Supporting Information for

Stereoselective Synthesis of New Selenium-Containing Heterocycles by Cyclocarbonylation of Aminoalkynes with Carbon Monoxide and Selenium

Shin-ichi Fujiwara,^{*,†} Yasukazu Shikano,[‡] Tsutomu Shin-ike,[†]

Nobuaki Kambe,^{*,‡} and Noboru Sonoda^{*,§}

Department of Chemistry, Osaka Dental University, Hirakata, Osaka 573-1121, Japan,

Department of Applied Chemistry, Faculty of Engineering, Osaka University, Suita,

Osaka 565-0871, Japan, and Department of Applied Chemistry, Faculty of Engineering,

Kansai University, Suita, Osaka 564-8680, Japan

Table of Content Graphic

Analytical Instrument.

Melting points were determined on a Yanagimoto Micro Melting Point apparatus. ^1H and ^{13}C NMR spectra were recorded on a JEOL JNM-ALICE-400 (400 MHz and 100 MHz, respectively) spectrometer using Me_4Si as an internal standard. IR spectra were determined on a Perkin Elmer Model 1600 spectrometer. Purification of products was usually performed on a recycling preparative HPLC (Japan Analytical Industry Co. Ltd., Model LC-908) equipped with JAIGEL-1H and -2H columns (GPC) using CHCl_3 as an eluent. If necessary, preparative TLC was conducted by using Wakogel B-5F silica gel (325 mesh). Mass spectra (EI) were taken on a SHIMADZU GCMC-QP2000 operating in the electron impact mode (70 eV) equipped with CBP1-M25-025 column. High-resolution mass spectra (HRMS) were obtained on a JEOL JMS-DX303 in the Instrumental Analysis Center of the Faculty of Engineering, Osaka University. Elemental analyses were performed on Perkin Elmer 240C apparatus.

Butyl(3-phenylprop-2-ynyl)amine (2h).

Yellow liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.93 (t, $J = 7.3$ Hz, 3 H), 1.38 (sextet, $J = 7.3$ Hz, 2 H), 1.44-1.55 (m, 3 H), 2.75 (t, $J = 7.3$ Hz, 2 H), 3.64 (s, 2 H), 7.27-7.31 (m, 3 H), 7.39-7.43 (m, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 14.0, 20.4, 32.0, 39.0, 48.5, 83.1, 87.6, 123.0, 127.6, 127.9, 131.3; IR (neat) 2957, 2928, 2872, 1490, 1442, 1327, 1141, 755, 691 cm^{-1} ; MS (EI) m/e (relative intensity) 115 (100), 144 (62), 187 (M^+ , 7). Anal. Calcd for $\text{C}_{13}\text{H}_{17}\text{N}$: C, 83.37; H, 9.15; N, 7.48. Found: C, 83.03; H, 9.02; N, 7.52.

Butyl(pent-2-ynyl)amine (2i).

Colorless liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.92 (t, $J = 7.3$ Hz, 3 H), 1.31 (t, $J = 7.6$ Hz, 3 H), 1.32-1.51 (m, 5 H), 2.19 (q, $J = 7.6$ Hz, 2 H), 2.66 (t, $J = 7.3$ Hz, 2 H), 3.38 (t, $J = 2.2$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 12.4, 14.0, 14.1, 20.4, 32.0, 38.6, 48.4, 77.4, 84.6; IR (neat) 2959, 2929, 2874, 1456, 1319, 1132, 1107, 774 cm^{-1} ; MS (EI) m/e (relative intensity) 67 (26), 96 (100), 139 (M^+ , 2). Anal. Calcd for $\text{C}_9\text{H}_{17}\text{N}$: C, 77.64; H, 12.31; N, 10.06. Found: C, 77.30; H, 12.17; N, 9.97.

Butyl(3-trimethylsilanylprop-2-ynyl)amine (2j).

Colorless liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.16 (s, 9 H), 0.92 (t, $J = 7.3$ Hz, 3 H), 1.30 (brs, 1 H), 1.36 (sext, $J = 7.3$ Hz, 2 H), 1.48 (quint, $J = 7.3$ Hz, 2 H), 2.67 (t, $J = 7.2$ Hz, 2 H), 3.43 (s, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 0.0, 13.9, 20.3, 31.8, 39.2, 48.3, 87.4, 104.4; IR (neat) 2959, 2929, 1250, 986, 842, 760 cm^{-1} ; MS (EI) m/e (relative intensity) 83 (26), 111 (28), 140 (100), 183 (M^+ , 3); HRMS (EI) calcd for $\text{C}_{10}\text{H}_{21}\text{NSi}$ 183.1443, found 183.1443

Butyl(but-3-ynyl)amine (7).

