



Supporting Information

for

Metal-free nucleophilic trifluoromethylselenolation via an iodide-mediated umpolung reactivity of trifluoromethylselenotoluenesulfonate

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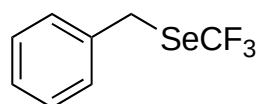
Beilstein J. Org. Chem. **2020**, *16*, 3032–3037. doi:10.3762/bjoc.16.252

Additional experimental and analytical data

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Synthesis of benzyl(trifluoromethyl)selane (**3a**)



Colorless liquid

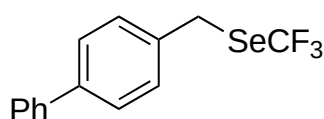
Eluent for flash chromatography: pentane 100%

^1H NMR (300 MHz, CDCl_3) δ = 7.36-7.27 (massif, 5H), 4.25 (s, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ = -34.48 (s, 3F).

Characterization data matched that reported in the literature[1].

Synthesis of ([1,1'-biphenyl]-4-ylmethyl)(trifluoromethyl)selane (**3c**)



White solid

Melting point: 70°C.

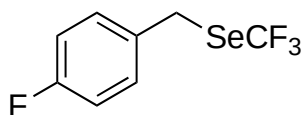
Eluent for flash chromatography: pentane 100%

^1H NMR (300 MHz, CDCl_3) δ = 7.61-7.54 (massif, 4H), 7.47-7.32 (massif, 5H), 4.30 (s, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ = -34.38 (s, 3F).

Characterization data matched that reported in the literature[2].

Synthesis of (4-fluorobenzyl)(trifluoromethyl)selane (**3d**)



Colorless liquid

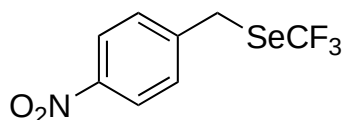
Eluent for flash chromatography: pentane 100%

^1H NMR (300 MHz, CDCl_3) δ = 7.31 (m, 2H), 7.01 (m, 2H), 4.22 (s, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ = -34.38 (s, 3F), -114.11 (tt, J = 8.5, 5.3 Hz, 1F).

Characterization data matched that reported in the literature[3].

Synthesis of (4-nitrobenzyl)(trifluoromethyl)selane (**3e**)



Yellow oil

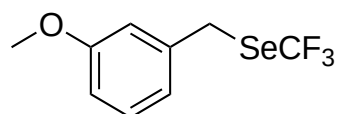
Eluent for flash chromatography: pentane/ Et_2O 8:2 to 7:3

^1H NMR (300 MHz, CDCl_3) δ = 8.20 (m, 2H), 7.51 (m, 2H), 4.28 (s, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ = -34.11 (s, 3F).

Characterization data matched that reported in the literature[4].

Synthesis of (3-methoxybenzyl)(trifluoromethyl)selane (**3f**)



Colorless liquid

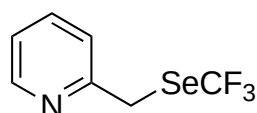
Eluent for flash chromatography: pentane/Et₂O 97:3

¹H NMR (300 MHz, CDCl₃) δ = 7.24 (t, J = 8.0 Hz, 1H), 6.93 (m, 1H), 6.88 (t, J = 2.3 Hz, 1H), 6.82 (ddd, J = 7.9, 2.2, 0.9 Hz, 1H), 4.22 (s, 2H), 3.81 (s, 3H).

¹⁹F NMR (282 MHz, CDCl₃) δ = -34.50 (s, 3F).

Characterization data matched that reported in the literature[4].

Synthesis of 2-(((trifluoromethyl)selanyl)methyl)pyridine (**3g**)



Yellowish oil

Only 1 eq. of alkyl halide was used instead of 2 eq.

Saturated aqueous NaHCO₃ was used instead of water during work-up

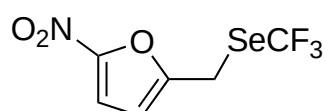
Eluent for flash chromatography: pentane/Et₂O 8:2 to 7:3

¹H NMR (300 MHz, CDCl₃) δ = 8.55 (d, J = 4.9 Hz, 1H), 7.67 (td, J = 7.7, 1.8 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.20 (ddd, J = 7.6, 4.9, 1.1 Hz, 1H), 4.37 (s, 2H).

