Supporting Information

Acyclic Selenoiminium Salts: Isolation, First Structural Characterization, and Reactions

Yuichiro Mutoh and Toshiaki Murai*

Department of Chemistry, Faculty of Engineering, Gifu University, Yanagido, Gifu 501-1193, Japan

Characterization. Melting points were measured by a Yanagimoto micro melting point apparatus (uncorrected). The IR spectra were obtained on a JASCO FT / IR 410 spectrophotometers. ^1H (399.7 MHz), ^{13}C (100.4 MHz), ^{19}F (376.0 MHz), ^{77}Se (76.2 MHz), and ^{125}Te (126.0 MHz) NMR spectra were measured on the spectrometer JEOL *a*-400. The ^1H and the ^{13}C chemical shifts are reported in δ values referred to Me_4Si or CD_2Cl_2 and CDCl_3 or CD_2Cl_2 as an internal standard, respectively. The ^{19}F , the ^{77}Se , and the ^{125}Te chemical shifts are expressed in δ values deshielded with respect to CF_3COOH , Me_2Se , and Me_2Te as an external standard, respectively. Phase sensitive NOESY spectra were measured with a Varian Inova 500 NMR. All spectra were acquired in the proton-decoupled mode. The mass spectra (MS) were taken on SHIMADZU GCMS QP1000 (EI mode) or GCMS 9020DF high-resolution mass spectrometers. The FAB mass spectra were measured on JEOL GC-mate II mass spectrometers. Elemental analyses were carried out by Elemental Analysis Center of Kyoto University.

Materials. Diethyl ether (Et_2O) and tetrahydrofuran (THF) were distilled from sodium/benzophenone ketyl prior to use. Methyl trifluoromethanesulfonate (methyl triflate) was purchased from Aldrich Chemical Company, Inc., and used without further purification. *n*-Butyllithium 1.6 M hexane solution and lithium aluminum hydride (LiAlH_4) were purchased from Nacalai Tesque, Inc., and used without further purification. Tellurium was purchased from Nacalai Tesque, Inc., and was finely mashed prior to use. Selenoamides **1a**^{7e}, **1b**^{5a}, **1c**^{5a}, **1d**^{5f}, **1e**^{5f}, **1f**^{5g}, **1g**, **1h**^{5c}, **1i**^{5c}, **1j**^{7e}, **1k**^{7a}, **1l**^{5a}, and **1m**^{7e} were prepared according to literature methods. Silica gel used on column chromatography was silica gel 60N (Spherical, Neutral, 100–210 μm) and Florisil used on column chromatography was Florisil (150–250 μm) from Kanto Chemical Co., Inc.

Selenoiminium Salts 2

Dimethyl-*N*-(1-methylselenenylmethylidene)aminium trifluoromethanesulfonate (2a)

A pale yellow solid: mp 41.5–42.5 °C; IR (KBr) 3042, 1633, 1421, 1260, 1226, 1161, 1031, 933, 772, 640 cm^{-1} ; ^1H NMR (CDCl_3) δ 2.87 (s, 3H, SeCH_3), 3.44 (s, 3H, CH_3), 3.78 (s, 3H, CH_3), 10.0 (s, 1H, CHSe); ^{13}C NMR (CDCl_3) δ 10.0 (SeCH_3), 43.9, 50.0 (CH_3), 120.0 (q, $^1J_{\text{C-F}} = 319.5$ Hz, CF_3), 187.0 (CSe , $^1J_{\text{C-SeMe}} = 161.9$ Hz); ^{19}F NMR (CDCl_3) δ -79.2; ^{77}Se NMR (CDCl_3) δ 367.8; MS (FAB+) m/z 152 ($\text{M}^+ - \text{OTf}$); Anal.

Calcd for $\text{C}_5\text{H}_{10}\text{F}_3\text{NO}_3\text{SSe}$: C, 20.01; H, 3.36. Found: C, 19.96; H, 3.38.

