(1970) were included in F_c. All calculations were performed on the CDC-Cyber 962-31 computer of the University of Groningen with the program packages *Xtal* (Hall & Stewart, 1990) and *PLATON* (Spek, 1990); Figs. 1 and 2 were produced using a program by Meetsma (1991), a modified version of *PLUTO* (Motherwell & Clegg, 1978).

Related literature. 1,5,7-Triazabicyclo[4.4.0]dec-5-ene (tbd) as a strong base is a good catalyst for nitroalkanes in C—C bond forming reactions. In its protonated form the structure of the guanidinium cation is complementary to that of a nitronate and nitrite anion. tbd is therefore used as a model catalyst for its chiral analogue as synthesized by Echavarren, Galan, Mendoza, Salmeron & Lehn (1988) and Kurzmeier & Schmidtchen (1990).

Acknowledgement is made to the Dutch foundation for Chemical Research (SON) and the Dutch Organization for Scientific Research (NWO) for funding this research.

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Structure of 1,1-Dibromo-2-phenylseleno-3-*p*-tolylcyclopropane

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(*Received* 2 *September* 1991; *accepted* 21 *February* 1992)

Abstract. $C_{16}H_{14}Br_2Se$, $M_r = 445.07$, monoclinic, $P2_1/n$, $a = 12.755$ (1), $b = 11.221$ (2), $c = 21.770$ (2) Å, $\beta = 94.16$ (2)°, $V = 3107$ (1) Å^3, $Z = 8$, $D_x = 1.903$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 74.72$ cm^{-1}, $F(000) = 1712$, $T = 296$ K, final $R = 0.053$ for 1768 independent observed reflections. The two independent molecules in the asymmetric unit are essentially identical. Bond lengths and angles involving selenium are: Se—C(Ph) = 1.92 (1), 1.91 (2) Å, Se—C(sp^3) = 1.94 (1), 1.94 (2) Å and C—Se—C = 95.0 (7), 97.6 (7)°.

Experimental. The synthesis of the title compound is described by Comasseto, Stefani & Silveira (1990); crystals were obtained from chloroform at 277 K. The data collection and refinement parameters are summarized in Table 1.

The structure was solved using standard direct methods and difference Fourier techniques. In the final cycles of the blocked-matrix least-squares refinement, all non-H atoms were treated anisotropically. H atoms included, as fixed contributors, at positions found from a difference Fourier synthesis, all with a common isotropic temperature factor that refined to $U = 0.086$ (4) Å^2. The data were corrected for Lp and absorption with maximum and minimum transmission factors of 1.01 and 0.94 (Walker & Stuart, 1983). Scattering factors for non-H atoms were taken from Cromer & Mann (1968) with corrections for anomalous dispersion from Cromer &

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Table 1. *Crystallographic summary*

Data collection$^{\text{i}}$	
Mode	ω–2θ
Scan rate (° min^{-1})	2.8–10.0
θ range (°)	0–25
Range of *hkl*	$-15 \le h \le 15$, $0 \le k \le 13$, $0 \le l \le 25$
Total reflections measured	4203
Unique reflections	4094
R_{int}	0.029
Standard reflections (h^{-1})	1
Variation	Not significant
Crystal dimensions (mm)	~0.15 × 0.10 × 0.10
Diffractometer	Enraf–Nonius CAD-4, graphite monochromator
Structure determination$^{\text{ii}}$	
Reflections used [$I > 3\sigma(I)$]	1768
No. of variables	344
R, wR	0.053, 0.046
w	$1/[\sigma^2(F_o) + 0.0003F_o^2]$
Max. shift/e.s.d.	0.006
Max., min. density in final difference map (e Å^{-3})$^{\text{iii}}$	0.64, −0.66
S	1.25

Notes: (i) Unit-cell parameters by least-squares refinement of the setting angles of 23 reflections with $8 < \theta < 18°$. (ii) Function minimized was $\sum w(|F_o| - |F_c|)^2$. (iii) Less than 1.0 Å from the Br(1′) atom.

