

Supporting Information for

Photoinduced Group Transfer Radical Addition of Carbamotelluroates to Acetylenes

Shin-ichi Fujiwara,* Yoshihiko Shimizu, Tsutomu Shin-ike, and Nobuaki Kambe*

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

Department of Applied Chemistry, Faculty of Engineering,

Osaka University, Suita, Osaka 565-0871, Japan.

General Comments.

Carbamotelluroates **1a-c**^{S1} and 2,4,6-trimethylphenylacetylene^{S2} were synthesized according to the reported procedure. Other acetylenes were obtained commercially and used after distillation or recrystallization.

Melting points were determined on a Yanagimoto Micro Melting Point apparatus. ¹H and ¹³C NMR spectra were recorded on a JEOL JNM-ALICE-400 (400 MHz and 100 MHz, respectively) spectrometer using Me₄Si as an internal standard. IR spectra were determined on a Perkin Elmer Model 1600 spectrometer. Purification of products was performed on a recycling preparative HPLC (Japan Analytical Industry Co. Ltd., Model LC-908) equipped with JAIGEL-1H and -2H columns (GPC) using CHCl₃ as an eluent. 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.

***Te*-Phenyl *N,N*-dimethylcarbamotelluroate (**1a**).**

^1H NMR (400 MHz, CDCl_3) δ 2.89 (s, 3 H), 3.02 (s, 3 H), 7.25-7.39 (m, 3 H), 7.79-7.81 (m, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 36.0, 38.1, 114.2, 128.5, 129.0, 140.1, 156.9; IR (NaCl) 3052, 2927, 1650, 1474, 1434, 1251, 1083, 1017, 880, 734, 691, 666 cm^{-1} ; MS (EI), m/z (relative intensity, %) 279 (M^+ , 2), 278 (15), 72 (100). HRMS calcd for $\text{C}_9\text{H}_{11}\text{NOTe}$: 278.9903. Found 278.9901.

***Te*-Phenyl *N,N*-diethylcarbamotelluroate (**1b**).**

^1H NMR (400 MHz, CDCl_3) δ 1.14 (t, $J = 7.2$ Hz, 3 H), 1.23 (t, $J = 7.1$ Hz, 3 H), 3.17 (q, $J = 7.1$ Hz, 2 H), 3.44 (q, $J = 7.2$ Hz, 2 H), 7.23-7.39 (m, 3 H), 7.81 (d, $J = 7.1$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.4, 14.7, 41.7, 44.3, 114.1, 128.4, 128.9, 140.2, 155.0; IR (NaCl) 3053, 2972, 2933, 1651, 1474, 1434, 1396, 1242, 1211, 1105, 1094, 832, 733, 690, 646 cm^{-1} ; MS (EI), m/z (relative intensity, %) 307 (M^+ , 1), 100 (100). Anal. Calcd for $\text{C}_{11}\text{H}_{15}\text{NOTe}$: C, 43.34; H, 4.96; N, 4.59. Found: C, 43.36; H, 4.75; N, 4.31.

***N,N*-Dimethyl-3-phenyl-3-phenyltelluroacrylamide (**2a**).** Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and phenylacetylene (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, excess phenylacetylene was removed *in vacuo* and the residue was purified by preparative recycling HPLC to provide *N,N*-dimethyl-3-phenyl-3-phenyltelluroacrylamide (**2a**) in 72% yield. After the *E/Z* ratio was determined by ^1H NMR (*E/Z* = 42/58), (*Z*)-**2a** was separated by preparative TLC eluted with *n*-hexane/ Et_2O = 5/1. An attempt for isolation of (*E*)-**2a** failed, so the spectra data of (*E*)-**2a** were obtained from the *E/Z* mixture. (*Z*)-**2a**: mp 76-77 °C. ^1H NMR (400 MHz, CDCl_3) δ 3.10 (s, 6 H), 6.86-7.02 (m, 9 H), 7.39 (d, $J = 7.8$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 36.1, 37.2, 119.37, 119.40, 121.2, 126.9, 127.0, 127.8, 128.0, 140.0, 141.5, 152.9, 167.0; IR (NaCl) 3051, 2928, 1614 (C=O), 1490, 1398, 1150, 736, 695 cm^{-1} ; MS (EI), m/z (relative intensity, %) 381 (M^+ , 60), 379 (55), 335 (16), 304 (100), 302 (90). Anal. Calcd for $\text{C}_{17}\text{H}_{17}\text{NOTe}$: C, 53.88; H, 4.52; N, 3.70. Found:

