C(35*A*)—C(36)—Cl(2)	120.2 (7)	C(18)—C(25)—C(26)	119.6 (6)
C(18)—C(25)—C(26*A*)	121.6 (5)	C(26)—C(25)—C(26*A*)	118.8 (4)
C(25)—C(26)—C(27)	120.7 (8)	C(25)—C(26*A*)—C(27*A*)	118.6 (6)
C(26)—C(27)—C(28)	121.0 (7)	C(26*A*)—C(27*A*)—C(28)	122.8 (8)
C(27)—C(28)—C(27*A*)	118.0 (6)		

Intensities were corrected for Lorentz, polarization and absorption effects. The structure was solved by extracting the positions of the Cl and S atoms from a sharpened Patterson map and extending the structure with a tangent expansion. All H atoms were located by difference synthesis and refined with displacement factors of H fixed to $U(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$ or $1.5U_{\mathrm{eq}}(\mathrm{C_{methyl}})$ or $1.5U_{\mathrm{eq}}(\mathrm{O})$ using a riding model with C—H = 0.96 Å. The coordinates of the hydroxyl H atom were refined with the O—H distance restrained to 0.8500 (1) Å. Refinement was carried out with *XLS* (Sheldrick, 1987). The absolute configuration was determined by η refinement (Rogers, 1981) starting from both configurations [η = 1.0 (1) for the correct structure]. The molecular plot was prepared with *XP* (*SHELXTL-Plus*; Sheldrick, 1991).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SH1080). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A γ-Hydroxyvinylsulfoximine, $C_{23}H_{31}NO_3S$

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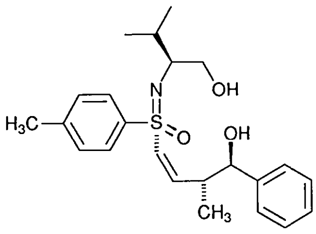
Abstract

The structure of [*S*(S),1*Z*,*N*(1*S*),3*R*,4*R*]-1-{*N*-[1-(hydroxymethyl)-2-methylpropyl]-*S*-(*p*-tolyl)sulfonimidoyl}-3-methyl-4-phenyl-1-buten-4-ol {or *N*-[1-(hydroxymethyl)-2-methylpropyl]-*S*-(4-hydroxy-3-methyl-4-phenyl-1-butenyl)-*S*-(*p*-tolyl)sulfoximide} has been determined. The C=C double bond is *cis* configured. Both hydroxyl groups form intramolecular hydrogen bonds.

Comment

The geometrical parameters of the two intramolecular hydrogen bonds are as follows: O(41)···O(61) 2.915 (3), H(41)···O(61) 2.080 (9) Å, O(41)—H(41)···O(61) 168 (1)° and O(61)···O(1) 2.902 (3), H(61)···O(1) 2.088 (8) Å, O(61)—H(61)···O(6) 160 (1)°. The title compound, (I), is the product of a diastereoselective γ-hydroxyalkylation of an enantiomerically pure crotylsulfoximine (Reggelin & Weinberger, 1994).



(I)

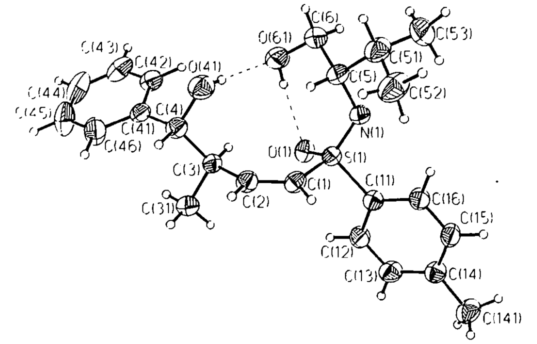


Fig. 1. Perspective view with the atom-numbering scheme, with heavy atoms represented as 30% probability ellipsoids and H atoms as spheres of arbitrary radii.

