Supporting Information

MeOTf-Mediated Alkynylation of Selenoamides Leading to β-Methylselenenyl α,β-Unsaturated Ketones and Their Characterization

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Characterization of the products 3

(*Z*)-1-Methylselenenyl-3-oxo-3-phenyl-1-trimethylsilyl-1-propene (3a)

IR (KBr) 3054, 2951, 2898, 1644, 1622, 1596, 1497, 1234, 1021, 952, 754, 709 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.40 (s, 9H, $SiMe_3$), 2.31 (s, 3H, SeMe), 7.46-7.54 (m, 3H, Ar), 7.80 (s, 1H, C<u>H</u>=C) 7.96-7.98 (m, 2H, Ar); ^{13}C NMR ($CDCl_3$) δ 1.1 ($SiMe_3$), 7.4 (SeMe), 127.4, 128.1, 128.3 (Ar), 132.2 (<u>C</u>H=C), 138.5 (Ar), 169.3 (CSe), 188.1 (C=O); ^{77}Se NMR ($CDCl_3$) δ 419.6; EIMS *m*/*z* 298 (M^+), 283 (M^+-CH_3).

1-(1-Cyclohexenyl)-1-methylselenenyl-3-oxo-3-phenyl-1-propene (3b)

IR (KBr) 2993, 2860, 1623, 1596, 1519, 1445, 1340, 1232, 1044, 706 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 1.63-1.67 (br, m, 2H, CH_2(Cyclohexenyl)), 1.72-1.76 (br, m, 2H, CH_2(Cyclohexenyl)), 2.06 (s, 3H, SeMe), 2.13-2.23 (br, 4H, Cyclohexenyl), 5.69 (br, 1H, CH=C), 7.36 (s, 1H, C<u>H</u>=C(SeMe)), 7.42-7.51 (m, 3H, Ar), 7.97-8.00 (m, 2H, Ar); ^{13}C NMR ($CDCl_3$) δ 6.3 (SeMe), 21.8, 22.3, 24.9, 30.0 (CH_2), 118.7 (<u>C</u>H=C), 126.9, 127.9, 128.5 132.1 (Ar), 138.2 (<u>C</u>H=C(SeMe)), 138.4 (CH=<u>C</u>), 169.1 (CSe), 189.0 (C=O); ^{77}Se NMR ($CDCl_3$) δ 365.6; EIMS *m*/*z* 306 (M^+), 291 (M^+-CH_3).

1-Methylselenenyl-3-oxo-3-(4-methoxyphenyl)-1-trimethylsilyl-1-propene (3c)

IR (KBr) 2958, 2838, 1621, 1600, 1571, 1500, 1239, 1169, 954, 854, 712 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.39 (s, 9H, $SiMe_3$), 2.29 (s, 3H, SeMe), 3.86 (s, 3H, OCH_3), 6.94 (d, *J* = 8.8 Hz, 2H, Ar), 7.78 (s, 1H, C<u>H</u>=C) 7.97 (d, *J* = 9.3 Hz, 2H, Ar); ^{13}C NMR ($CDCl_3$) δ 1.1 ($SiMe_3$), 7.3 (SeMe), 55.4 (OCH_3), 113.8 (Ar), 127.6 (<u>C</u>H=C), 130.4, 131.4, 162.9 (Ar), 167.3 (CSe), 186.9 (C=O); ^{77}Se NMR ($CDCl_3$) δ 407.9; EIMS *m*/*z* 328 (M^+), 313 (M^+-CH_3), 297 (M^+-OCH_3).

1-Methylselenenyl-3-oxo-3-(4-bromophenyl)-1-trimethylsilyl-1-propene (3d)

IR (KBr) 2938, 2360, 2342, 1622, 1584, 1498, 1479, 1237, 1229, 952, 843, 816 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.39 (s, 9H, $SiMe_3$), 2.32 (s, 3H, SeMe), 7.59 (d, *J* = 8.8 Hz, 2H, Ar), 7.74 (s, 1H, C<u>H</u>=C) 7.83 (d, *J* = 8.3 Hz, 2H, Ar); ^{13}C NMR ($CDCl_3$) δ 1.0 ($SiMe_3$), 7.5 (SeMe), 126.8 (<u>C</u>H=C), 127.1, 129.7, 131.9, 137.3 (Ar), 170.9 (CSe), 186.8 (C=O); ^{77}Se NMR ($CDCl_3$) δ 427.5; EIMS *m*/*z* 376 (M^+), 361 (M^+-CH_3).

