

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(3*aR*,6*S*,7*aR*)-7*a*-Bromo-2-[(4-methylphenyl)sulfonyl]-1,2,3,6,7,7*a*-hexahydro-3*a*,6-epoxyisoindole

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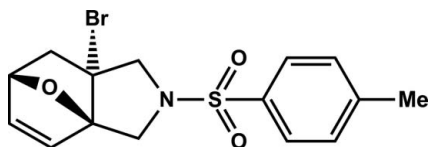
Received 5 March 2011; accepted 22 March 2011

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.048; wR factor = 0.126; data-to-parameter ratio = 16.6.

In the title compound, $\text{C}_{15}\text{H}_{16}\text{BrNO}_3\text{S}$, the boat form of the six-membered ring is almost symmetrical with respect to the epoxy bridge. The two five-membered rings generated by the epoxy bridge of the six-membered ring adopt envelope conformations, whereas the N-containing five-membered ring adopts a twisted conformation. In the crystal, molecules are linked by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For general background to intramolecular Diels–Alder reactions and heteroaromatic Diels–Alder reactions, see: Dell (1998); Kappe *et al.* (1997); Arai *et al.* (2010); Lohse & Hsung (2009). For related structures, see: Koşar *et al.* (2006, 2007*a,b*). For the synthesis of the title compound and related compounds, see: Carlini *et al.* (1997); Hart *et al.* (1997); Shing *et al.* (1996); Karaarslan *et al.* (2007); Pontén & Magnusson (1997); Demircan *et al.* (2006); Arslan & Demircan (2008); Demircan & Parsons (1998). For puckering analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{16}\text{BrNO}_3\text{S}$
 $M_r = 370.26$
Monoclinic, $P2_1/c$

$a = 16.5136$ (6) Å
 $b = 6.2186$ (3) Å
 $c = 16.3487$ (7) Å

$\beta = 113.802$ (3)°
 $V = 1536.07$ (12) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 2.82$ mm⁻¹
 $T = 296$ K
 $0.58 \times 0.44 \times 0.31$ mm

Data collection

STOE IPDS 2 CCD diffractometer
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)
 $T_{\min} = 0.310$, $T_{\max} = 0.495$

7305 measured reflections
3163 independent reflections
2353 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.126$
 $S = 1.07$
3163 reflections

190 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.44$ e Å⁻³

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C6}-\text{H6A}\cdots\text{O1}^i$	0.97	2.50	3.382 (6)	151

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *OLEX2*, *PUBLICIF* (Westrip, 2010) and *Mercury* (Macrae *et al.*, 2006).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the diffractometer (purchased under grant F.279 of University Research Fund) and also the Scientific & Technological Research Council of Turkey (TÜBİTAK) for financial support of this work (PN: 107 T831).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2354).

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supplementary materials

Acta Cryst. (2011). E67, o994-o995 [doi:10.1107/S1600536811010750]

(3a*R*,6*S*,7a*R*)-7a-Bromo-2-[(4-methylphenyl)sulfonyl]-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole

B. Kosar, A. Demircan, H. Arslan and O. Büyükgüngör

Comment

Thermal intramolecular [4 + 2] type cycloaddition processes, or intramolecular Diels Alder (IMDA) reactions, have been a highly useful tool for the construction of many cycloaddition products (Dell, 1998). The IMDA reaction is especially useful for asymmetrical syntheses towards natural products such as, (\pm)-xestoquinone (Carlini *et al.*, 1997), (+)-himbelive (Hart *et al.*, 1997) and (S)-(\pm)-carvone (Shing *et al.*, 1996). In this context, the use of heteroaromatic compounds has been gaining popularity (Kappe *et al.*, 1997). IMDA reactions with furan derivatives, called IMDAF, have been widely used for the construction of some new molecules (Karaarslan *et al.*, 2007; Pontén & Magnusson, 1997; Demircan *et al.*, 2006; Koşar *et al.*, 2007a; Koşar *et al.*, 2007b; Arslan & Demircan, 2008; Demircan & Parsons, 1998; Koşar *et al.*, 2006). These compounds have been used as strategic intermediates in combinatorial synthesis.