Dimethyl-*N*-(1-methylselenenylethylidene)aminium trifluoromethanesulfonate (2b)

A colorless oil: ^1H NMR (CDCl_3) **major** δ 2.68 (s, 3H, SeCH_3), 2.73 (br s, 3H, CH_3), 3.58 (br s, 3H, NCH_3), 3.66 (br s, 3H, NCH_3); **minor** δ 2.61 (s, 3H, CH_3), 2.68 (br s, 3H, SeCH_3), 3.48 (br s, 3H, NCH_3), 3.55 (br s, 3H, NCH_3); ^{13}C NMR (CDCl_3) **major** δ 11.9 (SeCH_3), 24.0 (CH_3), 47.0, 47.5 (NCH_3), 120.8 (q, $^1J_{\text{C-F}} = 320.3$ Hz, CF_3), 195.5 (CSe , $^1J_{\text{C-SeMe}} = 164.3$ Hz); ^{19}F NMR (CDCl_3) δ -79.0; ^{77}Se NMR (CDCl_3) δ 433.4; MS (FAB+) m/z 166 ($\text{M}^+ - \text{OTf}$).

Dimethyl-*N*-(1-methylselenenylpropylidene)aminium trifluoromethanesulfonate (2c)

A colorless oil: IR (neat) 3114, 1736, 1606, 1258, 1226, 1164, 1031, 639 cm^{-1} ; ^1H NMR (CDCl_3) **major** δ 1.24–1.27 (m, 3H, CH_3), 2.70 (s, 3H, SeCH_3), 3.01–3.07 (m, 2H, CH_2), 3.56 (s, 3H, NCH_3), 3.66 (s, 3H, NCH_3); **minor** δ 1.26–1.30 (m, 3H, CH_3), 2.71 (s, 3H, SeMe), 3.05–3.12 (m, 2H, CH_2), 3.61 (s, 3H, NCH_3), 3.71 (s, 3H, NCH_3); ^{13}C NMR (CDCl_3) δ 10.3 (SeCH_3), 10.8 (CH_3), 29.6 (CH_2), 45.8, 47.2 (NCH_3), 120.4 (q, $^1J_{\text{C-F}} = 320.3$ Hz, CF_3), 199.7 (CSe); ^{19}F NMR (CDCl_3) **major** δ -78.9; **minor** δ -79.0; ^{77}Se NMR (CDCl_3) **major** δ 410.6; **minor** δ 409.5; MS (FAB+) m/z 180 ($\text{M}^+ - \text{OTf}$); Anal. Calcd for $\text{C}_7\text{H}_{14}\text{F}_3\text{NO}_3\text{SSe}$: C, 25.62; H, 4.30. Found: C, 25.84; H, 4.12.

Dimethyl-*N*-(1-methylselenenyl-2-methyl-4-pentenylidene)aminium trifluoromethanesulfonate (2d)

A slightly yellow oil: IR (neat) 2981, 2940, 1641, 1604, 1456, 1419, 1263, 1225, 1156, 1031, 929, 639 cm^{-1} ; ^1H NMR (CDCl_3) δ 1.39 (d, $J = 6.8$ Hz, 3H, CH_3), 2.44 (dt, $J = 7.3, 14.6$ Hz, 1H, $\text{CH}_2 = \text{CHCH}_2$), 2.58 (dt, $J = 7.3, 14.2$ Hz, 1H, $\text{CH}_2 = \text{CHCH}_2$), 2.71 (s, 3H, SeCH_3), 3.42 (sextet, $J = 6.8$ Hz, 1H, CH_3CH),

3.75 (s, 6H, N(CH₃)₂), 5.14–5.21 (m, 2H, CH₂=CH), 5.74 (ddt, *J* = 6.8, 10.3, 17.1 Hz, 1H, CH₂=CH); ¹³C NMR (CDCl₃) δ 12.5 (SeCH₃), 16.7 (CH₃), 37.9 (CH₂=CHCH₂), 42.8 (CH₃CH), 46.9, 50.6 (NCH₃), 119.3 (CH₂=CH), 120.1 (q, ¹*J*_{C-F} = 320.8 Hz, CF₃), 132.9 (CH₂=CH), 200.1 (CSe, ¹*J*_{C-SeMe} = 180.0 Hz); ¹⁹F NMR (CDCl₃) δ -79.0; ⁷⁷Se NMR (CDCl₃) δ not observed; MS (FAB+) *m/z* 220 (M⁺-OTf); Anal. Calcd for C₁₀H₁₈F₃NO₃SSe: C, 32.61; H, 4.93. Found: C, 32.52; H, 4.84.