(*Z*)-1-Methylselenenyl-3-oxo-1-phenyl-1-butene (3e)

IR (KBr) 2926, 1653, 1538, 1486, 1442, 1421, 1231, 1181, 983, 767, 708, 630 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 1.62 (s, 3H, CH_3), 2.11 (s, 3H, SeMe), 6.74 (s, 1H, C<u>H</u>=C), 7.20 (d, *J* = 8.3 Hz, 2H, Ar), 7.33-7.42 (m, 3H Ar); ^{13}C NMR ($CDCl_3$) δ 7.3 (SeMe), 30.3 (CH_3), 125.0 (<u>C</u>H=C), 127.8, 128.3, 128.4, 139.5 (Ar), 162.4 (CSe), 196.3 (C=O); ^{77}Se NMR ($CDCl_3$) δ 372.6; EIMS *m*/*z* 240 (M^+), 225 (M^+-CH_3); Anal. Calcd for $C_{10}H_{12}OSe$: C, 55.24; H, 5.06. Found: C, 55.22; H, 5.06.

(*Z*)-1-Methylselenenyl-3-oxo-1-phenyl-1-pentene (3f)

IR (neat) 3057, 2974, 2933, 1655, 1543, 1487, 1226, 1129, 1046, 760, 701 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 1.16 (t, *J* = 7.3 Hz, 3H, CH_3), 1.62 (s, 3H, SeMe), 2.54 (q, *J* = 7.3 Hz, 2H, $CH_3C\underline{H}_2$), 6.73 (s, 1H, C<u>H</u>=C), 7.18-7.21 (m, 2H, Ar), 7.32-7.41 (m, 3H Ar); ^{13}C NMR ($CDCl_3$) δ 7.2 (SeMe), 8.3 (CH_3), 36.3 (CH_2), 124.3, 127.8, 128.3, (Ar), 128.3 (<u>C</u>H=C), 139.6 (Ar), 161.7 (CSe), 199.5 (C=O); ^{77}Se NMR ($CDCl_3$) δ 369.4; EIMS *m*/*z* 254 (M^+), 239 (M^+-CH_3), 225 (M^+-CH_3CH_2); Anal. Calcd for $C_{11}H_{14}OSe$: C, 56.92; H, 5.57. Found: C, 57.17; H, 5.64.

1-Methylselenenyl-3-oxo-4-phenyl-1-trimethylsilyl-1-butene (3g)

IR (neat) 3061, 3028, 2954, 1651, 1496, 1251, 1096, 974, 857, 842, 750, 702 cm^{-1}; ^{1}H NMR ($CDCl_3$) *E*-isomer δ 0.25 (s, 3H, $SiMe_3$), 2.07 (s, 3H, SeMe), 3.73 (s, 2H, $PhC\underline{H}_2$), 6.59 (s, 1H, C<u>H</u>=C(SeMe)), 7.21-7.27 (m, 5H, Ar); *Z*-isomer δ 0.27 (s, 3H, $SiMe_3$), 2.23 (s, 3H, SeMe), 3.78 (s, 2H, $PhC\underline{H}_2$), 7.02 (s, 1H, C<u>H</u>=C(SeMe)), 7.30-7.34 (m, 5H, Ar); ^{13}C NMR ($CDCl_3$) *E*-isomer δ -0.75 ($SiMe_3$), 6.8 (SeMe), 50.0 ($Ph\underline{C}H_2$), 126.8 (<u>C</u>H=C(SeMe)), 128.6, 129.4, 130.0, 134.9 (Ar), 167.4 (CSe), 192.6 (C=O); *Z*-isomer δ 0.9 ($SiMe_3$), 7.1 (SeMe), 50.0 ($Ph\underline{C}H_2$), 126.7 (<u>C</u>H=C(SeMe)), 128.7, 129.5, 130.1, 135.0 (Ar), 167.5 (CSe), 195.2 (C=O); ^{77}Se NMR ($CDCl_3$) *E*-isomer δ 300.1; *Z*-isomer δ 413.1;

EIMS *m*/*z* 312 (M^+), 297 (M^+-CH_3), 221 (M^+-$PhCH_2$); HRMS. Calcd for $C_{14}H_{20}OSeSi$: (M^+) 312.0449, Found: 312.4553.