C, 54.15; H, 4.41; N, 3.59. (*E*)-**2a**: ^1H NMR (400 MHz, CDCl_3) δ 2.62 (s, 3 H), 2.71 (s, 3 H), 6.07 (s, 1 H), 7.22-7.40 (m, 8 H), 7.84-7.86 (m, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 34.5, 37.7, 114.3, 127.5, 128.1, 128.2, 128.5, 128.6, 128.8, 129.6, 130.0, 140.3, 167.5; IR (NaCl) 1628 (C=O) cm^{-1} .

***N,N*-Dimethyl-3-(4-bromophenyl)-3-phenyltelluroacrylamide (2b)**. Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and *p*-bromophenylacetylene (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, the mixture was purified by preparative recycling HPLC to provide *N,N*-dimethyl-3-(4-bromophenyl)-3-phenyltelluroacrylamide (**2b**) in 84% yield. After the *E/Z* ratio was determined by ^1H NMR (*E/Z* = 35/65), (*Z*)-**2b** was separated by preparative TLC eluted with *n*-hexane/ Et_2O = 1/1 and subjected to X-ray analysis after recrystallization from *n*-hexane- CHCl_3 (1:1). An attempt for isolation of (*E*)-**2b** failed, so the spectra data of (*E*)-**2b** were obtained from the *E/Z* mixture. (*Z*)-**2b**: mp 127-128 °C; ^1H NMR (400 MHz, CDCl_3) δ 3.10 (s, 6 H), 6.78-6.82 (m 2 H), 6.91-6.96 (m 2 H), 7.03 (s, 1 H), 7.08-7.14 (m, 3 H), 7.38-7.42 (m, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 35.9, 37.1, 119.4, 120.7, 120.8, 127.2, 127.9, 129.4, 129.8, 139.9, 140.3, 151.2, 166.6; IR (NaCl) 3049, 1615 (C=O), 1482, 1400, 732 cm^{-1} ; MS (EI), *m/z* (relative intensity, %) 459 (M^+ , 100). Anal. Calcd for $\text{C}_{17}\text{H}_{16}\text{BrN}\text{OTe}$: C, 44.60; H, 3.52; N, 3.06. Found: C, 44.59; H, 3.43; N, 3.06. (*E*)-**2b**: ^1H NMR (400 MHz, CDCl_3) δ 2.68 (s, 3 H), 2.73 (s, 3 H), 6.14 (s, 1 H), 7.23-7.42 (m, 7 H), 7.80-7.84 (m 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 34.6, 37.6, 114.0, 122.1, 128.9, 129.1, 129.6, 131.1, 131.6, 139.3, 140.2, 166.8.

***N,N*-Dimethyl-3-(4-methoxyphenyl)-3-phenyltelluroacrylamide (2c)**. Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and *p*-methoxyphenylacetylene (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, the mixture was purified by preparative recycling HPLC to provide *N,N*-dimethyl-3-(4-methoxyphenyl)-3-phenyltelluroacrylamide (**2c**) in 18% yield. Although the *E/Z* ratio was determined by ^1H NMR

