Table 2. *Bond distances* (Å) *and angles* (°)

C(1)—C(2)	1·525 (5)	C(1)—C(9)	1·558 (3)
C(1)—C(11)	1·556 (5)	C(2)—C(3)	1·538 (6)
C(3)—C(4)	1·516 (5)	C(4)—C(5)	1·458 (6)
C(4)—C(12)	1·515 (4)	C(4)—O(17)	1·456 (5)
C(5)—C(6)	1·500 (5)	C(5)—O(17)	1·446 (5)
C(6)—C(7)	1·536 (5)	C(7)—C(8)	1·545 (5)
C(8)—C(9)	1·531 (4)	C(8)—C(13)	1·533 (5)
C(8)—O(16)	1·454 (3)	C(9)—C(10)	1·551 (5)
C(10)—C(11)	1·544 (4)	C(11)—C(14)	1·518 (7)
C(11)—C(15)	1·518 (6)	C(12)—C(13)	1·534 (5)

C(2)—C(1)—C(9)	120·0 (2)	C(2)—C(1)—C(11)	120·7 (3)
C(9)—C(1)—C(11)	88·5 (2)	C(1)—C(2)—C(3)	113·4 (3)
C(2)—C(3)—C(4)	111·4 (3)	C(3)—C(4)—C(5)	117·3 (3)
C(3)—C(4)—C(12)	115·2 (3)	C(3)—C(4)—O(17)	114·5 (2)
C(5)—C(4)—C(12)	122·4 (3)	C(5)—C(4)—O(17)	59·5 (3)
C(12)—C(4)—O(17)	115·5 (3)	C(4)—C(5)—C(6)	121·2 (2)
C(4)—C(5)—O(17)	60·2 (3)	C(6)—C(5)—O(17)	118·2 (3)
C(5)—C(6)—C(7)	111·0 (3)	C(6)—C(7)—C(8)	115·3 (3)
C(7)—C(8)—C(9)	114·1 (2)	C(7)—C(8)—C(13)	112·3 (3)
C(7)—C(8)—O(16)	103·9 (3)	C(9)—C(8)—C(13)	112·0 (3)
C(9)—C(8)—O(16)	106·7 (2)	C(13)—C(8)—O(16)	107·2 (2)
C(1)—C(9)—C(8)	125·3 (2)	C(1)—C(9)—C(10)	87·1 (2)
C(8)—C(9)—C(10)	119·5 (3)	C(9)—C(10)—C(11)	89·2 (3)
C(1)—C(11)—C(10)	87·3 (2)	C(1)—C(11)—C(14)	114·1 (4)
C(1)—C(11)—C(15)	114·6 (3)	C(10)—C(11)—C(14)	112·0 (3)
C(10)—C(11)—C(15)	117·0 (4)	C(14)—C(11)—C(15)	110·3 (3)
C(4)—C(12)—C(13)	119·2 (3)	C(8)—C(13)—C(12)	116·7 (2)
C(4)—O)17)—C(5)	60·3 (2)		

Related literature. The title compound was prepared in connection with our studies on the spectroscopic irradiations of the β-caryophyllene (Damodaran & Sukh Dev, 1968) derivatives. Its chemical structure was formulated from spectroscopic evidence (Matsubara, Uchida & Ono, 1985).

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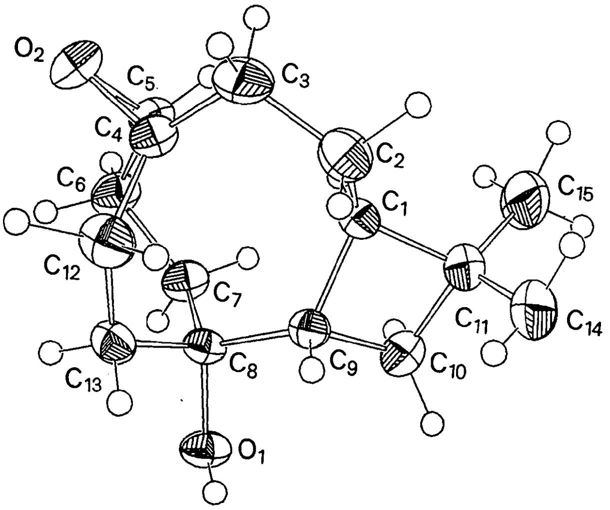

Fig. 1. View of the title compound showing the atomic numbering scheme.