In view of a recent literature research (Arai *et al.*, 2010; Lohse & Hsung, 2009), we would like to report here a thermal IMDAF reaction of an alkenyl furan with a nitrogen linked chain which undergoes intramolecular cycloaddition upon heating to 371 K for two days (Fig. 1 and 2). The product of the intramolecular thermal cycloaddition reaction of compound (I) was characterized by ^1H NMR, ^{13}C NMR, FT-IR, MS, elemental analysis and X-ray single crystal diffraction studies. Despite of the presence of three new stereocenters in the product molecules only one pair of mirror symmetric enantiomers was formed in the reaction, i.e. the intramolecular thermal cycloaddition of II to I is diastereoselective under the chosen reaction conditions.

Related with the above mentioned reaction, we presented here the crystal structure of the title compound, $\text{C}_{15}\text{H}_{16}\text{BrNO}_3\text{S}$. Fig. 1 shows the molecular structure of the title compound, I. The pyrrolidine (C4/C5/N1/C6/C7) ring adopts a twisted conformation with a total puckering parameter Q_{T} value of 0.329 (5) Å (Cremer & Pople, 1975). The tetrahydrofuran (O1/C1-C4) and bromo-attached tetrahydrofuran (O1/C4/C7/C8/C1) rings adopt envelope conformations with total puckering parameters of 0.514 (5) and 0.627 (5) Å, respectively.

The title compound displays an intramolecular hydrogen bond between atoms C10 and O2 and the crystal structure is stabilized by weak van der Waals interactions and a weak intermolecular hydrogen bond, C6—H6a \cdots O1 in a three dimensional network (Fig. 3). Geometrical parameters of the intra- and intermolecular H-bonds are listed in Table 1.

Experimental

N-(2-Bromoprop-2-en-1-yl)-4-methyl-*N*-[(5-methyl-2-furyl)methyl]benzenesulfonamide, II, (1 g, 2.7 mmol) was stirred and heated under reflux in water (25 mL) at 372 K for two days (Fig. 2). The mixture was poured into ethyl acetate (25 mL) and the aqueous phase was washed with excess ethyl acetate (2 x 25 mL). The combined organic phases were dried over magnesium sulphate and filtered off. The solvent was then removed under reduced pressure. The residue was subjected to flash column chromatography (R_{f} (Hexane:Ethyl acetate = 7:3): 0.47) to afford I (0.7 g, 70 % yield) as yellow crystals. M. p.: 396-398 K, ν_{max} (Thin film) / cm^{-1} : 2932 (s, CH), 2161 (m, SO), 1977 (m, S=O), 1453, 1159, 1065 (s, C-O). δ_{H} (400 MHz, CDCl_3): 7.67 (d, 2H, $J = 8$ Hz), 7.24 (d, 2H, $J = 8$ Hz, H10-H13), 6.40 (dd, 1H, $J = 5.6$ Hz, $J = 1.8$ Hz, AB), 6.34

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(d, 1H, $J = 5.6$ Hz, AB), 4.95 (dd, 1H, $J = 4.5$ Hz, $J = 1.8$ Hz), 4.06 (d, 1H, $J = 12$ Hz), 4.01 (d, 1H, $J = 12$ Hz), 3.67 (d, 1H, $J = 12$ Hz), 3.43 (d, 1H, $J = 12$ Hz), 2.39 (dd, 1H, $J = 4.5$ Hz, $J = 12$ Hz), 2.36 (s, 3H), 1.63 (d, 1H, $J = 12$ Hz). δ_C (100 MHz, $CDCl_3$): 143.8, 137.2, 134.7, 134.5, 129.9 (2 x C), 127.7 (2 x C), 97.2, 81.0, 64.0, 63.3, 47.5, 41.4, 21.7. m/z (70 eV, EI): 371,00 [$M^+(\text{}^{81}\text{Br})$, 42%], 369, [$M^+(\text{}^{79}\text{Br})$, 42%], 216,00 [$M^+(\text{}^{81}\text{Br})\text{-Ts}$, 100%], 214 [$M^+(\text{}^{79}\text{Br})\text{-H+Ts}$, 100%]. Elemental Analysis ($C_{15}H_{16}BrNO_3S$): % Calculated (Found): C, 48.66 (48.72); H, 4.36 (4.39); N, 3.78 (3.74).

Refinement

H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.96, 0.97, 0.98 and 0.93 Å for CH_3 , CH_2 , CH and CH (aromatic), respectively. The displacement parameters of the H atoms were constrained with $U_{iso}(H) = 1.2U_{eq}$ (aromatic, methylene or methine C) or $1.5U_{eq}$ (methyl C).

Figures

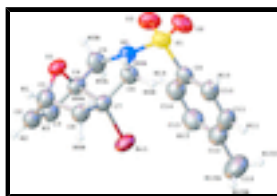


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.



