022 (13)	0.0172 (17)	−0.0090 (16)
S1	0.0290 (4)	0.0460 (5)	0.0476 (5)	0.0002 (4)	0.0041 (3)	0.0030 (5)

Geometric parameters (Å, º)

C1—N1	1.477 (4)	C10—S1	1.783 (4)
C1—C6	1.535 (6)	C10—H10A	0.9700
C1—C2	1.547 (5)	C10—H10B	0.9700
C1—H1	0.9800	C11—O3	1.209 (5)
C2—C3	1.539 (6)	C11—N1	1.371 (5)
C2—H2A	0.9700	C11—C12	1.528 (5)
C2—H2B	0.9700	C12—C14	1.518 (6)
C3—C7	1.544 (6)	C12—C13	1.544 (8)
C3—C4	1.545 (6)	C12—H12	0.9800
C3—H3	0.9800	C13—H13A	0.9600
C4—C5	1.549 (6)	C13—H13B	0.9600
C4—H4A	0.9700	C13—H13C	0.9600
C4—H4B	0.9700	C14—C15	1.377 (6)
C5—C6	1.541 (5)	C14—C19	1.380 (6)
C5—H5A	0.9700	C15—C16	1.395 (7)
C5—H5B	0.9700	C15—H15	0.9300
C6—C10	1.521 (5)	C16—C17	1.351 (7)
C6—C7	1.561 (5)	C16—H16	0.9300
C7—C9	1.522 (7)	C17—C18	1.360 (6)
C7—C8	1.538 (6)	C17—Cl1	1.749 (4)
C8—H8A	0.9600	C18—C19	1.384 (6)
C8—H8B	0.9600	C18—H18	0.9300
C8—H8C	0.9600	C19—H19	0.9300
C9—H9A	0.9600	N1—S1	1.706 (3)
C9—H9B	0.9600	O1—S1	1.415 (4)
C9—H9C	0.9600	O2—S1	1.417 (3)
N1—C1—C6	107.4 (3)	C7—C9—H9C	109.5

N1—C1—C2	116.2 (3)	H9A—C9—H9C	109.5
C6—C1—C2	103.4 (3)	H9B—C9—H9C	109.5
N1—C1—H1	109.8	C6—C10—S1	107.0 (3)
C6—C1—H1	109.8	C6—C10—H10A	110.3
C2—C1—H1	109.8	S1—C10—H10A	110.3
C3—C2—C1	102.2 (3)	C6—C10—H10B	110.3
C3—C2—H2A	111.3	S1—C10—H10B	110.3
C1—C2—H2A	111.3	H10A—C10—H10B	108.6
C3—C2—H2B	111.3	O3—C11—N1	119.5 (4)
C1—C2—H2B	111.3	O3—C11—C12	121.7 (4)
H2A—C2—H2B	109.2	N1—C11—C12	118.6 (4)
C2—C3—C7	102.7 (3)	C14—C12—C11	112.3 (3)
C2—C3—C4	107.8 (4)	C14—C12—C13	110.8 (4)
C7—C3—C4	102.3 (4)	C11—C12—C13	108.9 (4)
C2—C3—H3	114.3	C14—C12—H12	108.2
C7—C3—H3	114.3	C11—C12—H12	108.2
C4—C3—H3	114.3	C13—C12—H12	108.2
C3—C4—C5	103.6 (3)	C12—C13—H13A	109.5
C3—C4—H4A	111.0	C12—C13—H13B	109.5
C5—C4—H4A	111.0	H13A—C13—H13B	109.5
C3—C4—H4B	111.0	C12—C13—H13C	109.5
C5—C4—H4B	111.0	H13A—C13—H13C	109.5
H4A—C4—H4B	109.0	H13B—C13—H13C	109.5
C6—C5—C4	102.0 (3)	C15—C14—C19	117.4 (4)
C6—C5—H5A	111.4	C15—C14—C12	118.3 (4)
C4—C5—H5A	111.4	C19—C14—C12	124.2 (4)
C6—C5—H5B	111.4	C14—C15—C16	121.6 (4)
C4—C5—H5B	111.4	C14—C15—H15	119.2
H5A—C5—H5B	109.2	C16—C15—H15	119.2
C10—C6—C1	108.4 (3)	C17—C16—C15	118.9 (4)
C10—C6—C5	116.8 (3)	C17—C16—H16	120.5
C1—C6—C5	105.4 (3)	C15—C16—H16	120.5
C10—C6—C7	118.5 (3)	C16—C17—C18	121.1 (4)
C1—C6—C7	104.5 (3)	C16—C17—Cl1	119.6 (3)
C5—C6—C7	101.9 (3)	C18—C17—Cl1	119.3 (3)
C9—C7—C8	106.9 (4)	C17—C18—C19	119.7 (4)
C9—C7—C3	115.0 (4)	C17—C18—H18	120.1
C8—C7—C3	113.4 (4)	C19—C18—H18	120.1
C9—C7—C6	113.1 (4)	C14—C19—C18	121.1 (4)
C8—C7—C6	116.1 (3)	C14—C19—H19	119.4
C3—C7—C6	92.2 (3)	C18—C19—H19	119.4
C7—C8—H8A	109.5	C11—N1—C1	119.5 (3)
C7—C8—H8B	109.5	C11—N1—S1	124.2 (3)
H8A—C8—H8B	109.5	C1—N1—S1	111.8 (3)
C7—C8—H8C	109.5	O1—S1—O2	116.8 (2)
H8A—C8—H8C	109.5	O1—S1—N1	109.7 (2)
H8B—C8—H8C	109.5	O2—S1—N1	109.0 (2)
C7—C9—H9A	109.5	O1—S1—C10	112.6 (2)