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Structure of (3*SR*,4*SR*,S*SR*)-Methyl 4-(*tert*-Butylsulfinyl)-3-methyl-5-phenylvalerate

By Alan D. Redhouse

Department of Chemistry and Applied Chemistry, University of Salford, Salford, M5 4WT, England

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Abstract. $C_{17}H_{26}O_3S$, $M_r = 310{\cdot}4$, triclinic, $P\bar{1}$, $a = 9{\cdot}022$ (3), $b = 9{\cdot}088$ (3), $c = 12{\cdot}265$ (4) Å, $\alpha = 106{\cdot}49$ (2), $\beta = 106{\cdot}12$ (2), $\gamma = 100{\cdot}71$ (2)°, $V = 887{\cdot}1$ (5) Å^3, $Z = 2$, $D_x = 1{\cdot}162$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}7107$ Å, $\mu = 0{\cdot}181$ mm^{-1}, $F(000) = 336$, $T = 293$ K, $R = 0{\cdot}051$ for 2150 observed reflections. The orientation of the O(1)—S—C(2)—C(4) fragment is eclipsed [torsion angle 4·8 (2)°] whereas in studies of *tert*-butyl phenethyl sulfoxides the corresponding system is staggered (torsion angles 55, 72°) [Kodama, Nishihata, Nishio & Iitaka (1976). *J. Chem. Soc. Perkin Trans.* 2, pp. 1490–1495]. This difference is presumably the result of unacceptable steric interactions between a methyl group of the *tert*-butyl func-

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tion and either C(4) or the phenyl group if the staggered arrangement was adopted in the present compound.

Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}(Å^2)
S	0·1300 (1)	0·5334 (1)	0·8933 (1)	0·042 (1)
O(1)	0·1874 (3)	0·4601 (2)	0·9860 (2)	0·060 (1)
O(2)	0·4652 (3)	0·7659 (3)	1·3355 (2)	0·083 (2)
O(3)	0·2508 (3)	0·8034 (3)	1·3816 (2)	0·070 (1)
C(1)	0·2391 (4)	0·4868 (3)	0·7856 (3)	0·047 (1)
C(11)	0·1709 (5)	0·5458 (5)	0·6834 (3)	0·076 (2)
C(12)	0·1941 (5)	0·3040 (4)	0·7385 (4)	0·071 (2)
C(13)	0·4206 (4)	0·5581 (4)	0·8476 (4)	0·069 (2)
C(2)	0·2161 (3)	0·7543 (3)	0·9693 (2)	0·041 (1)
C(3)	0·0750 (4)	0·8293 (4)	0·9611 (3)	0·050 (1)
C(31)	−0·0295 (4)	0·8050 (3)	0·8337 (3)	0·046 (1)
C(32)	−0·1823 (4)	0·6961 (4)	0·7809 (3)	0·059 (2)
C(33)	−0·2811 (5)	0·6745 (5)	0·6652 (3)	0·072 (2)
C(34)	−0·2292 (5)	0·7615 (5)	0·6006 (3)	0·074 (2)
C(35)	−0·0784 (5)	0·8698 (5)	0·6520 (3)	0·069 (2)
C(36)	0·0203 (4)	0·8927 (4)	0·7678 (3)	0·059 (2)
C(4)	0·3322 (3)	0·7976 (3)	1·1010 (3)	0·043 (1)
C(5)	0·4558 (5)	0·9610 (4)	1·1438 (3)	0·074 (2)
C(6)	0·2403 (4)	0·7921 (4)	1·1880 (3)	0·049 (1)
C(7)	0·3345 (4)	0·7853 (4)	1·3071 (3)	0·048 (1)
C(8)	0·3220 (6)	0·7937 (6)	1·4983 (3)	0·089 (2)

Table 2. *Bond lengths* (Å) *and angles* (°)