Table 2. *Final atomic coordinates and equivalent isotropic temperature factors* (Å^2)

$$B_{\text{eq}} = (4/3)\textstyle\sum_i \sum_j B_{ij}(\mathbf{a}_i{}^*\mathbf{a}_j{}^*).$$

	x	y	z	B_{eq}
Se(1)	0.4810 (1)	0.2083 (2)	0.1543 (1)	3.90 (7)
Br(1)	0.4200 (2)	0.1555 (2)	0.3073 (1)	4.24 (8)
Br(2)	0.1843 (1)	0.2166 (2)	0.2630 (1)	4.38 (8)
C(1)	0.356 (1)	0.272 (1)	0.1877 (7)	2.8 (3)
C(2)	0.330 (1)	0.247 (1)	0.2526 (7)	2.8 (3)
C(3)	0.358 (1)	0.371 (1)	0.2347 (6)	2.0 (3)
C(4)	0.459 (1)	0.433 (1)	0.2594 (8)	2.9 (3)
C(5)	0.474 (1)	0.457 (2)	0.3223 (8)	3.4 (3)
C(6)	0.560 (1)	0.524 (2)	0.3441 (7)	3.2 (3)
C(7)	0.636 (1)	0.561 (1)	0.3053 (8)	3.3 (3)
C(8)	0.621 (1)	0.535 (2)	0.2456 (7)	3.2 (3)
C(9)	0.533 (1)	0.473 (2)	0.2207 (7)	3.1 (3)
C(10)	0.730 (1)	0.630 (2)	0.3326 (9)	5.7 (3)
C(11)	0.407 (1)	0.094 (2)	0.1017 (8)	3.7 (3)
C(12)	0.351 (1)	0.003 (2)	0.1261 (8)	4.6 (3)
C(13)	0.298 (1)	−0.081 (2)	0.090 (1)	5.1 (3)
C(14)	0.304 (1)	−0.072 (2)	0.0264 (9)	5.6 (3)
C(15)	0.354 (1)	0.024 (2)	0.0012 (8)	6.2 (3)
C(16)	0.408 (1)	0.103 (2)	0.0377 (8)	4.7 (3)
Se(1′)	0.8940 (1)	0.4734 (2)	0.0978 (1)	3.77 (7)
Br(1′)	0.6334 (2)	0.3950 (2)	0.0538 (1)	3.74 (7)
Br(2′)	0.6826 (2)	0.4619 (2)	−0.0826 (1)	4.39 (8)
C(1′)	0.824 (1)	0.531 (2)	0.0213 (7)	4.1 (3)
C(2′)	0.711 (1)	0.497 (1)	0.0041 (6)	2.3 (3)
C(3′)	0.735 (1)	0.620 (2)	0.0205 (7)	3.1 (3)
C(4′)	0.702 (1)	0.681 (1)	0.0795 (8)	3.1 (3)
C(5′)	0.774 (1)	0.731 (2)	0.1201 (8)	3.6 (3)
C(6′)	0.741 (1)	0.793 (2)	0.1713 (7)	3.6 (3)
C(7′)	0.635 (1)	0.803 (1)	0.1787 (7)	3.3 (3)
C(8′)	0.561 (1)	0.757 (2)	0.1361 (8)	3.5 (3)
C(9′)	0.593 (1)	0.693 (2)	0.0858 (7)	3.0 (3)
C(10′)	0.596 (1)	0.872 (2)	0.2334 (8)	4.4 (3)
C(11′)	0.965 (1)	0.341 (2)	0.0643 (7)	2.6 (3)
C(12′)	1.054 (1)	0.291 (2)	0.0972 (8)	4.1 (3)
C(13′)	1.105 (1)	0.193 (2)	0.078 (1)	5.2 (3)
C(14′)	1.075 (1)	0.150 (2)	0.0193 (9)	4.7 (3)
C(15′)	0.989 (1)	0.197 (2)	−0.0141 (7)	4.1 (3)
C(16′)	0.934 (1)	0.292 (2)	0.0080 (7)	3.6 (3)

Liberman (1970), and for H atoms from Stewart, Davidson & Simpson (1965). Programs used: *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1965). Most of the calculations were performed on a VAX 6420 computer at the Instituto de Física e Química de São Carlos.

Table 3. *Interatomic bond distances* (Å) *and angles* (°)