Dimethyl-*N*-(1-methylselenenyl-2-phenyl-4-pentenylidene) trifluoromethanesulfonate (2e)

A slightly yellow oil: IR (neat) 3030, 1641, 1599, 1450, 1418, 1263, 1225, 1155, 1031, 638 cm⁻¹; ¹H NMR (CDCl₃) δ 2.59 (s, 3H, SeCH₃), 2.89 (dt, *J* = 7.8, 14.6 Hz, 1H, CH₂=CHCH₂), 3.11 (dt, *J* = 6.8 Hz, 14.6 Hz, 1H, CH₂=CHCH₂), 3.62 (s, 3H, NCH₃), 3.79 (s, 3H, NCH₃), 4.83 (t, *J* = 7.3 Hz, 1H, PhCH), 5.19–5.31 (m, 2H, CH₂=CH), 5.89 (ddt, *J* = 6.8, 9.8, 16.6 Hz, 1H, CH₂=CH) 7.30–7.43 (m, 5H Ar); ¹³C NMR (CDCl₃) δ 13.0 (SeCH₃), 34.5 (CH₂=CHCH₂), 47.6, 50.1 (NCH₃), 53.4 (PhCH), 115.8 (CH₂=CH), 120.1 (q, ¹*J*_{C-F} = 320.8 Hz, CF₃), 127.4 (Ar), 128.7 (CH₂=CH), 129.5, 132.3, 134.0 (Ar), 199.0 (CSe, ¹*J*_{C-SeMe} = 174.0 Hz); ¹⁹F NMR (CDCl₃) δ -78.9; ⁷⁷Se NMR (CDCl₃) δ 421.6; MS (FAB+) *m/z* 282 (M⁺-OTf); Anal. Calcd for C₁₅H₂₀F₃NO₃SSe: C, 41.86; H, 4.68. Found: C, 41.92; H, 4.73.

Dimethyl-*N*-(1-methylselenenyl-5-oxo-2,3,3-trimethylhexanylidene) trifluoromethanesulfonate (2f)

A white solid: mp 70.5–72.0 °C; IR (KBr) 2965, 1705, 1598, 1265, 1225, 1158, 1032, 639 cm⁻¹; ¹H NMR (CDCl₃) δ 1.13 (s, 3H, CCH₃), 1.17 (s, 3H, CH₃), 1.31 (d *J* = 6.8 Hz, 3H, CHCH₃), 2.16 (s, 3H, CH₃C=O), 2.45 (d, *J* = 18.1 Hz, 1H, CH₂), 2.70 (d, *J* = 18.1 Hz, 1H, CH₂), 2.72 (s, 3H, SeCH₃), 3.90 (s, 3H, NCH₃), 3.92 (s, 3H, NCH₃), 4.03 (q, *J* = 6.8 Hz, 1H, CH); ¹³C NMR (CDCl₃) δ 13.6 (SeCH₃), 14.9 (CHCH₃), 24.9, 25.7 (CCH₃), 31.8 (CH₃C=O), 37.7 (CCH₃), 47.4, 48.4 (NCH₃), 52.5 (CH₂), 52.1 (CHCH₃), 120.6 (q, ¹*J*_{C-F} = 320.3 Hz, CF₃), 200.6 (CSe, ¹*J*_{C-SeMe} = 160.4 Hz), 208.3 (C=O); ¹⁹F NMR (CDCl₃) δ -78.9; ⁷⁷Se NMR (CDCl₃) δ 333.9; MS (FAB+) *m/z* 278 (M⁺-OTf).

(*E*)-*N*-[1-Methylselenenyl-3-(4-methylphenyl)-2-propenylidene]pyrrolidinium trifluoromethanesulfonate (2h)