Colorless liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.92 (t, $J = 7.3$ Hz, 3 H), 1.27-1.44 (m, 3 H), 1.49 (quint, $J = 7.3$ Hz, 2 H), 1.99 (t, $J = 2.7$ Hz, 1 H), 2.39 (dt, $J = 2.7, 6.6$ Hz, 2

H), 2.62 (t, $J = 7.3$ Hz, 2 H), 2.78 (t, $J = 6.6$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 14.0, 19.5, 20.4, 32.2, 47.9, 49.0, 69.2, 82.4; IR (neat) 3311, 2958, 2930, 2873, 2823, 1465, 1129 cm^{-1} ; MS (EI) m/e (relative intensity) 30 (49), 82 (56), 86 (100), 125 (M^+ , 8); HRMS (EI) calcd for $\text{C}_8\text{H}_{15}\text{N}$ 125.1204, found 125.1208.

3-Butyl-5-methyleneselenazolidin-2-one (3a).

Yellow liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.94 (t, $J = 7.3$ Hz, 3 H), 1.29-1.40 (m, 2 H), 1.51-1.61 (m, 2 H), 3.38 (t, $J = 7.3$ Hz, 2 H), 4.27 (t, $J = 2.2$ Hz, 2 H), 5.26 (q, $J = 2.2$ Hz, 1 H), 5.63 (q, $J = 2.2$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.6, 19.8, 29.3, 44.6, 56.3, 110.4 ($^2J_{\text{Se-C}} = 6.9$ Hz), 134.8 ($^1J_{\text{Se-C}} = 98.7$ Hz), 166.1 ($^1J_{\text{Se-C}} = 109.3$ Hz); IR (neat) 2958, 2930, 2871, 1686 (C=O), 1621, 1464, 1416, 1204 cm^{-1} ; MS (EI) m/e (relative intensity) 120 (82), 217 (52), 219 (M^+ , 100). Anal. Calcd for $\text{C}_8\text{H}_{13}\text{NOSe}$: C, 44.04; H, 6.01; N, 6.42. Found: C, 43.91; H, 6.00; N, 6.51.

3-Methyl-5-methyleneselenazolidin-2-one (3b).

Yellow liquid; ^1H NMR (400 MHz, CDCl_3) δ 2.95 (s, 3 H), 4.25 (t, $J = 2.3$ Hz, 2 H), 5.27 (q, $J = 2.3$ Hz, 1 H), 5.63 (q, $J = 2.2$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 31.4, 58.1, 110.5 ($^2J_{\text{Se-C}} = 12.0$ Hz), 134.4 ($^1J_{\text{Se-C}} = 59.0$ Hz), 166.2; IR (neat) 1682 (C=O), 1621, 1478, 1419, 1386, 1227, 1177, 913, 871 cm^{-1} ; MS (EI) m/e (relative intensity) 39 (81), 96 (100), 120 (61), 177 (M^+ , 82). Anal. Calcd for $\text{C}_5\text{H}_7\text{NOSe}$: C, 34.11; H, 4.01; N,

7.95. Found: C, 34.32; H, 4.07; N, 8.00.

3-Isopropyl-5-methyleneselenazolidin-2-one (3c).

Yellow liquid; ^1H NMR (400 MHz, CDCl_3) δ 1.23 (d, $J = 6.8$ Hz, 6 H), 4.23 (t, $J = 2.2$ Hz, 2 H), 4.47 (heptet, $J = 6.8$ Hz, 1 H), 5.26 (q, $J = 2.2$ Hz, 1 H), 5.65 (q, $J = 2.2$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 19.9, 45.9, 51.4, 110.5 ($^2J_{\text{Se-C}} = 12.0$ Hz), 135.0 ($^1J_{\text{Se-C}} = 98.2$ Hz), 165.9 ($^1J_{\text{Se-C}} = 107.9$ Hz); IR (neat) 2975, 1682 (C=O), 1621, 1461, 1416, 1401, 1197, 1177, 814 cm^{-1} ; MS (EI) m/e (relative intensity) 43 (100), 120 (68), 205 (M^+ , 76). Anal. Calcd for $\text{C}_7\text{H}_{11}\text{NOSe}$: C, 41.19; H, 5.43; N, 6.86. Found: C, 41.45; H, 5.37; N, 6.90.