S—O(1)	1·495 (3)	S—C(1)	1·860 (4)
S—C(2)	1·860 (3)	O(2)—C(7)	1·194 (5)
O(3)—C(7)	1·332 (5)	O(3)—C(8)	1·431 (5)
C(1)—C(11)	1·520 (6)	C(1)—C(12)	1·527 (4)
C(1)—C(13)	1·520 (4)	C(2)—C(3)	1·544 (5)
C(2)—C(4)	1·551 (4)	C(3)—C(31)	1·511 (4)
C(31)—C(32)	1·390 (4)	C(31)—C(36)	1·388 (6)
C(32)—C(33)	1·386 (5)	C(33)—C(34)	1·376 (7)
C(34)—C(35)	1·374 (6)	C(33)—C(36)	1·383 (5)
C(4)—C(5)	1·530 (4)	C(4)—C(6)	1·530 (5)
C(6)—C(7)	1·497 (5)		
O(1)—S—C(1)	106·3 (2)	O(1)—S—C(2)	107·2 (1)
C(1)—S—C(2)	102·1 (1)	C(7)—O(3)—C(8)	117·1 (3)
S—C(1)—C(11)	107·4 (3)	S—C(1)—C(12)	103·3 (3)
C(11)—C(1)—C(12)	110·4 (3)	S—C(1)—C(13)	112·2 (2)
C(11)—C(1)—C(13)	112·6 (3)	C(12)—C(1)—C(13)	110·5 (3)
S—C(2)—C(3)	108·1 (2)	S—C(2)—C(4)	110·6 (2)
C(3)—C(2)—C(4)	113·9 (2)	C(2)—C(3)—C(31)	115·1 (3)
C(3)—C(31)—C(32)	120·1 (3)	C(3)—C(31)—C(36)	121·9 (3)
C(32)—C(31)—C(36)	118·0 (3)	C(31)—C(32)—C(33)	120·9 (4)
C(32)—C(33)—C(34)	120·3 (3)	C(33)—C(34)—C(35)	119·4 (4)
C(34)—C(35)—C(36)	120·6 (4)	C(31)—C(36)—C(35)	120·8 (3)
C(2)—C(4)—C(5)	110·6 (3)	C(2)—C(4)—C(6)	111·5 (2)
C(5)—C(4)—C(6)	111·3 (3)	C(4)—C(6)—C(7)	115·3 (3)
O(2)—C(7)—O(3)	122·7 (3)	O(2)—C(7)—C(6)	127·2 (4)
O(3)—C(7)—C(6)	110·1 (3)		

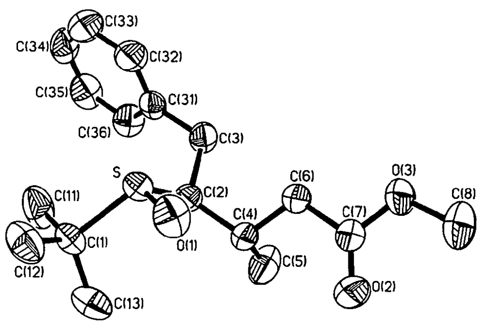

Fig. 1. Molecular structure and numbering scheme for ^{t}BuSO(PhCH$_2$)CHCH(Me)CH$_2$CO(OMe).

Experimental. Colourless crystals were obtained from flash chromatography on silica (petroleum ether: ethyl acetate) on the crude compound. Crystal size for data collection 0·5 × 0·16 × 0·12 mm, Nicolet *R*3*m*/*V* diffractometer with graphite monochromator. Cell dimensions from setting angles of 25 reflections with 2θ values 30–34°. Total of 3368 reflections measured to $2\theta = 50°$ using 2θ–θ scans in the range $0 \le h \le 10$, $-10 \le k \le 10$, $-14 \le l \le 14$. No absorption correction. Three reference reflections monitored periodically showed no significant change. Structure solution, refinement and graphics using *SHELXTL-Plus* (Sheldrick, 1988). Structure determined using direct methods, refined by full-matrix least squares on F with anisotropic thermal parameters for C, O and S, H atoms included in the model in their calculated positions but not refined. 3149 unique reflections, $R_{\rm int} = 0{\cdot}049$, 2150 with $F > 4\sigma(F)$. At convergence $R = 0{\cdot}051$, $wR = 0{\cdot}052$ (on all data $R = 0{\cdot}082$, $wR = 0{\cdot}057$), $w = [\sigma^2(F) + 0{\cdot}00038F^2]^{-1}$, $S = 1{\cdot}38$ for 205 parameters, $\Delta/\sigma < 0{\cdot}02$, $\Delta\rho_{\max} = 0{\cdot}29$, $\Delta\rho_{\min} = -0{\cdot}18$ e Å^{-3}. Scattering factors for all atoms from *SHELXTL-Plus.*

Atomic parameters are given in Table 1,* bond distances and bond angles in Table 2. Fig. 1 shows the molecule together with the numbering scheme used.

Related literature. The reaction of lithiated alkyl *tert*-butyl sulfoxides with $\alpha\beta$-unsaturated esters gives conjugate addition products in good yield, with high stereoselectivity (Casey, Manage & Nezhat, 1988). The relative stereochemistry of the title compound was determined in order to assist with the stereochemical assignment of other conjugate addition products.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52758 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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