CH_2Cl_2 was used as a solvent for the synthesis of **2h**. A light yellow solid: dec. 94.0–94.6 °C; IR (KBr) 3035, 2992, 1622, 1604, 1550, 1260, 1151, 1031, 637 cm^{-1} ; ^1H NMR (CDCl_3) δ 2.21–2.31 (m, 4H, NCH_2CH_2), 2.39 (s, 3H, ArCH_3), 2.61 (s, 3H, SeCH_3), 3.92 (br, t, $J = 6.8$ Hz, 2H, NCH_2), 4.08 (br, t, $J = 6.8$ Hz, 2H, NCH_2), 6.97 (d, $J = 16.1$ Hz, 1H, CH), 7.24 (d, $J = 9.3$ Hz, 2H, Ar), 7.32 (d, $J = 16.1$ Hz, 1H, CH), 7.57 (d, $J = 8.3$ Hz, 2H, Ar); ^{13}C NMR (CDCl_3) δ 13.4 (SeCH_3), 21.6 (ArCH_3), 24.6, 25.4 (NCH_2CH_2), 57.1, 57.3 (NCH_2), 118.2 (CH), 120.8 (q, $^1J_{\text{C-F}} = 320.3$ Hz, CF_3), 129.0, 130.0, 130.4, 142.8 (Ar), 148.3 (CH), 185.1 (CSe , $^1J_{\text{C-SeMe}} = 158.9$ Hz); ^{19}F NMR (CDCl_3) δ -78.9; ^{77}Se NMR (CDCl_3) δ 390.2; MS (FAB+) m/z 294 ($\text{M}^+ - \text{OTf}$); Anal. Calcd for $\text{C}_{16}\text{H}_{20}\text{F}_3\text{NO}_3\text{SSe} \cdot 0.2\text{CH}_2\text{Cl}_2$: C, 42.36; H, 4.48. Found: C, 42.59; H, 4.49.

(E)-N-[3-(4-Dimethylaminophenyl)-1-methylselenenyl-2-propenylidene]pyrrolidinium trifluoromethanesulfonate (2i)

CH_2Cl_2 was used as a solvent for the synthesis of **2i**. A red solid: dec. 101–104 °C; IR (KBr) 2918, 1611, 1575, 1521, 1440, 1382, 1310, 1277, 1161, 1028, 632 cm^{-1} ; ^1H NMR (CDCl_3) δ 2.24 (br, 4H, NCH_2CH_2), 2.59 (s, 3H, SeCH_3), 3.11 (s, 6H $\text{N}(\text{CH}_3)_2$), 4.00 (br, t, $J = 6.1$ Hz, 2H, NCH_2), 4.63 (br, t, $J = 6.1$ Hz, 2H, NCH_2), 6.75–6.79 (m, 3H, Ar, CH), 7.52 (d, $J = 15.1$ Hz, 1H, CH), 7.63 (d, $J = 9.3$ Hz, 2H, Ar); ^{13}C NMR (CDCl_3) δ 13.3 (SeCH_3), 24.5, 25.3 (NCH_2CH_2), 40.4 ($\text{N}(\text{CH}_3)_2$), 55.8, 57.4 (NCH_2), 112.5 (CH), 112.9 (Ar), 120.7 (q, $^1J_{\text{C-F}} = 320.8$ Hz, CF_3), 132.4, 150.0 (Ar), 153.3 (CH), 179.9 (CSe , $^1J_{\text{C-SeMe}} = 153.1$ Hz); ^{19}F NMR (CDCl_3) δ -78.8; ^{77}Se NMR (CDCl_3) δ 423.9; MS (FAB+) m/z 323 ($\text{M}^+ - \text{OTf}$); Anal. Calcd for $\text{C}_{17}\text{H}_{23}\text{F}_3\text{NO}_3\text{SSe} \cdot 0.3\text{CH}_2\text{Cl}_2$: C, 41.82; H, 4.79. Found: C, 41.71; H, 4.70.

Dimethyl-N-(1-methylselenenyl-1-phenylmethylidene)aminium trifluoromethanesulfonate (2j)

A white solid: mp 79.5–82.0 °C; IR (KBr) 2924, 1615, 1446, 1253, 1223, 1155, 1031, 763, 703, 639 cm^{-1} ; ^1H NMR (CDCl_3) δ 2.06 (s, 3H, SeCH_3), 3.49 (s, 3H, CH_3), 3.82 (s, 3H, CH_3), 7.44–7.46 (m, 2H, Ar), 7.59–7.66 (m, 3H, Ar); ^{13}C NMR (CDCl_3) δ 13.2 (SeCH_3), 47.1, 48.4 (CH_3), 120.8 (q, $^1J_{\text{C-F}} = 320.6$ Hz, CF_3), 126.0, 130.1, 131.7, 132.2 (Ar), 195.6 (C=Se , $^1J_{\text{C-SeMe}} = 164.3$ Hz); ^{19}F NMR (CDCl_3) δ -78.8; ^{77}Se NMR

(CDCl₃) δ 449.9; MS (FAB+) m/z 228 (M⁺–OTf); Anal. Calcd for C₁₁H₁₄F₃NO₃SSe: C, 35.11; H, 3.75. Found: C, 35.40; H, 3.77.