Experimental

Crystal data

$C_{23}H_{31}NO_3S$	Cu *Kα* radiation
M_r = 401.5	λ = 1.5418 Å
Orthorhombic	Cell parameters from 25 reflections
$P2_12_12_1$	θ = 13–42°
a = 9.707 (1) Å	μ = 1.39 mm^{-1}
b = 10.116 (1) Å	T = 293 K
c = 23.262 (2) Å	Transparent block
V = 2284.2 (4) Å^3	

$Z = 4$
$D_x = 1.168$ Mg m^{-3}

0.6 × 0.6 × 0.4 mm
Colourless
Crystal source: ether

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: empirical
$T_{\min} = 0.79$, $T_{\max} = 1.00$
4197 measured reflections
3839 independent reflections
3839 observed reflections

$R_{\rm int} = 0.032$
$\theta_{\max} = 65°$
$h = -11 \rightarrow 11$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 27$
3 standard reflections
frequency: 90 min
intensity variation: none

Refinement

Refinement on F
$R = 0.034$
$wR = 0.047$
$S = 2.60$
3839 reflections
266 parameters
$w = 1/[\sigma^2(F) + 0.0002F^2]$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.39$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}

Extinction correction: empirical
$F^* = F[1 + (0.002\chi \times F^2/\sin2\theta)]^{-1/4}$
Extinction coefficient: $\chi = 0.027(1)$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{\rm eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	$U_{\rm eq}$
S(1)	0.6852 (1)	0.5856 (1)	0.6439 (1)	0.052 (1)
O(1)	0.6301 (2)	0.6992 (1)	0.6747 (1)	0.063 (1)
N(1)	0.8383 (2)	0.5659 (2)	0.6385 (1)	0.061 (1)
C(5)	0.9217 (2)	0.5107 (2)	0.6855 (1)	0.066 (1)
C(51)	1.0457 (3)	0.4389 (3)	0.6592 (1)	0.085 (1)
C(52)	0.9984 (4)	0.3174 (3)	0.6269 (1)	0.106 (1)
C(53)	1.1329 (3)	0.5294 (4)	0.6217 (1)	0.114 (1)
C(6)	0.9637 (2)	0.6168 (3)	0.7280 (1)	0.081 (1)
O(61)	0.8481 (2)	0.6679 (2)	0.7590 (1)	0.089 (1)
C(1)	0.6058 (2)	0.4420 (2)	0.6708 (1)	0.059 (1)
C(2)	0.5453 (2)	0.4263 (2)	0.7215 (1)	0.062 (1)
C(3)	0.5140 (2)	0.5221 (2)	0.7690 (1)	0.056 (1)
C(31)	0.3582 (2)	0.5423 (3)	0.7726 (1)	0.076 (1)
C(4)	0.5753 (2)	0.4691 (2)	0.8253 (1)	0.061 (1)
O(41)	0.7195 (2)	0.4485 (2)	0.8200 (1)	0.085 (1)
C(41)	0.5394 (2)	0.5544 (2)	0.8760 (1)	0.059 (1)
C(42)	0.6076 (2)	0.6726 (2)	0.8864 (1)	0.070 (1)
C(43)	0.5714 (3)	0.7490 (2)	0.9327 (1)	0.092 (1)
C(44)	0.4678 (4)	0.7142 (3)	0.9680 (1)	0.110 (1)
C(45)	0.4007 (4)	0.5953 (4)	0.9587 (1)	0.120 (1)
C(46)	0.4363 (3)	0.5173 (3)	0.9135 (1)	0.092 (1)
C(11)	0.6244 (2)	0.5942 (2)	0.5726 (1)	0.054 (1)
C(12)	0.4927 (2)	0.6412 (2)	0.5630 (1)	0.066 (1)
C(13)	0.4419 (2)	0.6431 (2)	0.5076 (1)	0.074 (1)
C(14)	0.5194 (2)	0.6012 (2)	0.4615 (1)	0.064 (1)
C(141)	0.4627 (3)	0.5993 (3)	0.4013 (1)	0.092 (1)
C(15)	0.6523 (2)	0.5561 (2)	0.4720 (1)	0.070 (1)
C(16)	0.7048 (2)	0.5518 (2)	0.5269 (1)	0.064 (1)

Table 2. *Selected geometric parameters* (Å, °)