(*Z*)-1-(1-Cyclohexenyl)-1-methylselenenyl-3-oxo-4-phenyl-1-butene (3h)

IR (neat) 3060, 3026, 2929, 2857, 2183, 1662, 1617, 1531, 1495, 1311, 1187, 1000, 716, 695 cm^{-1}; ^1H NMR ($CDCl_3$) δ 1.57-1.62 (br, 2H, CH_2(Cyclohexenyl)), 1.63-1.70 (br, 2H, CH_2(Cyclohexenyl)), 1.98 (s, 3H, SeMe), 2.03 (br 2H, CH_2(Cyclohexenyl)), 2.12 (br 2H, CH_2(Cyclohexenyl)), 3.74 (s, 2H, Ph$\underline{C}H_2$), 5.54 (br, 1H, CH=C), 6.59 (s, 1H, C$\underline{H}$=C(SeMe)), 7.22-7.25 (m, 3H, Ar), 7.29-7.32 (m, 2H, Ar); ^{13}C NMR ($CDCl_3$) δ 6.1 (SeMe), 21.7, 22.2, 24.8, 29.8 (CH_2), 49.9 (Ph$\underline{C}H_2$), 121.2 ($\underline{C}$H=C), 126.7 ($\underline{C}$H=C(SeMe)), 126.8, 128.5, 129.5 134.9 (Ar), 137.5 ($\underline{C}$H=C(SeMe)), 167.0 (CSe), 196.2 (C=O).

(*Z*)-4-Methyl-1-methylselenenyl-3-oxo-1-phenylhepta-1,6-diene (3i)

IR (neat) 3074, 2972, 2928, 1651, 1539, 1487, 1442, 1227, 1072, 915, 765, 701 cm^{-1}; ^1H NMR ($CDCl_3$) δ 1.16 (d, *J* = 6.8 Hz, 3H, CH_3), 1.62 (s, 3H, SeMe), 2.16 (dt, *J* = 7.3, 14.5 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.49 (dt, *J* = 6.5, 13.3 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.69 (sextet, *J* = 7.0 Hz, 1H, $CH_3C\underline{H}$), 5.00-5.08 (m, 2H, C$\underline{H}_2$=CH), 5.77 (ddt, *J* = 7.0,10.0, 17.1 Hz, 1H, CH_2=C$\underline{H}$), 6.77 (s, 1H, C$\underline{H}$=C(SeMe)), 7.20-7.22 (m, 2H, Ar), 7.33-7.43 (m, 3H, Ar); ^{13}C NMR ($CDCl_3$) δ 7.4 (SeMe), 16.1 (CH_3), 37.4 (CH_2=CH$\underline{C}H_2$), 45.9 ($CH_3\underline{C}H$), 116.6 ($\underline{C}H_2$=CH), 123.7, 127.9, 128.3 (Ar), 128.4 ($\underline{C}$H=C(SeMe)), 136.0 (Ar), 139.7 ($\underline{C}$H=C(SeMe)), 163.0 (CSe), 201.7 (C=O); ^{77}Se NMR ($CDCl_3$) δ 372.6; EIMS *m*/*z* 294 (M^+), 279 (M^+-CH_3), 225 (M^+-CH_2=$CHCH_2CHCH_3$); Anal. Calcd for $C_{15}H_{18}OSe$: C, 61.40; H, 6.19. Found: C, 61.56; H, 6.19.