(Z)-Benzyl-N-(1-methylselenenyl-1-phenylmethylidene)aminium trifluoromethanesulfonate (2k)

A pale yellow solid: mp 106–114 °C; IR (KBr) 3192, 3066, 2967, 1717, 1700, 1685, 1595, 1281, 1242, 1225, 1029, 638 cm⁻¹; ¹H NMR (CDCl₃) δ 2.25 (s, 3H, SeCH₃), 5.02 (s, 2H PhCH₂), 7.29–7.79 (m, 10H, Ar), 12.6 (br, s, 1H, NH); ¹³C NMR (CDCl₃) δ 13.1 (SeCH₃), 54.6 (PhCH₂), 120.2 (q, ¹J_{C–F} = 320.0 Hz, CF₃), 128.3, 128.6, 129.0, 129.2, 129.7, 131.6, 131.9, 134.3 (Ar), 198.1 (CSe, ¹J_{C–SeMe} = 167.7 Hz); ¹⁹F NMR (CDCl₃) δ –78.9; ⁷⁷Se NMR (CDCl₃) δ 382.9; MS (FAB+) m/z 290 (M⁺–OTf); Anal. Calcd for C₁₆H₁₆F₃NO₃SSe: C, 43.84; H, 3.68. Found: C, 43.85; H, 3.53.

(Z)-4-Methoxyphenyl-N-(1-methylselenenylethylidene)aminium trifluoromethanesulfonate (2l)

A red-yellow oil: IR (neat) 2939, 2845, 1737, 1725, 1610, 1580, 1512, 1256, 1170, 1030, 639 cm⁻¹; ¹H NMR (CDCl₃) δ 2.56 (s, 3H, SeCH₃), 2.91 (s, 3H CH₃), 3.82 (s, 3H, OCH₃), 6.96 (d, *J* = 8.8 Hz, 2H, Ar), 7.32 (d, *J* = 8.8 Hz, 2H, Ar), 13.0 (br, s, 1H NH); ¹³C NMR (CDCl₃) δ 9.6 (SeCH₃), 26.9 (CH₃), 55.5 (OCH₃), 115.2 (Ar), 120.1 (q, ¹J_{C–F} = 318.8 Hz, CF₃), 125.4, 129.0, 160.9 (Ar), 200.8 (CSe, ¹J_{C–SeMe} = 162.8 Hz); ¹⁹F NMR (CDCl₃) δ –79.1; ⁷⁷Se NMR (CDCl₃) δ 416.8; MS (FAB+) m/z 244 (M⁺–OTf); Anal. Calcd for C₁₁H₁₄F₃NO₃SSe•0.05hexane: C, 34.22; H, 3.74. Found: C, 34.36; H, 3.72.

1-Methyl-2-methylselenenylpyrrolidinium trifluoromethanesulfonate (2m)

A brown solid: mp 46.0–47.5 °C; IR (KBr) 2360, 1621, 1264, 1159, 1032, 639 cm⁻¹; ¹H NMR (CDCl₃) δ 2.40 (quint, *J* = 8.0 Hz, 2H, CH₂), 2.72 (s, 3H, SeCH₃), 3.41 (s, 3H NCH₃), 3.43 (t, *J* = 7.6 Hz, 2H, CH₂), 4.24 (t, *J* = 7.6 Hz, 2H, CH₂); ¹³C NMR (CDCl₃) δ 9.8 (SeCH₃), 19.5 (CH₂), 39.0 (NCH₃), 41.0 (CH₂), 63.2 (CH₂), 120.7 (q, ¹J_{C–F} = 320.7 Hz, CF₃), 195.2 (CSe, ¹J_{C–SeMe} = 170.1 Hz); ¹⁹F NMR (CDCl₃) δ –79.0; ⁷⁷Se NMR (CDCl₃) δ 343.4; MS (FAB+) m/z 179 (M⁺–OTf); Anal. Calcd for C₇H₁₂F₃NO₃SSe: C, 25.77; H, 3.71. Found: C, 25.73; H, 3.48.