Se(1)—C(1)	1.94 (1)	Se(1′)—C(1′)	1.94 (2)
Se(1)—C(11)	1.92 (2)	Se(1′)—C(11′)	1.91 (2)
Br(1)—C(2)	1.90 (2)	Br(1′)—C(2′)	1.90 (1)
Br(2)—C(2)	1.92 (1)	Br(2′)—C(2′)	1.94 (1)
C(1)—C(2)	1.50 (2)	C(1′)—C(2′)	1.51 (2)
C(1)—C(3)	1.51 (2)	C(1′)—C(3′)	1.51 (2)
C(2)—C(3)	1.50 (2)	C(2′)—C(3′)	1.45 (2)
C(3)—C(4)	1.53 (2)	C(3′)—C(4′)	1.54 (2)
C(4)—C(5)	1.40 (2)	C(4′)—C(5′)	1.35 (2)
C(4)—C(9)	1.38 (2)	C(4′)—C(9′)	1.41 (2)
C(5)—C(6)	1.38 (2)	C(5′)—C(6′)	1.40 (2)
C(6)—C(7)	1.39 (2)	C(6′)—C(7′)	1.38 (2)
C(7)—C(8)	1.33 (2)	C(7′)—C(8′)	1.37 (2)
C(7)—C(10)	1.51 (2)	C(7′)—C(10′)	1.53 (2)
C(8)—C(9)	1.40 (2)	C(8′)—C(9′)	1.40 (2)
C(11)—C(12)	1.37 (3)	C(11′)—C(12′)	1.41 (2)
C(11)—C(16)	1.40 (2)	C(11′)—C(16′)	1.37 (2)
C(12)—C(13)	1.37 (3)	C(12′)—C(13′)	1.36 (3)
C(13)—C(14)	1.40 (3)	C(13′)—C(14′)	1.39 (3)
C(14)—C(15)	1.39 (3)	C(14′)—C(15′)	1.38 (2)
C(15)—C(16)	1.35 (3)	C(15′)—C(16′)	1.38 (2)

C(1)—Se(1)—C(11)	95.0 (7)	C(1′)—Se(1′)—C(11′)	97.6 (7)
Se(1)—C(1)—C(2)	122 (1)	Se(1′)—C(1′)—C(2′)	120 (1)
Se(1)—C(1)—C(3)	124 (1)	Se(1′)—C(1′)—C(3′)	122 (1)
C(2)—C(1)—C(3)	60 (1)	C(2′)—C(1′)—C(3′)	57 (1)
Br(1)—C(2)—Br(2)	112.2 (8)	Br(1′)—C(2′)—Br(2′)	111.3 (7)
Br(1)—C(2)—C(1)	122 (1)	Br(1′)—C(2′)—C(1′)	122 (1)
Br(1)—C(2)—C(3)	122 (1)	Br(1′)—C(2′)—C(3′)	123 (1)
Br(2)—C(2)—C(1)	115 (1)	Br(2′)—C(2′)—C(1′)	114 (1)
Br(2)—C(2)—C(3)	117 (1)	Br(2′)—C(2′)—C(3′)	117 (1)
C(1)—C(2)—C(3)	60 (1)	C(1′)—C(2′)—C(3′)	61 (1)
C(1)—C(3)—C(2)	60 (1)	C(1′)—C(3′)—C(2′)	61 (1)
C(1)—C(3)—C(4)	123 (1)	C(1′)—C(3′)—C(4′)	122 (1)
C(2)—C(3)—C(4)	123 (1)	C(2′)—C(3′)—C(4′)	124 (1)
C(3)—C(4)—C(5)	119 (1)	C(3′)—C(4′)—C(5′)	121 (1)
C(3)—C(4)—C(9)	122 (1)	C(3′)—C(4′)—C(9′)	117 (1)
C(5)—C(4)—C(9)	119 (1)	C(5′)—C(4′)—C(9′)	122 (1)
C(4)—C(5)—C(6)	119 (1)	C(4′)—C(5′)—C(6′)	120 (1)
C(5)—C(6)—C(7)	121 (1)	C(5′)—C(6′)—C(7′)	119 (1)
C(6)—C(7)—C(8)	118 (1)	C(6′)—C(7′)—C(8′)	121 (1)
C(6)—C(7)—C(10)	119 (1)	C(6′)—C(7′)—C(10′)	121 (1)
C(8)—C(7)—C(10)	123 (1)	C(8′)—C(7′)—C(10′)	118 (1)
C(7)—C(8)—C(9)	123 (1)	C(7′)—C(8′)—C(9′)	120 (1)
C(4)—C(9)—C(8)	119 (1)	C(4′)—C(9′)—C(8′)	118 (1)
Se(1)—C(11)—C(12)	121 (1)	Se(1′)—C(11′)—C(12′)	120 (1)
Se(1)—C(11)—C(16)	120 (1)	Se(1′)—C(11′)—C(16′)	122 (1)
C(12)—C(11)—C(16)	119 (1)	C(12′)—C(11′)—C(16′)	117 (1)
C(11)—C(12)—C(13)	122 (1)	C(11′)—C(12′)—C(13′)	123 (1)
C(12)—C(13)—C(14)	117 (1)	C(12′)—C(13′)—C(14′)	117 (1)
C(13)—C(14)—C(15)	121 (1)	C(13′)—C(14′)—C(15′)	120 (1)
C(14)—C(15)—C(16)	121 (1)	C(14′)—C(15′)—C(16′)	121 (1)
C(11)—C(16)—C(15)	120 (1)	C(11′)—C(16′)—C(15′)	120 (1)

Atomic coordinates are listed in Table 2,* bond lengths and bond angles in Table 3. Fig. 1 is a projection of the title compound showing the atom labeling.