(*Z*)-1-(1-Cyclohexenyl)-1-methylselenenyl-3-oxo-4-methylhepta-1,6-diene (3j)

IR (neat) 3074, 2968, 2929, 2858, 2837, 1643, 1604, 1537, 1448, 1437, 1184, 1066, 916, 825 cm^{-1}; ^1H NMR ($CDCl_3$) δ 1.08 (d, *J* = 6.8 Hz, 3H, CH_3), 1.56-1.62 (br,m, 2H), 1.63-1.69 (br,m, 2H), 1.96 (s, 3H, SeMe), 2.02-2.06 (br,m, 2H), 2.10-2.15 (br,m, 2H), 2.10-2.15 (m, 1H, CH_2=CHC$\underline{H}_2$), 2.41 (dt, *J* = 6.6, 12.7 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.58 (sextet, *J* = 7.0 Hz, 1H, $CH_3C\underline{H}$), 4.94-5.02 (m, 2H, C$\underline{H}_2$=CH), 5.55-5.58 (br,m, 1H, CH=C), 5.70 (ddt, *J* = 7.3, 9.8, 17.1 Hz, 1H, CH_2=C$\underline{H}$), 6.59 (s, 1H, C$\underline{H}$=C(SeMe)); ^{13}C NMR ($CDCl_3$) δ 6.1 (SeMe), 16.1 (CH_3), 21.8, 22.3, 24.9, 30.3 ($\underline{C}H_2$), 37.4 (CH_2=CH$\underline{C}H_2$),

45.7 ($CH_3\underline{C}H$), 116.4 ($\underline{C}H_2$=CH), 121.0 ($\underline{C}$H=C), 126.8 (CH=$\underline{C}$(SeMe)), 136.1 ($\underline{C}$H=C(SeMe)), 137.8 (CH_2=$\underline{C}$H), 166.1 (CSe), 202.0 (C=O); ^{77}Se NMR ($CDCl_3$) δ 353.1; EIMS *m*/*z* 298 (M^+), 283 (M^+-CH_3), 229 (M^+-CH_2=$CHCH_2CHCH_3$); Anal. Calcd for $C_{15}H_{22}OSe$: C, 60.60; H, 7.46. Found: C, 60.66; H, 7.31.

(*Z*)-2,6-Dimethyl-3-methylselenenyl-5-oxonona-1,3,8-triene (3k)

IR (neat) 3078, 2972, 2929, 1653, 1535, 1456, 1421, 1371, 1300, 1263, 1080, 910, 833, 741, 606 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 1.07 (d, *J* = 7.3 Hz, 3H, CH_3), 1.86 (s, 3H, CCH_3), 1.98 (s, 3H, SeMe), 2.09 (dt, *J* = 7.3, 15.1 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.40 (dt, *J* = 6.4, 14.2 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.59 (sextet, *J* = 6.8 Hz, 1H, $CH_3C\underline{H}$), 4.81 (s, 1H, C$\underline{H}_2$=C), 4.94-5.01 (m, 2H, C$\underline{H}_2$=CH), 5.01 (s, 1H, C$\underline{H}_2$=C), 5.70 (ddt, *J* = 7.3, 10.3, 17.6 Hz, 1H, CH_2=C$\underline{H}$), 6.63 (s, 1H, C$\underline{H}$=C(SeMe)); ^{13}C NMR ($CDCl_3$) δ 6.2 (SeMe), 16.0 (CCH_3), 23.8 (CH_3), 37.3 (CH_2=$CH\underline{C}H_2$), 45.7 ($CH_3\underline{C}H$), 114.9 ($\underline{C}H_2$=C), 116.5 ($\underline{C}H_2$=CH), 120.8 ($\underline{C}$H=C(SeMe)), 130.6 (CH_2=$\underline{C}$H), 143.9 ($CH_3\underline{C}$), 165.2 (CSe), 202.0 (C=O); ^{77}Se NMR ($CDCl_3$) δ 340.3; EIMS *m*/*z* 258 (M^+), 243 (M^+-CH_3), 189 (M^+-CH_2=$CHCH_2CH$+CH_3); Anal. Calcd for $C_{12}H_{18}OSe$: C, 56.03; H, 7.05. Found: C, 56.28; H, 7.20.