Reaction of selenoiminium salt 2j with BuLi.

To an Et₂O solution of BuLi (1.6 M hexane solution, 0.94 mL, 1.5 mmol) was added seleniminium salt **2j** (0.188 g, 0.5 mmol) at –78 °C, and this was stirred for 1.5 h at this temperature. After warming up to room temperature over 1.5 h, the resulting mixture was poured into a saturated aqueous solution of NaHCO₃, and extracted with Et₂O. The organic layer was dried over MgSO₄ and concentrated in vacuo. The residue was purified by column chromatography (SiO₂, hexane : CH₂Cl₂ = 1 : 1) to give ketone **5** (0.044 g, 70 %) and ketone **6** (0.029, 26%).

Phenyl 1-pentyl ketone (5) A colorless oil: *R_f* = 0.63; ¹H NMR (CDCl₃) δ 0.86 (t, *J* = 7.1 Hz, 3H, CH₃), 1.16–1.43 (m, 4H, CH₂CH₂CH₃), 1.78–1.87 (br, m, 1H, CH₂CH₂CH₂CH₃), 2.14–2.23 (br, m, 1H, CH₂CH₂CH₂CH₃), 4.54 (t, *J* = 7.3 Hz, 1H, CH), 7.17–7.21 (m, 1H Ar), 7.26–7.32 (m, 4H Ar), 7.36–7.40 (m, 2H Ar), 7.46–7.50 (m, 1H Ar), 7.95–7.97 (m, 2H Ar); ¹³C NMR (CDCl₃) δ 14.0 (CH₃), 22.7, 22.9, 33.8 (CH₂), 53.7 (CH), 126.9, 128.2, 128.5, 128.7, 128.9, 132.8, 137.0, 139.9 (Ar), 200.2 (C=O); MS (EI) *m/z* 252 (M⁺), 196 (M⁺-Bu).

Butyl phenyl ketone (6) A slightly yellow oil: *R_f* = 0.50; ¹H NMR (CDCl₃) δ 0.95 (t, *J* = 7.3 Hz, 3H, CH₃), 1.41 (sextet, *J* = 7.3 Hz, 2H, CH₂CH₃), 1.72 (quint, *J* = 7.5 Hz, 2H, CH₂CH₂CH₃), 2.97 (t, *J* = 7.6 Hz, 2H, CH₂CH₂CH₂CH₃), 7.44–7.48 (m, 2H Ar), 7.53–7.57 (m, 1H Ar), 7.94–7.97 (m, 2H Ar); ¹³C NMR (CDCl₃) δ 14.0 (CH₃), 22.5, 26.5, 38.4 (CH₂), 128.1, 128.6, 132.9, 137.1 (Ar), 200.6 (C=O).

Telluroamides **7**

N,N-Dimethyl Telluroformamide (**7a**)

A red solid: ¹H NMR (CD₂Cl₂) δ 3.21 (s, 3H, NCH₃), 3.53 (s, 3H, NCH₃), 12.7 (s, 1H, CH=Te); ¹³C NMR (CD₂Cl₂) δ 46.8, 50.8 (NCH₃), 179.0 (C=Te); ¹²⁵Te NMR (CD₂Cl₂) δ 549.1.

N,N-Dimethyl Tellurobenzamide (**7b**)

A dark red solid: ¹H NMR (CD₂Cl₂) δ 2.96 (s, 3H, CH₃), 3.78 (s, 3H, CH₃), 7.23–7.36 (m, 5H, Ar); ¹³C NMR (CD₂Cl₂) δ 44.7, 55.2 (NCH₃), 123.1, 128.0, 128.3, 152.6 (Ar), 197.5 (C=Te); ¹²⁵Te NMR (CD₂Cl₂) δ 894.0.