3-Cyclohexyl-5-methyleneselenazolidin-2-one (3d).

White solid: mp 57-58 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 0.98-1.17 (m, 1 H), 1.09-1.51 (m, 4 H), 1.64-1.72 (m, 1 H), 1.76-1.86 (m, 4 H), 4.00-4.10 (m, 1 H), 4.20-4.28 (m, 2 H), 5.21-5.27 (m, 1 H), 5.61-5.66 (m, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 25.2, 25.6, 30.4, 52.5, 54.0, 110.3 ($^2J_{\text{Se-C}} = 8.3$ Hz), 135.3 ($^1J_{\text{Se-C}} = 98.2$ Hz), 165.9 ($^1J_{\text{Se-C}} = 107.9$ Hz); IR (neat) 2931, 2852, 1663 (C=O), 1619, 1413, 1221, 1200, 1173, 856 cm^{-1} ; MS (EI) m/e (relative intensity) 55 (68), 83 (100), 245 (M^+ , 78). Anal. Calcd for $\text{C}_{10}\text{H}_{15}\text{NOSe}$: C, 49.19; H, 6.19; N, 5.74. Found: C, 49.37; H, 6.22; N, 5.76.

3-*tert*-Butyl-5-methyleneselenazolidin-2-one (3e).

Yellow solid: mp 31-34 °C; ^1H NMR (400 MHz, CDCl_3) δ 1.46 (s, 9 H), 4.37 (t, $J = 2.1$ Hz, 2 H), 5.19 (q, $J = 2.1$ Hz, 1 H), 5.60 (q, $J = 2.1$ Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 28.1, 55.5, 57.8, 109.9 ($^2J_{\text{Se-C}} = 11.5$ Hz), 135.2 ($^1J_{\text{Se-C}} = 97.7$ Hz), 166.1; IR (neat) 2976, 1682 (C=O), 1620, 1364, 1195, 1133 cm^{-1} ; MS (EI) m/e (relative intensity) 41 (22), 57 (100), 219 (M^+ , 21); HRMS (EI) calcd for $\text{C}_8\text{H}_{13}\text{NOSe}$ 219.0162, found 219.0153.

5-Methyleneselenazolidin-2-one (3g).

White solid: mp 105-107 °C; ^1H NMR (400 MHz, CDCl_3) δ 4.23-4.29 (m, 2 H), 5.25-5.31 (m, 1 H), 5.63 (q, $J = 2.1$ Hz, 1 H), 6.77 (br, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 50.8, 110.9, 138.2 ($^1J_{\text{Se-C}} = 100.0$ Hz), 171.4; IR (KBr) 3208, 3084, 1676 (C=O), 1654, 1613, 1560, 1250, 1066 cm^{-1} ; MS (EI) m/e (relative intensity) 39 (97), 118 (50), 120 (96), 161 (50), 163 (M^+ , 100); HRMS (EI) calcd for $\text{C}_4\text{H}_5\text{NOSe}$ 162.9536, found 162.9534

(Z)-5-Benzylidene-3-butylselenazolidin-2-one (3h).

Colorless crystals: mp 82 °C; ^1H NMR (400 MHz, CDCl_3) δ 0.95 (t, $J = 7.3$ Hz, 3 H), 1.31-1.41 (m, 2 H), 1.55-1.63 (m, 2 H), 3.42 (t, $J = 7.4$ Hz, 2 H), 4.36 (d, $J = 2.2$ Hz, 2 H), 6.87 (t, $J = 2.1$ Hz, 1 H), 7.22-7.28 (m, 3H), 7.36 (t, $J = 7.7$ Hz, 2 H); NOE experiment: irradiation of the allyl methylene doublet at δ 4.36 resulted in 15% enhancement of the signal at δ 6.87 (vinyl triplet); ^{13}C NMR (100 MHz, CDCl_3) δ 13.6, 19.9, 29.4, 44.6, 57.3, 124.1, 127.0, 127.1, 127.4, 128.3, 136.0, 166.0 ($^1J_{\text{Se-C}} = 109.2$ Hz); IR (KBr) 1693, 1677, 1460, 1442, 1222, 1206, 687, 516 cm^{-1} ; MS (EI) m/e (relative intensity) 115 (100), 195 (73), 196 (68), 295 (M^+ , 87). Anal. Calcd for $\text{C}_{14}\text{H}_{17}\text{NOSe}$: C, 57.15; H, 5.82; N, 4.76. Found: C, 57.09; H, 5.79; N, 4.79.