Fig. 2. Synthesis of the title compound.

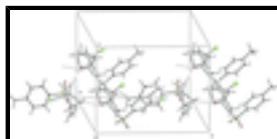


Fig. 3. A packing diagram of the title compound. Dashed lines indicate the O—H...O intermolecular hydrogen bonds.

(3a*R*,6*S*,7a*R*)-7a-Bromo-2-[(4-methylphenyl)sulfonyl]-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole

Crystal data

$C_{15}H_{16}BrNO_3S$

$M_r = 370.26$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 16.5136$ (6) Å

$b = 6.2186$ (3) Å

$c = 16.3487$ (7) Å

$\beta = 113.802$ (3)°

$V = 1536.07$ (12) Å³

$Z = 4$

$F(000) = 752$

$D_x = 1.601$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 10108 reflections

$\theta = 1.5\text{--}28.0^\circ$

$\mu = 2.82$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.58 \times 0.44 \times 0.31$ mm

Data collection

STOE IPDS 2 CCD

3163 independent reflections

diffractometer
 Radiation source: fine-focus sealed tube
 plane graphite
 Detector resolution: 6.67 pixels mm⁻¹
 rotation method scans
 Absorption correction: integration
 (*X-RED32*; Stoe & Cie, 2002)
 $T_{\min} = 0.310$, $T_{\max} = 0.495$
 7305 measured reflections

2353 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$
 $\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 2.5^\circ$
 $h = -20 \rightarrow 20$
 $k = -7 \rightarrow 7$
 $l = -20 \rightarrow 20$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.126$
 $S = 1.07$
 3163 reflections
 190 parameters
 0 restraints

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
 $w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 0.5082P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.44 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.9623 (3)	0.6757 (7)	0.0923 (3)	0.0640 (11)
H1	1.0211	0.7174	0.0966	0.077*
C2	0.9042 (3)	0.5742 (8)	0.0062 (3)	0.0681 (12)
H2	0.9082	0.5913	-0.0485	0.082*
C3	0.8459 (3)	0.4559 (7)	0.0218 (3)	0.0617 (10)
H3	0.8013	0.3717	-0.0189	0.074*
C4	0.8668 (3)	0.4857 (6)	0.1192 (3)	0.0537 (9)
C5	0.8358 (3)	0.3394 (6)	0.1725 (3)	0.0642 (11)
H5A	0.7765	0.2875	0.1372	0.077*