N,N-Dimethyl 2-Phenyl-4-pentenetelluroamide (7c)

A reddish-orange solid: IR 3060, 2924, 1638, 1598, 1511, 1493, 1389, 1250, 1151, 1054, 998, 916, 766, 701 cm^{-1} ; 1H NMR (CD_2Cl_2) δ 2.84 (dt, $J = 7.6$, 14.0 Hz, 1H, $CH_2=CHCH_2$), 3.13–3.22 (m, 1H, 4H, $CH_2=CHCH_2$, NCH_3), 3.69 (s, 3H, NCH_3), 3.90 (t, $J = 7.2$ Hz, 1H, PhCH), 4.97 (dt, $J = 2.5$, 10.4 Hz, 1H, $CH_2=CHCH_2$), 5.06 (dq, $J = 1.6$, 17.3 Hz, 1H, $CH_2=CHCH_2$), 5.77 (ddt, $J = 6.4$, 10.4, 17.2 Hz, 1H, $CH_2=CHCH_2$), 7.23–7.32 (m, 3H, Ar), 7.51–7.53 (m, 2H, Ar); ^{13}C NMR (CD_2Cl_2) δ 42.8 (NCH_3), 47.8 ($CH_2=CHCH_2$), 58.1 (NCH_3), 60.7 (PhCH), 116.9 ($CH_2=CHCH_2$), 127.4, 128.7, 129.1 (Ar), 136.4 ($CH_2=CHCH_2$), 138.9 (Ar), 206.0 (C=Te); ^{125}Te NMR (CD_2Cl_2) 620.4; MS (EI) m/z 317 (M^+ , ^{130}Te); HRMS Calcd for $C_{13}H_{17}NTe$: 317.0423, Found: 317.0420.

X-ray Structure Analysis. The measurement of selenoiminium salt **2j** was carried out on a Rigaku AFC7R four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71069$ Å). The structure was solved and refined using the teXsan® crystallographic software package of Molecular Structure Corporation. The X-ray quality crystals were obtained by slow diffusion of hexane and Et_2O into Et_2O/CH_2Cl_2 (1/1) solution of **2j** (0.020 g). The crystal was cut from the grown crystals and was mounted on a glass fiber. The cell dimensions were determined from a least-squares refinement of the setting diffractometer angles for 25 automatically centered reflections. Three standard reflections were measured every 150 reflections and showed no significant intensity variations during the data collection. Lorentz and polarization corrections were applied to the data, and empirical absorption corrections ψ -Scan were also applied. The structures were solved by direct method using SHELXS86¹ and expanded using DIRDIF94². Scattering factors for neutral atoms were from Cromer and Waber³, and anomalous dispersion effects⁴ were used. The function minimized was $\sum w(F_o^2 - F_c^2)^2$ and the weighting scheme employed was $w = [\sigma_c^2(F_o^2) + (p(\max(F_o^2, 0) + 2F_c^2/3)^2)]^{-1}$. A full-matrix least-squares refinement was executed with non-hydrogen atoms being anisotropic. The final least square cycle included fixed hydrogen atoms at calculated positions of which each isotropic thermal parameter was set to 1.2 times of that of the connecting atom. Crystal data and measurement description are summarized in Table 3. Atomic coordinates, B(iso)/B(eq) are listed in Table 4.

References:

- (1) Sheldrick, G. M. *Crystallographic Computing 3*; Sheldrick, G. M.; Kruger, C.; Goddard, R., Eds. Oxford University Press, 1985, pp. 175–189.

- (2) The DIRDIF94 program system was used: Beuiskens, P. T.; Admiraal, G.; Beurskiens, G.; Bosman, W. P.; de Gelder, R.; Israel, R.; Smits, J. M. M. *Technical Report of the Crystallography Laboratory*; University of Nijmegen; The Netherlands, 1994.
- (3) Cromer, D. T.; Waber, J. T. *International Tables for X-ray Crystallography*; Ibers, J. A.; Hamilton, W. C., Eds.; The Kynoch Press: Birmingham, England, 1974; Vol. IV, Table 2.2A.
- (4) Creagh, D. C.; McAuley, W. J. *International Tables for X-ray Crystallography*; Wilson, A. J. C., Ed.; Kluwer Academic Publishers, Boston, 1992; Vol. C, Table 4.2.6.8, pp. 219–222.