(Z)-Butyl-5-propylideneselenazolidin-2-one (3i).

Yellow liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.94 (t, $J = 7.3$ Hz, 3 H), 1.02 (t, $J = 7.4$ Hz, 3 H), 1.34 (sextet, $J = 7.4$ Hz, 2 H), 1.55 (quint, $J = 7.4$ Hz, 2 H), 1.99 (tquint, $J = 1.6, 7.4$ Hz, 2 H), 3.36 (t, $J = 7.4$ Hz, 2 H), 4.22 (q, $J = 1.9$ Hz, 2 H), 5.79 (tt, $J = 6.8, 2.2$ Hz, 1 H). NOE experiment: irradiation of the allyl methylene quartet at δ 4.22 resulted in 8% enhancement of the signal at δ 5.79 (vinyl triplet-triplet); ^{13}C NMR (100 MHz, CDCl_3) δ 13.1, 13.7, 19.9, 26.5, 29.4, 44.7, 55.7, 125.7, 126.20, 166.0; IR (neat) 2962, 2931, 2872, 1690 (C=O), 1654, 1466, 1409, 1192 cm^{-1} ; MS (EI) m/e

(relative intensity) 41 (28), 67 (100), 106 (38), 133 (41), 148 (33), 166 (35), 245 (33), 247 (M^+ , 65); HRMS (EI) calcd for $C_{10}H_{17}NOSe$ 247.0475, found 247.0490

3-Butyl-5-trimethylsilylmethyleneselenazolidin-2-one (3j).

Brown liquid; 1H NMR (400 MHz, $CDCl_3$) δ 0.14 (s, 9 H), 0.94 (t, $J = 7.3$ Hz, 3 H), 1.29-1.40 (m, 2 H), 1.51-1.60 (m, 2 H), 3.38 (t, $J = 7.3$ Hz, 2 H), 4.27 (d, $J = 2.2$ Hz, 2 H), 5.98 (t, $J = 2.2$ Hz, 1 H). NOE experiment: irradiation of the allyl methylene doublet at δ 4.27 resulted in 16% enhancement of the signal at δ 5.98 (vinyl triplet); ^{13}C NMR (100 MHz, $CDCl_3$) δ -1.43, 13.7, 19.9, 29.4, 44.3, 59.3, 123.2, 143.0 ($^1J_{Se-C} = 100.0$ Hz), 166.6; IR (neat) 2957, 2932, 1694 (C=O), 1591, 1464, 1406, 1248, 1206, 864, 839 cm^{-1} ; MS (EI) m/e (relative intensity) 73 (100), 169 (26), 210 (24), 211 (38), 291 (M^+ , 26). Anal. Calcd for $C_{11}H_{21}NOSeSi$: C, 45.51; H, 7.29; N, 4.82. Found: C, 45.91; H, 7.30; N, 4.85.

3-Butyl-6-methylene-[1,3]selenazinan-2-one (8).

Colorless liquid; 1H NMR (400 MHz, $CDCl_3$) δ 0.94 (t, $J = 7.4$ Hz, 3 H), 1.33 (sextet, $J = 7.4$ Hz, 2 H), 1.55 (quintet, $J = 7.4$ Hz, 2 H), 2.76 (t, $J = 5.4$ Hz, 2 H), 3.41 (t, $J = 5.4$ Hz, 2 H), 3.48 (t, $J = 7.4$ Hz, 2 H), 5.09 (s, 1 H), 5.39 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 20.0, 29.8, 35.3, 49.0, 49.6, 111.0 ($^2J_{Se-C} = 20.8$ Hz), 138.9 ($^1J_{Se-C} =$

102.6 Hz), 161.4 ($^1J_{\text{Se-C}} = 122.6$ Hz); IR (neat) 2957, 2930, 1652 (C=O), 1616, 1468, 1409, 1236, 1173, 1145 cm^{-1} ; MS (EI) m/e (relative intensity) 86 (64), 134 (57), 233 (M^+ , 100). Anal. Calcd for $\text{C}_9\text{H}_{15}\text{NOSe}$: C, 46.56; H, 6.51; N, 6.03. Found: C, 46.86; H, 6.56; N, 6.07.