(*Z*)-5-methylselenenyl-7-oxo-8-phenylundeca-5,10-diene (3l)

IR (neat) 3075, 3027, 2957, 2931, 2872, 1651, 1600, 1538, 1494, 1246, 1032, 912, 732, 700 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 0.87 (t, *J* = 7.1 Hz, 3H, CH_3), 1.29 (sextet, *J* = 7.3 Hz, 2H, C$\underline{H}_2CH_3$), 1.42 (quint, *J* = 7.4 Hz, 2H, C$\underline{H}_2CH_2CH_3$), 2.07 (s, 3H, SeMe), 2.43 (t, *J* = 7.8 Hz, 2H, CCH_2), 2.50 (dt, *J* = 7.2, 14.6 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.87 (dt, *J* = 7.2 14.6 Hz, 1H, CH_2=CHC$\underline{H}_2$), 3.71 (t, *J* = 7.3 Hz, 1H, PhC$\underline{H}$), 4.93 (dd, *J* = 1.4, 10.3 Hz, 1H, C$\underline{H}_2$=CH), 5.00 (dd, *J* = 1.4, 17.4 Hz, 1H, C$\underline{H}_2$=CH), 5.69 (ddt, *J* = 6.8, 10.3, 17.4 Hz, 1H, CH_2=C$\underline{H}$) 6.50 (s, 1H, C$\underline{H}$=C(SeMe)(Bu)) 7.21-7.31 (m, 5H Ar); ^{13}C NMR ($CDCl_3$) δ 4.6 (SeMe), 13.8 (CH_3), 22.0, 32.1, 36.6 ($\underline{C}H_2$), 37.0 (CH_2=$CH\underline{C}H_2$), 58.3 (PhCH), 116.3 ($\underline{C}H_2$=CH), 121.9 (C$\underline{H}$=C(SeMe)(Bu)), 126.9, 128.4, 128.7 (Ar), 136.2 (CH_2=$\underline{C}$H), 139.2 (Ar), 165.3 (CSe), 197.2 (C=O); ^{77}Se NMR ($CDCl_3$) δ 376.9; EIMS *m*/*z* 336 (M^+), 321 (M^+-CH_3); Anal. Calcd for $C_{12}H_{18}OSe$: C, 61.40; H, 6.19. Found: C, 61.56; H, 6.25.

1-(1-Cyclohexenyl)-1-methylselenenyl-3-oxo-4-phenylhepta-1,6-diene (3m)

IR (neat) 3074, 3026, 2929, 2857, 1658, 1643, 1538, 1494, 1181, 1089, 915, 700 cm^{-1}; ^{1}H NMR

($CDCl_3$) δ 1.55-1.67 (m, 4H), 1.98 (br, 2H), 1.98 (s, 3H, SeMe), 2.09 (br, 2H), 2.47-2.54 (m, 1H, CH_2=CHC$\underline{H}_2$), 2.84-2.91 (m, 1H, CH_2=CHC$\underline{H}_2$), 3.71 (t, *J* = 7.6 Hz, 1H, PhC$\underline{H}$), 4.92 (dd *J* = 1.2, 10.3 Hz, 1H, C$\underline{H}_2$=CH), 5.00 (dd, *J* = 1.2, 17.1 Hz, 1H, C$\underline{H}_2$=CH), 5.50 (br, 1H, CH=C), 5.69 (ddt, *J* = 6.8, 10.3, 17.1 Hz, 1H, CH_2=C$\underline{H}$), 6.50 (s, 1H, C$\underline{H}$=C(SeMe)), 7.21-7.32 (m, 5H, Ar); ^{13}C NMR ($CDCl_3$) δ 6.2 (SeMe), 21.8, 22.3, 24.8, 29.8 ($\underline{C}H_2$), 36.7 (CH_2=CH$\underline{C}H_2$), 58.4 (PhCH), 116.3 ($\underline{C}H_2$=CH), 121.8 ($\underline{C}$H=C), 126.9 (CH=$\underline{C}$(SeMe)), 127.0, 128.5, 128.7 (Ar), 136.2 ($\underline{C}$H=C(SeMe)), 137.6 (CH_2=$\underline{C}$H), 139.1 (Ar), 166.4 (CSe), 197.8 (C=O); ^{77}Se NMR ($CDCl_3$) δ 353.4; EIMS *m*/*z* 360 (M^+), 345 (M^+-CH_3); Anal. Calcd for $C_{20}H_{24}OSe$: C, 66.84; H, 6.73. Found: C, 67.06; H, 6.73.

