Preliminary Communication

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Synthesis of first selenodecalines: 2-aryl-4-phenyl octahydroselenochromenes

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Abstract: The reaction of 2-aryl-4-phenyl-5,6,7,8-tetrahydro-4*H*-selenochromenes **1–3** with trifluoroacetic acid and triethylsilane furnished a novel class of compounds, 2-aryl-4-phenyloctahydroselenochromenes.

Keywords: 2-aryl-4-phenyloctahydroselenochromenes; synthesis; tetrahydro-4*H*-selenochromenes.

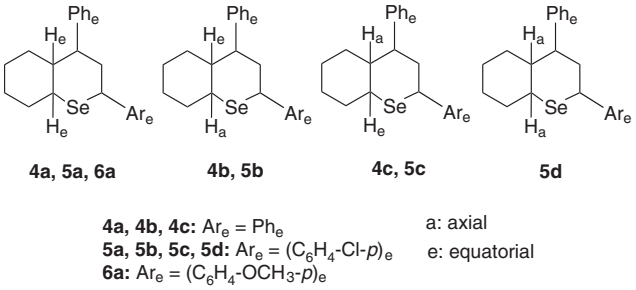
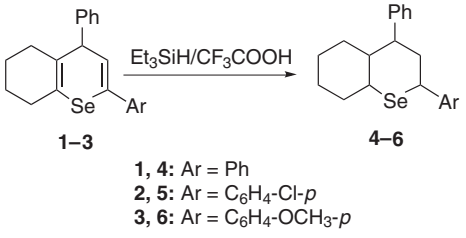


Figure 1 The suggested isomers **4a–c**, **5a–d**, **6a**.

Introduction

Selenium is an important ultramicroelement and its shortage in animal and people nutrition can lead to a variety of diseases [1–3]. Selenium-containing compounds have a wide spectrum of practical significancy [4, 5]. Previously, we have synthesized 2-aryl-4-phenyl-5,6,7,8-tetrahydro-4*H*-selenochromenes **1–3** [6]. In continuation of that work, we now report reduction of compounds **1–3** that does not lead to selenium elimination [7, 8] and furnishes the corresponding 2,4-diphenyloctahydroselenochromenes **4–6**. The reaction is carried out in the presence of triethylsilane and trifluoroacetic acid (Scheme 1).



Scheme 1

The diphenyloctahydroselenochromene **4** is composed of three isomers (Figure 1) that give three well-separated signals with different retention times (21.01, 21.58 and 22.05 min on a chromatogram and show identical molecular ion peaks at *m/z* 356 for isotope ^{80}Se in their mass spectra. It can be suggested that these are geometrical isomers that differ in the configuration at the ring junction but exhibit identical, most stable pseudo-equatorial conformation of the aryl substituents. Nevertheless, the given stereochemistry of **4a–c** is tentative and, at the present time, it is not possible to assign a physical characteristic, such as retention time, to a particular isomer.

In a similar way, a 4-chlorophenyl derivative is a mixture of four geometrical stereoisomers **5a**, **5b**, **5c, 5d**. Accordingly, the signals with different retention times (25.51, 26.22, 26.44 and 27.20 min) can be observed in the chromatogram and the mass spectra show identical molecular ion peak at *m/z* 390 for isotope ^{80}Se in each case.

The compound 2-(4-methoxyphenyl)-4-phenyloctahydroselenochromene (**6**) has only one isomer tentatively assigned the structure **6a** (Figure 1). Only one signal with retention time of 26.63 min can be observed in the chromatogram and the mass spectrum shows a molecular ion peak at *m/z* 386 for isotope ^{80}Se.

Experimental

A mixture of a 2-aryl-4-phenyl-5,6,7,8-tetrahydro-4*H*-selenochromene (**1–3**, 0.001 mol), triethylsilane (0.3 mL) and trifluoroacetic acid

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(0.37 mL), prepared in that order, was stirred biefly in the air and treated with diethyl ether (10 mL). The resultant homogeneous solution was washed with water to the neutral reaction and concentrated in the air to give the 2-aryl-4-phenyloctahydroselenochromene **4–6**. This synthesis was monitored by a capillary gas-liquid partition chromatography using mass-selective detector Agilent 5973: $T_{injector}$=200°C, $t_{initial}$=3 min, $T_{initial}$=50°C, T_{end}=280°C, gradient ΔT=10°C/min, carrier gas – helium, ν=1 mL/min. The ^{1}H NMR spectra were recorded in deuteriochloroform on a Bruker AV instrument operating at 600 MHz.

2,4-Diphenyloctahydroselenochromene (4) This compound was obtained in 79% yield as a brown powder; mp 115–117°C; ^{1}H NMR: δ 1.08–1.17 (m, 2H), 1.27 (m, 1H), 1.53 (dd, 1H, *J* = 7.1 Hz and 6.0 Hz), 1.62 (m, 2H), 1.86 (m, 1H), 1.92–1.99 (m, 4H), 2.58 (q, 1H, *J* = 8.0 Hz), 3.10–3.21 (m, 1H), 7.24–7.40 (m, 10H); MS (EI): *m/z* 356 (M^+). Anal. Calcd for $C_{21}H_{24}Se$: C, 70.79; H, 6.74. Found: C, 71.25; H, 7.17.

2-(4-Chlorophenyl)-4-phenyloctahydroselenochromene (5) This compound was obtained in 73% yield as brown powder; mp 42–44°C; ^{1}H NMR: δ 1.04–1.15 (m, 2H), 1.25 (m, 1H), 1.46 (m, 1H), 1.49 (m, 4H), 1.72 (m, 2H), 1.86 (m, 1H), 2.55 (q, 1H, *J* = 16.0 Hz), 2.90 (m, 1H), 7.18–7.36 (m, 9H); MS (EI): *m/z* 390 (M^+). Anal. Calcd for $C_{21}H_{23}SeCl$: C, 64.62; H, 5.90. Found: C, 65.03; H, 6.46.

2-(4-Methoxyphenyl)-4-phenyloctahydroselenochromene (6) This compound was obtained in 84% yield as a brown powder; mp 100–102°C; ^{1}H NMR: δ 1.14 (m, 2H), 1.19–1.30 (m, 1H), 1.42 (m, 1H), 1.65 (m, 2H), 1.77–2.2 (m, 4H), 2.08 (m, 1H), 2.40 (m, 1H), 2.96–3.30 (m, 1H), 3.77 (s, 3H), 6.51 (d, 1H, *J* = 8.0 Hz), 6.99 (d, 1H, *J* = 8.0 Hz), 7.15–7.43 (m, 7H); MS (EI): *m/z* 386 (M^+). Anal. Calcd for $C_{22}H_{26}SeO$: C, 68.39; H, 6.74. Found: C, 68.95; H, 7.23.

Supplementary material: The mass spectra of all isomers of compounds **4–6** observed by gas chromatography are given in the online supplementary material.

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Supplemental Material: The online version of this article (DOI: 10.1515/hc-2016-0076) offers supplementary material, available to authorized users.