Se-Butyl butyl(prop-2-ynyl)carbamosenoate (6).

Obtained as a *s-cis/trans* mixture. Brown liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.89-1.02 [overlapping m, 6 H (major, minor)], 1.28-1.49 [overlapping m, 4 H (major, minor)], 1.52-1.75 [overlapping m, 4 H (major, minor)], 2.25 [br. s, 1 H (major)], 2.31 [br. s, 1 H (minor)], 2.96 [t, $J = 7.3$ Hz, 2 H (major, minor)], 3.38 [br. s, 2 H (major)], 3.50 [br. s, 2 H (minor)], 4.08 [brs, 2 H (minor)], 4.23 [brs, 2 H (major)]; ^{13}C NMR (100 MHz, CDCl_3) δ 13.6 (major, minor), 13.7 (major, minor), 20.0 (major, minor), 23.1 (major, minor), 26.8 (major), 27.1 (minor), 29.6 (minor), 30.1 (major), 32.8 (major, minor), 35.6 (major), 38.0 (minor), 47.4 (minor), 48.0 (major), 71.9 (major), 72.6 (minor), 77.9 (minor), 78.3 (major), 164.6 (minor), 164.8 (major); IR (neat) 2959, 2932, 2872, 1656, 1397, 1187, 1106 cm^{-1} ; MS(EI) m/e (relative intensity) 57 (100), 82 (30), 138 (98), 275 (M^+ , 0.5); HRMS(EI) calcd for $\text{C}_{12}\text{H}_{21}\text{NOSe}$ 275.0788, found 275.0797. Anal. Calcd for $\text{C}_{12}\text{H}_{21}\text{NOSe}$: C, 52.55; H, 7.72; N, 5.11. Found: C, 52.64; H, 7.77; N, 5.23.

***Se*-Methyl butyl(but-3-ynyl)selenocarbamate**

Obatined as a *s-cis/trans* mixture. Pale yellow liquid; ^1H NMR (400 MHz, CDCl_3) δ 0.88-1.00 [overlapping m, 3 H (major, minor)], 1.25-1.40 [overlapping m, 2 H (major, minor)], 1.49-1.67 [overlapping m, 2 H (major, minor)], 2.00 [s, 1 H (major)], 2.06 [s, 1 H (minor)], 2.23 [s, 3 H, (major, minor)], 2.43-2.58 [overlapping m, 2 H (major, minor)], 3.32 [t, $J = 7.6$ Hz, 2 H (major)], 3.38-3.50 [overlapping m, 4 H (minor)], 3.53 [t, $J = 7.0$ Hz, 2 H, (major)]; ^{13}C NMR (100 MHz, CDCl_3) δ 6.2 (major), 6.3 (minor), 13.8 (major, minor), 17.8 (major), 18.9 (minor), 20.0 (major, minor), 29.9 (minor), 30.7 (major), 46.5 (major), 47.4 (minor), 47.9 (minor), 49.5 (major), 69.7 (major), 70.5 (minor), 80.3 (minor), 81.2 (major), 164.0 (minor), 164.3 (major); IR (neat) 2958, 2934, 1658, 1401, 1202, 1165, 1109 cm^{-1} ; MS(EI) m/e (relative intensity) 57 (68), 86 (100), 152 (83), 247 (M^+ , 7). Anal. Calcd for $\text{C}_{10}\text{H}_{17}\text{NOSe}$: C, 48.78; H, 6.96; N, 5.69. Found: C, 48.86; H, 6.90; N, 5.86.