2-Methyl-3-methylselenenyl-5-oxo-6-phenylnona-1,3,8-triene (3n)

IR (neat) 3078, 2930, 1659, 1651, 1538, 1454, 1372, 1262, 1134, 1097, 909, 834, 700 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 1.81 (s, 3H, CH_3), 2.00 (s, 3H, SeMe), 2.51 (dt, *J* = 7.2, 14.5 Hz, 1H, CH_2=CHC$\underline{H}_2$), 2.88 (dt, *J* = 7.2, 14.5 Hz, 1H, CH_2=CHC$\underline{H}_2$) 3.74 (t, *J* = 7.2 Hz, 1H, PhC$\underline{H}$), 4.74 (s, 1H, C$\underline{H}_2$=C), 4.97 (s, 1H, C$\underline{H}_2$=C), 4.91-5.02 (m, 2H, C$\underline{H}_2$=CH), 5.69 (ddt, *J* = 7.2, 10.3, 17.1 Hz, 1H, CH_2=C$\underline{H}$), 6.50 (s, 1H, C$\underline{H}$=C(SeMe)), 7.21-7.32 (m, 5H, Ar); ^{13}C NMR ($CDCl_3$) δ 6.3 (SeMe), 23.7 (CH_3), 36.5 (CH_2=CH$\underline{C}H_2$), 58.4 (Ph$\underline{C}$H), 115.0 ($\underline{C}H_2$=C)116.3 ($\underline{C}H_2$=CH), 121.6 ($\underline{C}$H=C(SeMe)), 127.0 (CH_2=$\underline{C}$H), 128.4, 128.7, 136.1 138.9 (Ar), 143.7($\underline{C}CH_3$), 165.4 (CSe), 197.6 (C=O); ^{77}Se NMR ($CDCl_3$) δ 346.2; EIMS *m*/*z* 320 (M^+), 305 (M^+-CH_3); Anal. Calcd for $C_{17}H_{20}OSe$: C, 63.95; H, 6.31. Found: C, 64.16; H, 6.41.

Experimental procedure for X-ray molecular structure analysis of 3b

X-ray Structure Analysis. The measurement was carried out on a Rigaku AFC7R four-circle diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71069 Å). The structure was solved and refined using the teXsan®, crystallographic software package. The X-ray quality crystal of **3b** was obtained by slow diffusion of hexane into hexane/CH_2Cl_2 (5/1) solution of the sample. The crystal was mounted on a glass fiber, and the crystal was coated with an epoxy resin. The cell dimensions were determined from a least-squares refinement of the setting diffractmeter 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 SHELXS86 and expanded using DIRDIF94. Scattering factors for neutral atoms were from Cromer and Waber, and anomalous dispersion was used. The function minimized was $\Sigma w(F_o^2-F_c^2)^2$, and the weighting scheme employed was $w=[\sigma^2_c(F_o^2)+(p(\max(F_o^2, 0)+2F_c^2/3)^2]^{-1}$. 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. The full-matrix least-squares refinement was executed with non-hydrogen atoms anisotropic. Crystal data and measurement description are summarized in Table 3. Atomic coodinates, B(iso)/B(eq) are listed in Table 4.