Table 3. Crystal data and experimental details for selenoiminium salt **2j**.

selenoiminium salt	2j
empirical formula	C ₁₁ H ₁₄ F ₃ NO ₃ SSe
formula weight	376.26
crystal color, habit	Colorless, prismatic
crystal system	monoclinic
unit-cell dimensions	a = 7.348(3) Å b = 17.768(3) Å c = 11.345(2) Å β = 94.68(2)°
volume of unit cell (Å ³)	1476.3(6)
space group	P2 ₁ /n (#14)
Z value	4
D _{calc} (g/cm ³)	1.693
crystal dimensions (mm)	0.14 x 0.20 x 0.33
μ (Mo Kα) (cm ⁻¹)	27.23
diffractometer	Rigaku AFC7R four-circle
temperature (°C)	-80
2θ _{max} (deg)	55.0
no. of reflections measured:	
total	4644
unique	3395
R _{int}	0.026
no. of Reflections (All, 2θ < 55.03)	3395
no. of variables	181
reflection / parameter ratio	18.76
residuals: R ^a , R _w ^b	0.097, 0.126
residuals: R1 ^c	0.047
p-factor	0.0500
Maximum peak in Final Diff. Map (e/Å ⁻³)	0.98
Minimum peak in Final Diff. Map (e/Å ⁻³)	-1.21
goodness of fit indicator	1.08

$$^a R = \Sigma(F_o^2 - F_c^2) / \Sigma F_o^2. \quad ^b R_w = [(\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w F_o^2)^2]^{1/2}. \quad ^c R1 = \Sigma |F_o| - |F_c| / \Sigma |F_o|. \quad w = 1 / [\Sigma^2(F_o)^2]$$

Table 4. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B _{eq}
Se(1)	0.14914(7)	0.31518(3)	0.56530(4)	3.35(1)
S(1)	0.1362(2)	0.13683(7)	0.2884(1)	3.06(3)
F(1)	0.4145(5)	0.0587(2)	0.2320(4)	8.3(1)
F(2)	0.3642(7)	0.0467(2)	0.4073(3)	9.4(1)
F(3)	0.1992(5)	-0.0076(2)	0.2732(4)	7.5(1)
O(1)	0.2522(5)	0.1967(2)	0.3290(4)	5.9(1)
O(2)	0.0801(6)	0.1387(2)	0.1658(3)	6.0(1)
O(3)	-0.0043(6)	0.1197(2)	0.3619(4)	7.3(1)
N(1)	-0.1767(5)	0.2427(2)	0.5070(3)	2.63(9)
C(1)	-0.0753(6)	0.2970(3)	0.4773(4)	2.35(10)
C(2)	0.2558(7)	0.3832(3)	0.4579(5)	3.9(1)
C(3)	-0.1353(6)	0.3493(3)	0.3799(4)	2.41(10)
C(4)	-0.1051(6)	0.3325(3)	0.2639(4)	2.9(1)
C(5)	-0.1627(7)	0.3818(3)	0.1747(4)	3.2(1)
C(6)	-0.2483(6)	0.4473(3)	0.1996(4)	3.1(1)
C(7)	-0.2816(7)	0.4640(3)	0.3149(4)	3.5(1)
C(8)	-0.2227(6)	0.4155(3)	0.4055(4)	3.1(1)
C(9)	-0.3575(7)	0.2264(3)	0.4453(5)	3.9(1)
C(10)	-0.1218(7)	0.1914(3)	0.6041(5)	3.8(1)
C(11)	0.2816(7)	0.0550(3)	0.3031(4)	3.5(1)
H(1)	-0.0405	0.2864	0.2464	3.6990
H(2)	-0.1414	0.3698	0.0927	4.0126
H(3)	-0.2852	0.4825	0.1364	3.8987
H(4)	-0.3465	0.5103	0.3328	4.1486
H(5)	-0.2417	0.4277	0.4880	3.8789
H(6)	0.3788	0.3932	0.4809	4.5920
H(7)	0.2465	0.3626	0.3786	4.5920
H(8)	0.1892	0.4304	0.4532	4.5920
H(9)	-0.3920	0.2642	0.3887	4.6444

H(10)	-0.4490	0.2239	0.5012	4.6444
H(11)	-0.3555	0.1788	0.4059	4.6444
H(12)	-0.1326	0.2157	0.6789	4.6748
H(13)	-0.2017	0.1483	0.6008	4.6748
H(14)	-0.0008	0.1748	0.6002	4.6748

$$B_{eq} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$