Figure S1. ORTEP Drawing of (Z)-3h

Table S1. Crystal Data and Structure Refinement for Compound (Z)-3h

empirical formula	C ₁₄ H ₁₇ NOSe
formula weight	294.25
crystal color, habit	colorless, prismatic
crystal system	Monoclinic
unit-cell dimensions	
a(Å)	10.5(1)
b(Å)	9.4(1)
c(Å)	28.03(9)
β(°)	99.6(5)
volume of unit cell (Å ³)	2724(29)
space group	P2 ₁ /c (#14)
Z value	8
Dcalc	1.435 g/cm ³
crystal dimension (mm)	0.70 x 0.70 x 0.10
μ(Mo-Kα)(cm ⁻¹)	27.10
F(000)	1200.00
2θmax (deg)	55.3
Temperature	296.2 K
no. of reflections measured:	
total	7022
unique	6282
Rint	0.055
no. of observations (I > -10.00σ(I))	6282
no. of variables	443
reflection / parameter ratio	14.18
residuals: R, Rw	0.099, 0.125
residuals: R _I	0.041
p-factor	0.0500
Maximum peak in Final Diff. Map (e/ Å ⁻³)	0.60
Minimum peak in Final Diff. Map (e/ Å ⁻³)	-0.50
goodness of fit indicator	1.01

Table S2. Positional Parameters and B(eq) for (Z)-**3h**

atom	x	y	z	B(eq)
Se(1)	0.56048(5)	0.26045(5)	0.03205(2)	0.0680(2)
O(1)	0.6994(4)	0.2259(4)	0.1253(1)	0.108(1)
N(1)	0.5280(4)	0.0772(4)	0.1037(1)	0.068(1)
C(1)	0.6086(5)	0.1815(6)	0.0965(2)	0.075(2)
C(2)	0.4233(5)	0.0384(6)	0.0655(2)	0.065(2)
C(3)	0.4165(4)	0.1362(5)	0.0229(2)	0.058(1)
C(4)	0.5492(6)	-0.0060(7)	0.1482(2)	0.079(2)
C(5)	0.4614(6)	0.0356(7)	0.1823(2)	0.086(2)
C(6)	0.4762(7)	-0.0631(9)	0.2264(2)	0.103(2)
C(7)	0.3844(9)	-0.029(1)	0.2600(3)	0.136(4)
C(8)	0.3212(4)	0.1268(5)	-0.0151(2)	0.057(1)
C(9)	0.2919(4)	0.2060(5)	-0.0602(2)	0.057(1)
C(10)	0.1812(5)	0.1692(6)	-0.0924(2)	0.074(2)
C(11)	0.1455(6)	0.2413(7)	-0.1355(2)	0.087(2)
C(12)	0.2204(6)	0.3498(6)	-0.1475(2)	0.082(2)
C(13)	0.3297(6)	0.3888(6)	-0.1164(2)	0.078(2)
C(14)	0.3658(5)	0.3172(5)	-0.0736(2)	0.067(2)
H(1)	0.343(4)	0.041(5)	0.078(1)	0.073(8)
H(2)	0.434(4)	-0.057(5)	0.055(2)	0.076(8)
H(3)	0.639(5)	0.005(5)	0.164(2)	0.098(8)
H(4)	0.535(5)	-0.106(6)	0.140(2)	0.095(8)
H(5)	0.481(5)	0.129(6)	0.194(2)	0.093(7)
H(6)	0.373(5)	0.035(6)	0.166(2)	0.101(7)
H(7)	0.565(5)	-0.063(6)	0.243(2)	0.118(6)
H(8)	0.459(6)	-0.161(7)	0.215(2)	0.126(6)
H(9)	0.399(8)	0.066(9)	0.270(3)	0.175(5)
H(10)	0.292(6)	-0.040(8)	0.241(2)	0.155(5)
H(11)	0.391(7)	-0.094(7)	0.287(2)	0.154(5)
H(12)	0.257(4)	0.054(4)	-0.012(1)	0.062(9)
H(13)	0.130(4)	0.094(5)	-0.084(2)	0.086(8)
H(14)	0.070(5)	0.213(6)	-0.156(2)	0.102(8)
H(15)	0.200(5)	0.397(5)	-0.177(2)	0.094(8)
H(16)	0.385(4)	0.467(5)	-0.124(2)	0.095(8)
H(17)	0.445(4)	0.347(5)	-0.053(2)	0.077(9)