Table 3. Crystal data and experimental details for **3b**

empirical formula	$C_{16}H_{18}NOSe$
formula weight	305.28
crystal color, habit	yellow, prismatic
crystal system	Monoclinic
unit-cell dimentions	a = 6.172(3) Å
	b = 8.825(2) Å
	c = 26.162(2) Å
	β = 95.81(1)°
volume of unit cell ($Å^3$)	1417.6(6)
space group	$P2_1$ / c (#14)
Z value	4
Dcalc (g/cm^3)	1.430
crystal dimensions (mm)	0.31 x 0.17 x 0.17
μ (Mo-Kα) (cm^{-1})	26.35
temperature (°C)	-80
2θmax (deg)	55.0
no. of reflections measured:	
total	4618
unique	3236
Rint	0.027
no. of observations (I > -10.00σ(I))	3236
no. of variables	163
reflection / parameter ratio	19.85
residuals: R^a, R_w^b	0.110, 0.146
residuals: $R1^c$	0.057
p- facter	0.0500
Maximum peak in Final Diff. Map ($e/Å^{-3}$)	1.27
Minimum peak in Final Diff. Map ($e/Å^{-3}$)	-1.59
goodness of fit indicator	1.24

[a] $R = \Sigma(Fo^2-Fc^2)/\Sigma Fo^2$. [b] $R_w = [(\Sigma w (Fo^2-Fc^2)^2/\Sigma wFo^2)^2]^{1/2}$. [c] $R1 = \Sigma|FOl-lFCl/\Sigma|FOl$. w = $1/[\Sigma^2(Fo)^2]$

Table 4. Atomic coordinates and B_{iso}/B_{eq} for **3b**

atom	x	y	z	B_{eq}
Se(1)	0.45540(10)	0.90644(6)	0.06086(2)	3.85(1)
O(1)	0.81 15(7)	0.9986(4)	0.1249(1)	5.4(1)
C(1)	0.5324(8)	0.7432(5)	0.1060(2)	2.6(1)
C(2)	0.6968(8)	0.7544(5)	0.1436(2)	2.7(1)
C(3)	0.8355(9)	0.8870(5)	0.1522(2)	3.1(1)
C(4)	1.0145(8)	0.8837(5)	0.1954(2)	3.0(1)
C(5)	1.2010(10)	0.9717(7)	0.1915(2)	4.6(2)
C(6)	1.370(1)	0.9697(9)	0.2300(4)	6.4(2)
C(7)	1.353(1)	0.8823(8)	0.2725(3)	6.7(2)
C(8)	1.175(1)	0.7949(7)	0.2774(2)	5.8(2)
C(9)	1.0020(9)	0.7947(6)	0.2385(2)	3.7(1)
C(10)	0.4081(7)	0.5984(5)	0.0988(2)	2.45(10)
C(11)	0.481(1)	0.4896(8)	0.0689(3)	8.3(2)
C(12)	0.377(2)	0.336(1)	0.0657(4)	12.6(4)
C(13)	0.192(1)	0.3166(9)	0.0945(3)	8.0(2)
C(14)	0.095(1)	0.4336(9)	0.1096(7)	16.6(5)
C(15)	0.219(1)	0.5757(7)	0.1239(3)	6.7(2)
C(16)	0.201(1)	0.8249(9)	0.0204(3)	7.3(2)
H(1)	0.7533	0.6594	0.1615	5.5423
H(2)	1.2140	1.0324	0.1625	5.5865
H(3)	1.5077	1.0213	0.2259	5.5423
H(4)	1.4662	0.8816	0.3002	7.8916

H(5)	1.1688	0.7338	0.3073	6.9823
H(6)	0.8781	0.7332	0.2418	4.4810
H(7)	0.6526	0.4832	0.0590	5.5423
H(8)	0.4886	0.2627	0.0812	12.7726
H(9)	0.3410	0.3094	0.0322	12.7726
H(10)	0.2352	0.2562	0.1240	9.2264
H(11)	0.0869	0.2641	0.0725	9.2264
H(12)	0.0332	0.4016	0.1406	18.3624
H(13)	-0.0139	0.4594	0.0845	18.3624
H(14)	0.2642	0.5758	0.161 1	8.0934
H(15)	0.1253	0.661 1	0.1 175	8.0934
H(16)	0.2389	0.7324	0.0023	8.2945
H(17)	0.0888	0.7973	0.041 1	8.2945
H(18)	0.1424	0.8941	-0.0055	8.2945

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