S(1)—O(1)	1.456 (1)	S(1)—N(1)	1.504 (1)
S(1)—C(1)	1.759 (2)	S(1)—C(11)	1.763 (2)
N(1)—C(5)	1.471 (2)	C(5)—C(51)	1.533 (3)
C(5)—C(6)	1.515 (3)	C(51)—C(52)	1.512 (4)
C(51)—C(53)	1.521 (4)	C(6)—O(61)	1.430 (3)
C(1)—C(2)	1.326 (3)	C(2)—C(3)	1.501 (2)
C(3)—C(31)	1.529 (3)	C(3)—C(4)	1.533 (3)
C(4)—O(41)	1.420 (3)	C(4)—C(41)	1.503 (3)
C(41)—C(42)	1.388 (3)	C(41)—C(46)	1.379 (3)
C(42)—C(43)	1.372 (3)	C(43)—C(44)	1.345 (5)
C(44)—C(45)	1.385 (5)	C(45)—C(46)	1.359 (4)
C(11)—C(12)	1.383 (3)	C(11)—C(16)	1.386 (2)
C(12)—C(13)	1.380 (3)	C(13)—C(14)	1.377 (3)
C(14)—C(141)	1.503 (3)	C(14)—C(15)	1.390 (3)
C(15)—C(16)	1.376 (3)		
O(1)—S(1)—N(1)	120.6 (1)	O(1)—S(1)—C(1)	108.4 (1)
N(1)—S(1)—C(1)	110.7 (1)	O(1)—S(1)—C(11)	107.5 (1)
N(1)—S(1)—C(11)	104.9 (1)	C(1)—S(1)—C(11)	103.2 (1)
S(1)—N(1)—C(5)	122.1 (1)	N(1)—C(5)—C(51)	108.4 (2)
N(1)—C(5)—C(6)	111.4 (2)	C(51)—C(5)—C(6)	112.6 (2)
C(5)—C(51)—C(52)	110.2 (2)	C(5)—C(51)—C(53)	112.3 (2)
C(52)—C(51)—C(53)	112.0 (2)	C(5)—C(6)—O(61)	111.9 (2)
S(1)—C(1)—C(2)	127.5 (1)	C(1)—C(2)—C(3)	131.8 (2)
C(2)—C(3)—C(31)	109.0 (2)	C(2)—C(3)—C(4)	108.9 (2)
C(31)—C(3)—C(4)	112.6 (2)	C(3)—C(4)—O(41)	111.1 (2)
C(3)—C(4)—C(41)	112.3 (2)	O(41)—C(4)—C(41)	112.3 (2)
C(4)—C(41)—C(42)	121.4 (2)	C(4)—C(41)—C(46)	120.5 (2)
C(42)—C(41)—C(46)	118.0 (2)	C(41)—C(42)—C(43)	120.0 (2)
C(42)—C(43)—C(44)	121.6 (3)	C(43)—C(44)—C(45)	118.9 (3)
C(44)—C(45)—C(46)	120.4 (3)	C(41)—C(46)—C(45)	121.0 (3)
S(1)—C(11)—C(12)	118.6 (1)	S(1)—C(11)—C(16)	121.2 (1)
C(12)—C(11)—C(16)	120.2 (2)	C(11)—C(12)—C(13)	119.1 (2)
C(12)—C(13)—C(14)	121.9 (2)	C(13)—C(14)—C(141)	121.9 (2)
C(13)—C(14)—C(15)	118.0 (2)	C(141)—C(14)—C(15)	120.0 (2)
C(14)—C(15)—C(16)	121.3 (2)	C(11)—C(16)—C(15)	119.5 (2)

Intensities were corrected for Lorentz, polarization and absorption effects. The structure was solved by extracting the position of the S atom from a sharpened Patterson map and extending the structure with a tangent expansion using *SHELXS*86 (Sheldrick, 1985). Refinement was by full-matrix least-squares methods with *XLS* (Sheldrick, 1987). All H atoms were located by a difference synthesis and refined with fixed individual displacement parameters [U(H) = $1.2U_{\rm eq}$(C), U(H) = $1.5U_{\rm eq}$($C_{\rm methyl}$) or U(H) = $1.2U_{\rm eq}$(O)] using a riding model with C—H = 0.96 Å; the coordinates of the hydroxyl H atoms were refined with the O—H distance restrained to 0.850 (1) Å. The absolute configuration was determined by η refinement (Rogers, 1981) starting from both configurations [η = 1.04 (3) for the correct structure].

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: NA1066). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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