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H5B	0.8753	0.2172	0.1945	0.077*
C6	0.8569 (3)	0.7032 (6)	0.2354 (3)	0.0519 (9)
H6A	0.9170	0.7400	0.2752	0.062*
H6B	0.8163	0.7984	0.2472	0.062*
C7	0.8443 (3)	0.7184 (6)	0.1376 (3)	0.0489 (8)
C8	0.9107 (3)	0.8549 (7)	0.1161 (3)	0.0571 (10)
H8A	0.9488	0.9380	0.1674	0.069*
H8B	0.8812	0.9506	0.0660	0.069*
C9	0.6718 (3)	0.5012 (6)	0.2434 (3)	0.0526 (9)
C10	0.6473 (3)	0.7028 (7)	0.2619 (3)	0.0617 (10)
H10	0.6869	0.7852	0.3082	0.074*
C11	0.5636 (4)	0.7800 (8)	0.2109 (4)	0.0736 (13)
H11	0.5473	0.9149	0.2236	0.088*
C12	0.5033 (3)	0.6607 (9)	0.1410 (3)	0.0724 (12)
C13	0.5291 (3)	0.4605 (9)	0.1249 (3)	0.0725 (12)
H13	0.4891	0.3777	0.0790	0.087*
C14	0.6117 (3)	0.3787 (7)	0.1743 (3)	0.0627 (11)
H14	0.6273	0.2429	0.1617	0.075*
C15	0.4125 (5)	0.7472 (12)	0.0862 (5)	0.117 (2)
H15A	0.3802	0.6448	0.0408	0.175*
H15B	0.4175	0.8799	0.0586	0.175*
H15C	0.3818	0.7722	0.1242	0.175*
N1	0.8373 (2)	0.4748 (5)	0.2466 (2)	0.0526 (8)
O1	0.96199 (18)	0.5098 (4)	0.15645 (19)	0.0589 (7)
O2	0.8163 (2)	0.5198 (5)	0.38595 (19)	0.0729 (8)
O3	0.7776 (2)	0.1766 (5)	0.3018 (2)	0.0707 (8)
S1	0.78021 (8)	0.40698 (16)	0.30290 (6)	0.0559 (3)
Br1	0.71982 (3)	0.78750 (8)	0.06223 (3)	0.06777 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.060 (3)	0.068 (3)	0.066 (3)	0.007 (2)	0.028 (2)	0.000 (2)
C2	0.082 (3)	0.067 (3)	0.057 (2)	0.019 (2)	0.030 (2)	-0.001 (2)
C3	0.072 (3)	0.057 (2)	0.055 (2)	0.006 (2)	0.024 (2)	-0.0128 (19)
C4	0.058 (2)	0.043 (2)	0.054 (2)	0.0055 (17)	0.0174 (19)	-0.0063 (17)
C5	0.088 (3)	0.041 (2)	0.069 (3)	-0.003 (2)	0.038 (3)	-0.0124 (19)
C6	0.062 (2)	0.0406 (19)	0.053 (2)	-0.0077 (17)	0.0232 (19)	-0.0103 (17)
C7	0.050 (2)	0.0403 (18)	0.052 (2)	0.0033 (16)	0.0160 (17)	-0.0051 (16)
C8	0.064 (3)	0.047 (2)	0.061 (2)	0.0017 (18)	0.026 (2)	-0.0006 (18)
C9	0.064 (2)	0.044 (2)	0.054 (2)	-0.0029 (18)	0.029 (2)	0.0008 (17)
C10	0.069 (3)	0.052 (2)	0.067 (3)	-0.002 (2)	0.031 (2)	-0.008 (2)
C11	0.084 (3)	0.059 (3)	0.090 (3)	0.013 (2)	0.048 (3)	0.003 (2)
C12	0.063 (3)	0.083 (3)	0.073 (3)	0.007 (2)	0.030 (2)	0.004 (3)
C13	0.066 (3)	0.078 (3)	0.069 (3)	-0.011 (2)	0.022 (2)	-0.009 (2)
C14	0.068 (3)	0.052 (2)	0.069 (3)	-0.006 (2)	0.029 (2)	-0.008 (2)
C15	0.087 (4)	0.140 (6)	0.113 (5)	0.038 (4)	0.029 (4)	0.004 (4)
N1	0.065 (2)	0.0388 (16)	0.0541 (18)	0.0059 (14)	0.0239 (16)	-0.0009 (13)

O1	0.0538 (16)	0.0582 (17)	0.0582 (16)	0.0158 (13)	0.0159 (13)	0.0002 (13)
O2	0.092 (2)	0.077 (2)	0.0429 (14)	-0.0032 (18)	0.0201 (15)	-0.0060 (14)
O3	0.089 (2)	0.0489 (17)	0.0693 (19)	0.0038 (15)	0.0267 (18)	0.0154 (14)
S1	0.0708 (7)	0.0462 (5)	0.0474 (5)	0.0020 (4)	0.0203 (5)	0.0036 (4)
Br1	0.0521 (2)	0.0697 (3)	0.0701 (3)	0.0172 (2)	0.01277 (19)	0.0041 (2)

Geometric parameters (Å, °)