C7—C9—H9B	109.5	O2—S1—C10	110.9 (2)
H9A—C9—H9B	109.5	N1—S1—C10	95.73 (16)
N1—C1—C2—C3	124.3 (3)	N1—C11—C12—C14	−103.2 (4)
C6—C1—C2—C3	6.9 (4)	O3—C11—C12—C13	−42.4 (6)
C1—C2—C3—C7	−41.2 (4)	N1—C11—C12—C13	133.6 (4)
C1—C2—C3—C4	66.3 (4)	C11—C12—C14—C15	163.0 (4)
C2—C3—C4—C5	−73.6 (4)	C13—C12—C14—C15	−75.0 (6)
C7—C3—C4—C5	34.3 (4)	C11—C12—C14—C19	−16.9 (6)
C3—C4—C5—C6	2.8 (5)	C13—C12—C14—C19	105.2 (5)
N1—C1—C6—C10	33.0 (4)	C19—C14—C15—C16	1.9 (8)
C2—C1—C6—C10	156.4 (3)	C12—C14—C15—C16	−178.0 (5)
N1—C1—C6—C5	158.8 (3)	C14—C15—C16—C17	−2.4 (9)
C2—C1—C6—C5	−77.8 (3)	C15—C16—C17—C18	3.0 (9)
N1—C1—C6—C7	−94.3 (3)	C15—C16—C17—Cl1	−179.2 (4)
C2—C1—C6—C7	29.1 (4)	C16—C17—C18—C19	−3.0 (8)
C4—C5—C6—C10	−169.3 (4)	Cl1—C17—C18—C19	179.2 (4)
C4—C5—C6—C1	70.3 (4)	C15—C14—C19—C18	−1.9 (7)
C4—C5—C6—C7	−38.6 (4)	C12—C14—C19—C18	178.0 (5)
C2—C3—C7—C9	173.1 (4)	C17—C18—C19—C14	2.4 (8)
C4—C3—C7—C9	61.4 (5)	O3—C11—N1—C1	−1.0 (6)
C2—C3—C7—C8	−63.5 (4)	C12—C11—N1—C1	−177.0 (3)
C4—C3—C7—C8	−175.2 (3)	O3—C11—N1—S1	−155.2 (4)
C2—C3—C7—C6	56.3 (4)	C12—C11—N1—S1	28.7 (5)
C4—C3—C7—C6	−55.5 (3)	C6—C1—N1—C11	177.1 (3)
C10—C6—C7—C9	69.0 (5)	C2—C1—N1—C11	61.9 (5)
C1—C6—C7—C9	−170.2 (4)	C6—C1—N1—S1	−25.7 (4)
C5—C6—C7—C9	−60.7 (4)	C2—C1—N1—S1	−140.9 (3)
C10—C6—C7—C8	−55.2 (5)	C11—N1—S1—O1	−78.3 (4)
C1—C6—C7—C8	65.6 (5)	C1—N1—S1—O1	125.7 (3)
C5—C6—C7—C8	175.1 (4)	C11—N1—S1—O2	50.7 (4)
C10—C6—C7—C3	−172.6 (3)	C1—N1—S1—O2	−105.2 (3)
C1—C6—C7—C3	−51.8 (3)	C11—N1—S1—C10	165.1 (3)
C5—C6—C7—C3	57.7 (4)	C1—N1—S1—C10	9.2 (3)
C1—C6—C10—S1	−26.2 (4)	C6—C10—S1—O1	−103.7 (3)
C5—C6—C10—S1	−145.0 (3)	C6—C10—S1—O2	123.2 (3)
C7—C6—C10—S1	92.5 (4)	C6—C10—S1—N1	10.3 (3)
O3—C11—C12—C14	80.8 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*B*···N1	0.96	2.54	3.129 (6)	120
C19—H19···O3	0.93	2.59	3.196 (6)	123
C12—H12···O1	0.98	2.49	3.268 (6)	137
C10—H10*A*···O3^{i}	0.97	2.36	3.292 (5)	161

Symmetry code: (i) *x*, *y*−1, *z*.