¹⁹F NMR (282 MHz, CDCl₃) δ = -34.58 (s, 3F).

Characterization data matched that reported in the literature[5].

Synthesis of 2-nitro-5-(((trifluoromethyl)selanyl)methyl)furan (**3h**)



Brownish oil

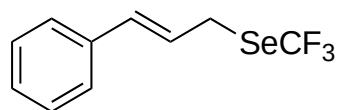
Eluent for flash chromatography: pentane/Et₂O 8:2

¹H NMR (300 MHz, CDCl₃) δ = 7.27 (d, J = 3.7 Hz, 1H), 6.53 (d, J = 3.7 Hz, 1H), 4.20 (s, 2H).

¹⁹F NMR (282 MHz, CDCl₃) δ = -34.43 (s, 3F).

Characterization data matched that reported in the literature[5].

Synthesis of cinnamyl(trifluoromethyl)selane (**3i**)



Colorless liquid

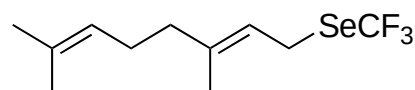
Eluent for flash chromatography: pentane 100%

^1H NMR (300 MHz, CDCl_3) δ = 7.39-7.23 (massif, 5H), 6.58 (d, J = 15.6 Hz, 1H), 6.33 (dt, J = 15.5, 7.7 Hz, 1H), 3.84 (d, J = 7.7 Hz, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ = -33.80 (s, 3F).

Characterization data matched that reported in the literature[4].

Synthesis of (3,7-dimethylocta-2,6-dienyl)(trifluoromethyl)selane (**3j**)



Colorless liquid

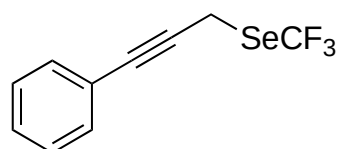
Eluent for flash chromatography: pentane 100%

^1H NMR (300 MHz, CDCl_3) δ = 5.37 (t, J = 8.4 Hz, 1H), 5.08-5.03 (m, 1H), 3.69 (d, J = 8.3 Hz, 2H), 2.14-2.00 (massif, 4H), 1.69 (s, 3H), 1.68 (s, 3H), 1.60 (s, 3H).

^{19}F NMR (282 MHz, CDCl_3) δ = -34.03 (s, 3F).

Characterization data matched that reported in the literature[6].

Synthesis of (3-phenylprop-2-yn-1-yl)(trifluoromethyl)selane (**3k**)



Colorless liquid

Eluent for flash chromatography: pentane 100%

^1H NMR (300 MHz, CDCl_3) δ = 7.42 (m, 2H), 7.35-7.29 (massif, 4H), 3.91 (s, 2H).

^{19}F NMR (282 MHz, CDCl_3) δ = -34.61 (s, 3F).

Characterization data matched that reported in the literature[4].

CC(=O)c1ccccc1SeC(F)(F)F

Characterization data matched that reported in the literature[4].

Cc1ccccn1C(F)(F)FSeC(F)(F)F

Characterization data matched that reported in the literature[5].

Characterization data matched that reported in the literature[7].

References:

1. Glenadel, Q.; Ismalaj, E.; Billard, T. *J. Org. Chem.* **2016**, *81*, 8268-8275.
2. Chen, X.-L.; Zhou, S.-H.; Lin, J.-H.; Deng, Q.-H.; Xiao, J.-C. *Chem. Commun.* **2019**, *55*, 1410-1413.
3. Ghiazza, C.; Khrouz, L.; Billard, T.; Monnereau, C.; Tlili, A. *Eur. J. Org. Chem.* **2020**, *2020*, 1559-1566.
4. Dong, T.; He, J.; Li, Z.-H.; Zhang, C.-P. *ACS Sustainable Chem. Eng.* **2018**, *6*, 1327-1335.
5. Ghiazza, C.; Kataria, A.; Tlili, A.; Toulgoat, F.; Billard, T. *Asian J. Org. Chem.* **2019**, *8*, 675-678.
6. Rong, M.; Huang, R.; You, Y.; Weng, Z. *Tetrahedron* **2014**, *70*, 8872-8878.
7. Glenadel, Q.; Ismalaj, E.; Billard, T. *Eur. J. Org. Chem.* **2017**, *2017*, 530-533.

NMR data :