C1—O1	1.472 (5)	C8—H8A	0.9700
C1—C2	1.487 (7)	C8—H8B	0.9700
C1—C8	1.544 (6)	C9—C10	1.388 (6)
C1—H1	0.9800	C9—C14	1.392 (6)
C2—C3	1.316 (7)	C9—S1	1.757 (4)
C2—H2	0.9300	C10—C11	1.380 (7)
C3—C4	1.498 (5)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.390 (8)
C4—O1	1.446 (5)	C11—H11	0.9300
C4—C5	1.487 (6)	C12—C13	1.375 (7)
C4—C7	1.553 (5)	C12—C15	1.502 (8)
C5—N1	1.467 (5)	C13—C14	1.373 (7)
C5—H5A	0.9700	C13—H13	0.9300
C5—H5B	0.9700	C14—H14	0.9300
C6—N1	1.484 (5)	C15—H15A	0.9600
C6—C7	1.530 (5)	C15—H15B	0.9600
C6—H6A	0.9700	C15—H15C	0.9600
C6—H6B	0.9700	N1—S1	1.616 (3)
C7—C8	1.535 (6)	O2—S1	1.427 (3)
C7—Br1	1.971 (4)	O3—S1	1.433 (3)
O1—C1—C2	101.0 (4)	C1—C8—H8A	111.7
O1—C1—C8	99.5 (3)	C7—C8—H8B	111.7
C2—C1—C8	109.5 (4)	C1—C8—H8B	111.7
O1—C1—H1	115.0	H8A—C8—H8B	109.5
C2—C1—H1	115.0	C10—C9—C14	119.7 (4)
C8—C1—H1	115.0	C10—C9—S1	120.1 (3)
C3—C2—C1	107.2 (4)	C14—C9—S1	120.1 (3)
C3—C2—H2	126.4	C11—C10—C9	119.5 (4)
C1—C2—H2	126.4	C11—C10—H10	120.3
C2—C3—C4	105.3 (4)	C9—C10—H10	120.3
C2—C3—H3	127.3	C10—C11—C12	121.4 (4)
C4—C3—H3	127.3	C10—C11—H11	119.3
O1—C4—C5	112.9 (3)	C12—C11—H11	119.3
O1—C4—C3	101.9 (3)	C13—C12—C11	117.8 (5)
C5—C4—C3	124.1 (4)	C13—C12—C15	121.5 (5)
O1—C4—C7	97.3 (3)	C11—C12—C15	120.7 (5)
C5—C4—C7	106.9 (3)	C14—C13—C12	122.3 (5)
C3—C4—C7	110.5 (3)	C14—C13—H13	118.8
N1—C5—C4	103.8 (3)	C12—C13—H13	118.8
N1—C5—H5A	111.0	C13—C14—C9	119.3 (4)
C4—C5—H5A	111.0	C13—C14—H14	120.4

supplementary materials

N1—C5—H5B	111.0	C9—C14—H14	120.4
C4—C5—H5B	111.0	C12—C15—H15A	109.5
H5A—C5—H5B	109.0	C12—C15—H15B	109.5
N1—C6—C7	104.1 (3)	H15A—C15—H15B	109.5
N1—C6—H6A	110.9	C12—C15—H15C	109.5
C7—C6—H6A	110.9	H15A—C15—H15C	109.5
N1—C6—H6B	110.9	H15B—C15—H15C	109.5
C7—C6—H6B	110.9	C5—N1—C6	112.2 (3)
H6A—C6—H6B	108.9	C5—N1—S1	120.1 (3)
C6—C7—C8	117.7 (3)	C6—N1—S1	121.8 (2)
C6—C7—C4	101.7 (3)	C4—O1—C1	95.1 (3)
C8—C7—C4	102.9 (3)	O2—S1—O3	120.16 (19)
C6—C7—Br1	109.5 (3)	O2—S1—N1	107.28 (19)
C8—C7—Br1	113.4 (3)	O3—S1—N1	105.97 (18)
C4—C7—Br1	110.7 (3)	O2—S1—C9	107.7 (2)
C7—C8—C1	100.1 (3)	O3—S1—C9	107.9 (2)
C7—C8—H8A	111.7	N1—S1—C9	107.18 (17)
O1—C1—C2—C3	31.5 (4)	C10—C11—C12—C13	1.0 (7)
C8—C1—C2—C3	-72.9 (5)	C10—C11—C12—C15	-180.0 (5)
C1—C2—C3—C4	0.8 (5)	C11—C12—C13—C14	-1.0 (7)
C2—C3—C4—O1	-33.6 (4)	C15—C12—C13—C14	-180.0 (5)
C2—C3—C4—C5	-162.1 (4)	C12—C13—C14—C9	0.2 (7)
C2—C3—C4—C7	68.9 (4)	C10—C9—C14—C13	0.6 (6)
O1—C4—C5—N1	80.2 (4)	S1—C9—C14—C13	-176.0 (3)
C3—C4—C5—N1	-156.0 (4)	C4—C5—N1—C6	7.1 (5)
C7—C4—C5—N1	-25.6 (4)	C4—C5—N1—S1	160.4 (3)
N1—C6—C7—C8	-139.8 (3)	C7—C6—N1—C5	14.3 (5)
N1—C6—C7—C4	-28.3 (4)	C7—C6—N1—S1	-138.6 (3)
N1—C6—C7—Br1	88.8 (3)	C5—C4—O1—C1	-174.3 (3)
O1—C4—C7—C6	-82.6 (3)	C3—C4—O1—C1	50.3 (3)
C5—C4—C7—C6	34.1 (4)	C7—C4—O1—C1	-62.5 (3)
C3—C4—C7—C6	171.8 (3)	C2—C1—O1—C4	-49.4 (3)
O1—C4—C7—C8	39.7 (4)	C8—C1—O1—C4	62.7 (3)
C5—C4—C7—C8	156.4 (4)	C5—N1—S1—O2	160.6 (3)
C3—C4—C7—C8	-65.9 (4)	C6—N1—S1—O2	-48.6 (4)
O1—C4—C7—Br1	161.2 (2)	C5—N1—S1—O3	31.1 (4)
C5—C4—C7—Br1	-82.2 (4)	C6—N1—S1—O3	-178.1 (3)
C3—C4—C7—Br1	55.6 (4)	C5—N1—S1—C9	-83.9 (3)
C6—C7—C8—C1	108.8 (4)	C6—N1—S1—C9	66.9 (3)
C4—C7—C8—C1	-2.0 (4)	C10—C9—S1—O2	23.2 (4)
Br1—C7—C8—C1	-121.5 (3)	C14—C9—S1—O2	-160.2 (3)
O1—C1—C8—C7	-35.8 (4)	C10—C9—S1—O3	154.3 (3)
C2—C1—C8—C7	69.5 (4)	C14—C9—S1—O3	-29.1 (4)
C14—C9—C10—C11	-0.6 (6)	C10—C9—S1—N1	-92.0 (3)
S1—C9—C10—C11	176.1 (3)	C14—C9—S1—N1	84.6 (3)
C9—C10—C11—C12	-0.3 (7)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C6—H6A···O1 ⁱ	0.97	2.50	3.382 (6)	151
C10—H10···O2	0.93	2.59	2.937 (6)	103

