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## Key indicators

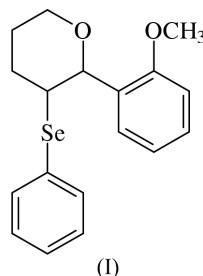
Single-crystal X-ray study  
 $T = 150\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.019  
 $wR$  factor = 0.052  
Data-to-parameter ratio = 15.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**cis-2-(2-Methoxyphenyl)-3-(phenylselenyl)-  
tetrahydropyran**The crystal structure of the title compound,  $\text{C}_{18}\text{H}_{20}\text{O}_2\text{Se}$ , shows that the tetrahydrofuran ring adopts a chair conformation, with the phenylselenenyl group occupying an axial position and the 2-methoxyphenyl group in an equatorial position.

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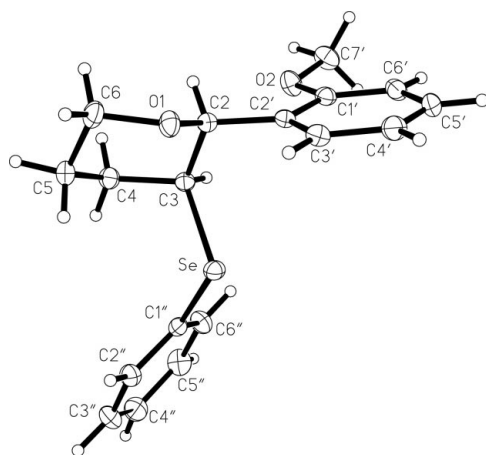
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## Comment

As part of a programme directed towards the synthesis of aryl C-glycosides (Brimble *et al.*, 2002), selenoetherification of  $\gamma$ -hydroxyalkenes was a key step. As analysis of the stereochemical outcome of the selenoetherification step was important for the overall synthetic strategy, we analysed the stereochemical outcome of the selenoetherification of a (*Z*)- $\gamma$ -hydroxyalkene and established the structure of the selenoetherification product by X-ray crystallography.Selenoetherification of (*Z*)-5-(2-methoxyphenyl)pent-4-en-1-ol gave the *cis*-selenide, (I), as only a minor product, the major product being a tetrahydrofuran which was formed *via* 5-*exo* cyclization of the transition state. The tetrahydrofuran was an oil and the structure was determined by NMR spectroscopy. The X-ray structure of the selenide (I) clearly shows that the tetrahydrofuran ring adopts a chair conformation, with the phenylselenenyl group occupying an axial position, whilst the 2-methoxyphenyl group occupies an equatorial position (Fig. 1 and Table 1).The product formed from (*E*)-5-naphthylpent-4-en-1-ol has a *trans* stereochemistry (Rickard *et al.*, 2002) and has a  $\pi$  interaction between the naphthyl and phenyl rings. For the selenide (I), a similar interaction is impossible with the equatorial-axial orientation of the substituents. For this molecule, both aromatic rings are involved in intermolecular interactions, leading to the formation of a  $\pi$  stack. Thus, the methoxyphenyl rings of adjacent molecules lie parallel, with a separation of 3.56 Å, and the phenyl rings of adjacent molecules are also parallel, with a separation of 3.46 Å.

## Experimental

Phenylselenenyl chloride (72 mg, 0.38 mmol) was added to a cooled solution (195 K) of *cis*-5-(2-methoxyphenyl)pent-4-en-1-ol (48 mg,