Related literature. This structure shows unambiguously that, starting from the *cis* vinylic selenide (Comasseto, Stefani & Silveira, 1990), the *cis* selenocyclopropane is obtained. The two independent molecules in the asymmetric unit are essentially identical; a least-squares fit (Kabsch, 1976) gives a mean deviation between equivalent atoms of 0.32 Å. The dihedral angles between the phenyl rings are 26 (1) and 38.9 (7)° for the unprimed and primed

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* Lists of H-atom positions, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55225 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0102]

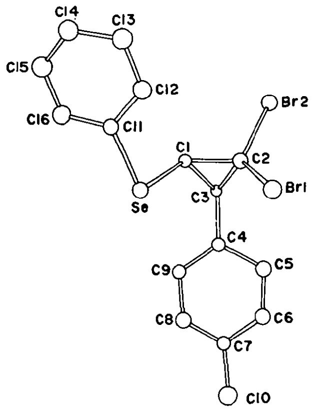

Fig. 1. Perspective view of one of the molecules showing the atom numbering.

molecules respectively. For an extensive review of the structural chemistry of organic compounds containing selenium, see Hargittai & Rozsondai (1986).

This work has received partial support from CNPq, CAPES, FAPESP and FINEP.

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Acta Cryst. (1992). C**48**, 1878–1880

Structure of a Chiral Intermediate in the Synthesis of (+)-19-Epiajmalicine

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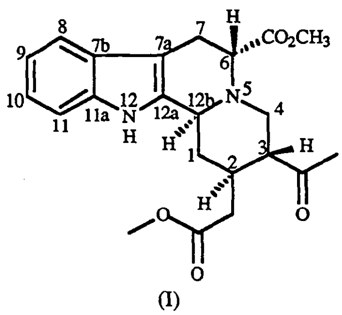
(*Received* 22 *October* 1991; *accepted* 19 *February* 1992)

Abstract. [2S^*-(2β,3α,6α,12bβ)]-Methyl 3-acetyl-1,2,3,4,6,7,12,12b-octahydro-6-methoxycarbonyl-indolo[2,3-*a*]quinolizine-3-ethanoate, $C_{22}H_{26}N_2O_5$, $M_r = 398.46$, orthorhombic, $P2_12_12_1$, $a = 9.463\,(2)$, $b = 11.251\,(3)$, $c = 18.871\,(6)$ Å, $V = 2009.2\,(9)$ Å^3, $Z = 4$, $D_x = 1.32$ g cm^{-3} (178 K), λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 0.8762$ cm^{-1}, $F(000) = 848$, $T = 178$ K, $R = 0.0536$ for 1673 reflections [$F_o \geq 6\sigma(F_o)$]. Molecules are hydrogen bonded along the 2_1-screw axis parallel to **a**. The hydrogen-bond geometric parameters for N12—H12···O19 (related by $0.5 + x$, $1.5 - y$, $1 - z$) are N···O 2.986 (6), H···O 2.30 (5) Å, N—H···O 161 (5)°. The *C* and *D* rings are *trans* fused with ring-junction torsion angles of $-39.6\,(5)$ and $63.8\,(5)^\circ$ for C12a—C12b—N5—C6 and C1—C12b—N5—C4, respectively. The conformation of the *C* ring is half chair with N5 and C6 $-0.168\,(4)$ and $0.552\,(5)$ Å, respectively, out of the plane defined by the remaining four atoms of the ring. The *D* ring is in the chair conformation.

Experimental. Compound (I) was synthesized *via* an intermolecular Michael addition (Hirai, Terada & Yamazaki, 1988) on an intermediate derived from D-tryptophan during studies directed toward the total synthesis of (+)-19-epiajmalicine (Melchio, Bouquet, Pais & Goutarel, 1977). The absolute configuration of (I) was deduced from the chiral center present in the optically pure starting material. Full details of the synthetic procedure will be published in due course (Martin & Corbett, 1991). Crystals were obtained by slow evaporation of a hexane–diethyl ether solution. The data crystal was a clear colorless needle of approximate dimensions 0.17 × 0.17 ×



(I)