Symmetry codes: (i) $-x+2, y+1/2, -z+1/2$.

Fig. 1

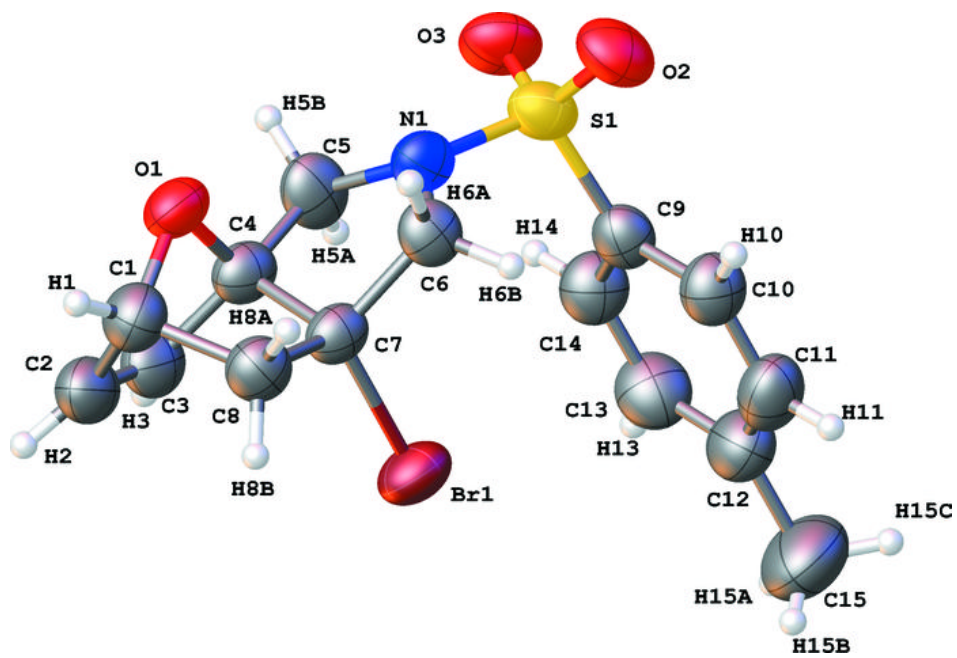


Fig. 2

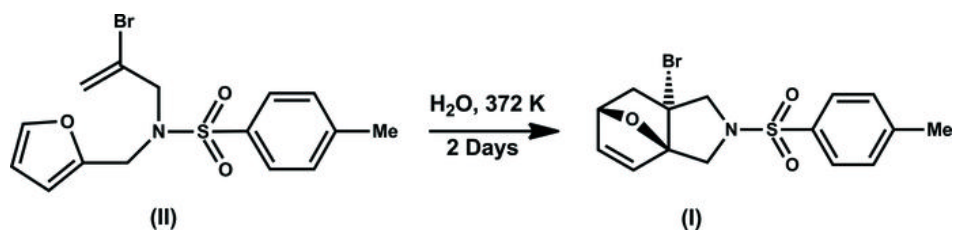


Fig. 3