Table S3. Unisotropic Displacement Parameters for (Z)-**3h**

	U11	U22	U33	U12	U13	U23
Se(1)	0.0633(3)	0.0669(3)	0.0745(4)	-0.0143(2)	0.0133(2)	-0.0026(3)
O(1)	0.094(3)	0.119(3)	0.098(3)	-0.036(2)	-0.020(2)	0.013(2)
N(1)	0.067(2)	0.076(3)	0.061(3)	-0.003(2)	0.011(2)	0.005(2)
C(1)	0.073(3)	0.074(3)	0.076(4)	-0.004(3)	0.007(3)	-0.001(3)
C(2)	0.067(3)	0.071(3)	0.062(3)	-0.008(3)	0.022(3)	-0.001(3)
C(3)	0.059(3)	0.060(3)	0.058(3)	-0.004(2)	0.023(2)	-0.005(2)
C(4)	0.086(4)	0.084(4)	0.069(4)	0.003(3)	0.017(3)	0.006(3)
C(5)	0.087(4)	0.104(5)	0.067(4)	-0.003(4)	0.012(3)	-0.005(4)
C(6)	0.115(5)	0.122(6)	0.074(4)	-0.002(5)	0.023(4)	0.005(4)

C(7)	0.148(7)	0.169(9)	0.099(6)	-0.007(7)	0.047(5)	0.018(6)
C(8)	0.058(3)	0.054(3)	0.061(3)	-0.009(2)	0.020(2)	-0.007(2)
C(9)	0.058(3)	0.054(3)	0.062(3)	0.003(2)	0.019(2)	-0.007(2)
C(10)	0.073(3)	0.072(3)	0.076(4)	-0.011(3)	0.013(3)	-0.005(3)
C(11)	0.078(4)	0.103(5)	0.076(4)	-0.003(4)	0.003(3)	-0.001(4)
C(12)	0.090(4)	0.085(4)	0.074(4)	0.014(3)	0.020(3)	0.013(3)
C(13)	0.083(4)	0.071(3)	0.083(4)	-0.003(3)	0.022(3)	0.004(3)
C(14)	0.065(3)	0.063(3)	0.073(4)	-0.004(2)	0.016(3)	-0.004(3)

Table S4. Bond Lengths for (Z)-3h

atom	atom	distance	atom	atom	distance
Se(1)	C(1)	1.939(5)	Se(1)	C(3)	1.89(1)
O(1)	C(1)	1.218(8)	N(1)	C(1)	1.332(8)
N(1)	C(2)	1.449(9)	N(1)	C(4)	1.455(6)
C(2)	C(3)	1.496(6)	C(2)	H(1)	0.97(4)
C(2)	H(2)	0.95(4)	C(3)	C(8)	1.337(8)
C(4)	C(5)	1.49(1)	C(4)	H(3)	0.98(5)
C(4)	H(4)	0.96(5)	C(5)	C(6)	1.530(9)
C(5)	H(5)	0.94(5)	C(5)	H(6)	0.97(5)
C(6)	C(7)	1.49(1)	C(6)	H(7)	0.97(5)
C(6)	H(8)	0.98(6)	C(7)	H(9)	0.93(8)
C(7)	H(10)	1.03(6)	C(7)	H(11)	0.97(7)
C(8)	C(9)	1.455(6)	C(8)	H(12)	0.97(4)
C(9)	C(10)	1.39(1)	C(9)	C(14)	1.389(8)
C(10)	C(11)	1.380(7)	C(10)	H(13)	0.94(5)
C(11)	C(12)	1.363(9)	C(11)	H(14)	0.94(5)
C(12)	C(13)	1.37(1)	C(12)	H(15)	0.93(5)
C(13)	C(14)	1.372(7)	C(13)	H(16)	0.97(5)
C(14)	H(17)	0.98(4)			

Table S5. Bond Angles for (Z)-3h

atom	atom	atom	angle
C(1)	Se(1)	C(3)	88.3(3)
C(1)	N(1)	C(2)	119.7(5)
C(1)	N(1)	C(4)	120.9(5)
C(2)	N(1)	C(4)	119.2(4)
C(3)	C(2)	H(1)	110(2)
C(3)	C(2)	H(2)	108(2)
H(1)	C(2)	H(2)	106(3)
Se(1)	C(3)	C(2)	109.7(3)
Se(1)	C(3)	C(8)	128.6(4)
C(2)	C(3)	C(8)	121.6(4)
N(1)	C(4)	C(5)	112.7(5)
N(1)	C(4)	H(3)	108(2)
N(1)	C(4)	H(4)	109(3)
C(5)	C(4)	H(3)	110(2)
C(5)	C(4)	H(4)	108(3)
H(3)	C(4)	H(4)	107(4)