**Figure 1**  
The structure of (I), showing 50% probability displacement ellipsoids (Siemens, 1995).

0.25 mmol) in dichloromethane (2 ml) under nitrogen. After 2 h, the reaction was diluted with dichloromethane (5 ml) and washed with saturated sodium bicarbonate solution. The aqueous portion was extracted with dichloromethane ( $3 \times 5$  ml) and the organic extracts were washed with brine and dried over  $\text{MgSO}_4$ . PLC (hexanes–EtOAc, 95:5) of the crude product afforded the title selenide, (I) (13 mg, 15%) which was recrystallized from ethyl acetate–hexane (1:19) as yellow prisms (m.p. 369–370 K). A sample, of suitable size for diffraction analysis, was cut from a prism. Analysis, found:  $M^+ = 348.0626$ ;  $\text{C}_{18}\text{H}_{20}\text{O}_2\text{Se}$  requires  $M = 348.0628$ ;  $\nu_{\text{max}}$  (film)/ $\text{cm}^{-1}$ : 1603, 1588, 1494, 1463, 1437, 1287, 1287, 1247, 1093, 1073, 1051, 1027, 754, 693;  $\delta_{\text{H}}$  (300 MHz,  $\text{CDCl}_3$ , p.p.m.): 2.21–2.27 (3H, *m*, H-4<sub>A</sub>, H-5<sub>A</sub>, H-5<sub>B</sub>), 2.25–2.29 (1H, *m*, H-4<sub>B</sub>), 3.64–3.73 (1H, *m*, H-3<sub>eq</sub>), 3.66 (3H, *s*, OCH<sub>3</sub>), 3.93 (1H, *m*, H-6<sub>ax</sub>), 4.22–4.27 (1H, *m*, H-6<sub>eq</sub>), 4.90 (1H, *d*,  $J_{2\text{ax},3\text{ax}} = 1.56$  Hz, H-2<sub>ax</sub>), 6.66–7.53 (9H, *m*, ArH);  $\delta_{\text{C}}$  (300 MHz, p.p.m.): 22.4 (CH<sub>2</sub>, C-4), 31.1 (CH<sub>2</sub>, C-5), 48.6 (CH, C-3), 54.9 (CH<sub>3</sub>, OMe), 69.4 (CH<sub>2</sub>, C-6), 77.1 (CH, C-2), 109.4 (CH, Ar), 120.2 (CH, Ar), 126.5 (CH, Ar), 127.3 (CH, Ar), 127.9 (CH, Ar), 128.3 (CH, Ar), 129.6 (quat, Ar), 130.6 (quat, Ar), 134.1 (CH, Ar), 155.1 (quat, Ar). The tetrahydrofuran (6) (36 mg, 41%) was also isolated from the reaction as a pale yellow oil.

#### Crystal data

$\text{C}_{18}\text{H}_{20}\text{O}_2\text{Se}$	$Z = 2$
$M_r = 347.30$	$D_x = 1.515 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.1823$ (4) Å	Cell parameters from 6450 reflections
$b = 7.7739$ (4) Å	$\theta = 2\text{--}26^\circ$
$c = 13.9367$ (7) Å	$\mu = 2.47 \text{ mm}^{-1}$
$\alpha = 97.180$ (2)°	$T = 150$ (2) K
$\beta = 97.654$ (2)°	Irregular fragment, yellow
$\gamma = 94.793$ (2)°	$0.36 \times 0.28 \times 0.14 \text{ mm}$
$V = 761.18$ (7) Å <sup>3</sup>	

#### Data collection

Siemens SMART diffractometer	2832 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.016$
Absorption correction: multi-scan (Blessing, 1995)	$\theta_{\text{max}} = 26.1^\circ$
$T_{\text{min}} = 0.460$ , $T_{\text{max}} = 0.709$	$h = -8 \rightarrow 8$
7048 measured reflections	$k = -9 \rightarrow 9$
2984 independent reflections	$l = 0 \rightarrow 17$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.2068P]$
$R[F^2 > 2\sigma(F^2)] = 0.019$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.052$	$(\Delta/\sigma)_{\text{max}} = 0.007$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
2984 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
193 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

Se–C1''	1.9244 (15)	C2–C3	1.539 (2)
Se–C3	1.9842 (15)	C3–C4	1.529 (2)
O1–C2	1.4289 (18)	C4–C5	1.526 (2)
O1–C6	1.4405 (18)	C5–C6	1.519 (2)
C2–C2'	1.5145 (19)		
C1''–Se–C3	99.14 (6)	C4–C3–Se	112.70 (10)
C2–O1–C6	110.71 (12)	C2–C3–Se	108.13 (10)
O1–C2–C2'	108.62 (12)	C5–C4–C3	111.69 (13)
O1–C2–C3	110.67 (11)	C6–C5–C4	110.60 (13)
C2'–C2–C3	114.91 (12)	O1–C6–C5	111.84 (13)
C4–C3–C2	109.31 (12)		

H atoms were clearly resolved in difference maps. They were refined using a riding model, with  $U_{\text{iso}}$  values constrained to be 1.2 times  $U_{\text{eq}}$  of the carrier atom.>

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1995); software used to prepare material for publication: *SHELXL97*.

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