C(4)	C(5)	C(6)	111.7(6)
C(4)	C(5)	H(5)	109(3)
C(4)	C(5)	H(6)	109(3)
C(6)	C(5)	H(5)	107(3)
C(6)	C(5)	H(6)	110(3)
H(5)	C(5)	H(6)	107(4)
C(5)	C(6)	C(7)	112.9(7)
C(5)	C(6)	H(7)	110(3)
C(5)	C(6)	H(8)	108(3)
C(7)	C(6)	H(7)	111(3)
C(7)	C(6)	H(8)	107(3)
H(7)	C(6)	H(8)	105(5)
C(6)	C(7)	H(9)	107(5)
C(6)	C(7)	H(10)	108(3)
C(6)	C(7)	H(11)	113(4)
H(9)	C(7)	H(10)	109(7)
H(9)	C(7)	H(11)	111(6)
H(10)	C(7)	H(11)	105(5)
C(3)	C(8)	C(9)	132.9(4)
C(3)	C(8)	H(12)	114(2)
C(9)	C(8)	H(12)	112(2)
C(8)	C(9)	C(10)	118.0(4)
C(8)	C(9)	C(14)	124.8(5)
C(10)	C(9)	C(14)	117.1(6)
C(9)	C(10)	C(11)	121.5(5)
C(9)	C(10)	H(13)	118(2)
C(11)	C(10)	H(13)	120(2)
C(10)	C(11)	C(12)	119.8(6)
C(10)	C(11)	H(14)	119(3)
C(12)	C(11)	H(14)	121(3)
C(11)	C(12)	C(13)	120.1(6)
C(11)	C(12)	H(15)	121(3)
C(13)	C(12)	H(15)	118(3)
C(12)	C(13)	C(14)	120.4(5)
C(12)	C(13)	H(16)	122(2)
C(14)	C(13)	H(16)	117(2)
C(9)	C(14)	C(13)	121.2(6)
C(9)	C(14)	H(17)	120(2)
C(13)	C(14)	H(17)	117(2)

Table S6. Torsion Angles for (Z)-**3h**

atom	atom	atom	atom	angle
Se(1)	C(1)	N(1)	C(2)	0.4(6)
Se(1)	C(1)	N(1)	C(4)	175.6(4)
Se(1)	C(3)	C(2)	N(1)	6.9(5)
Se(1)	C(3)	C(8)	C(9)	-2.0(7)
O(1)	C(1)	Se(1)	C(3)	-175.8(5)
O(1)	C(1)	N(1)	C(2)	179.3(5)
O(1)	C(1)	N(1)	C(4)	-5.6(8)
N(1)	C(1)	Se(1)	C(3)	3.1(4)
N(1)	C(2)	C(3)	C(8)	-174.9(4)

N(1)	C(4)	C(5)	C(6)	174.2(5)
C(1)	Se(1)	C(3)	C(2)	-5.6(3)
C(1)	Se(1)	C(3)	C(8)	176.4(4)
C(1)	N(1)	C(2)	C(3)	-4.9(6)
C(1)	N(1)	C(4)	C(5)	103.7(8)
C(2)	N(1)	C(4)	C(5)	-81.2(9)
C(2)	C(3)	C(8)	C(9)	-179.9(4)
C(3)	C(2)	N(1)	C(4)	179.8(4)
C(3)	C(8)	C(9)	C(10)	-179.0(5)
C(3)	C(8)	C(9)	C(14)	0.5(8)
C(4)	C(5)	C(6)	C(7)	-177.0(7)
C(8)	C(9)	C(10)	C(11)	178.7(5)
C(8)	C(9)	C(14)	C(13)	-178.5(4)
C(9)	C(10)	C(11)	C(12)	0.9(8)
C(9)	C(14)	C(13)	C(12)	-1.2(8)
C(10)	C(9)	C(14)	C(13)	1.0(7)
C(10)	C(11)	C(12)	C(13)	-1.1(9)
C(11)	C(10)	C(9)	C(14)	-0.9(7)
C(11)	C(12)	C(13)	C(14)	1.2(8)