(*E/Z* = 44/56), an attempt for isolation of isomers by PTLC failed, so the following spectra and analytical data were obtained from the *E/Z* mixture: ¹H NMR (400 MHz, CDCl₃) δ 2.63 (s, *E* (3 H)), 2.74 (s, *E* (3 H)), 3.10 (s, *E* (3 H)), 3.11 (s, *Z* (3 H)), 3.67 (s, *Z* (3 H)), 3.79 (s, *Z* (3 H)), 6.02 (s, *E* (1 H)), 6.50-6.54 (m, 2 H), 6.78-6.82 (m, 2 H), 6.87-6.95 (m, 4 H), 7.03-7.08 (m, 2 H), 7.04 (s, *Z* (1H)), 7.25-7.42 (m, 6 H), 7.83-7.87 (m, 2 H); ¹³C NMR (100 MHz, CDCl₃) δ 34.5 (*Z*), 36.1(*E*), 37.3 (*E*), 37.7 (*Z*), 55.3, 112.5, 113.5, 114.4, 119.2, 121.5, 127.0, 127.9, 128.7, 129.1, 129.5, 132.7, 134.2, 139.9, 140.2, 152.8, 159.3, 167.2 (*Z*), 167.9 (*E*); MS (EI), *m/z* (relative intensity, %) 411 (*M*⁺, 48), 365 (2), 334 (16), 204 (100), 72 (77). Anal. Calcd for C₁₈H₁₉NO₂Te: C, 52.87; H, 4.68; N, 3.43. Found: C, 52.93; H, 4.51; N, 3.31.

***N,N*-Dimethyl-3-(2,4,6-trimethylphenyl)-3-phenyltelluroacrylamide (2d).** Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and 2,4,6-trimethylphenylacetylene (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 48 h. After cooling to room temperature, the mixture was purified by preparative recycling HPLC to provide *N,N*-dimethyl-3-(2,4,6-trimethylphenyl)-3-phenyltelluroacrylamide (**2d**) in 31% yield. After the *E/Z* ratio was determined by ¹H NMR (*E/Z* = 7/93), (*Z*)-**2d** was separated by preparative TLC eluted with *n*-hexane/Et₂O = 5/1. An attempt for isolation of (*E*)-**2d** failed, so the spectra data of (*E*)-**2d** were obtained from the *E/Z* mixture. (*Z*)-**2d**: ¹H NMR (400 MHz, CDCl₃) δ 2.10 (s, 3 H), 2.13 (s, 6 H), 3.04 (s, 3 H), 3.10 (s, 3 H), 6.52 (s, 2 H), 6.82-6.87 (m, 2 H), 6.97 (s, 1 H), 7.01-7.06 (m, 1 H), 7.33-7.37 (m, 2 H); ¹³C NMR (100 MHz, CDCl₃) δ 20.4, 20.8, 36.0, 37.1, 118.0, 119.8, 127.1, 127.2, 127.4, 133.7, 136.4, 137.2, 139.5, 153, 5, 167.5; IR (NaCl) 2998, 2919, 1614 (C=O), 1474, 1162, 753, 632 cm⁻¹; MS (EI), *m/z* (relative intensity, %) 391 (*M*⁺, 53), 360 (100), 314 (14), 230 (10). Anal. Calcd for C₂₀H₂₃NOTe: C, 57.06; H, 5.51; N, 3.33. Found: C, 57.01; H, 5.27; N, 3.31. (*E*)-**2d**: ¹H NMR (400 MHz, CDCl₃) δ 2.21 (s, 3 H), 2.28 (s, 6 H), 2.74 (s, 3 H), 2.78 (s, 3 H), 6.26 (s, 1 H), 6.76 (s, 1 H), 7.24-7.39 (m, 4 H), 7.83-7.86 (m, 2 H); ¹³C NMR (100 MHz, CDCl₃) δ 19.9, 21.0, 34.7, 36.9, 113.9, 117.8, 125.7, 128.7, 129.2, 133.3, 135.8, 136.4, 137.4, 140.8, 164.4.

Methyl 3-dimethylcarbamoyl-2-phenyltelluroacrylate (2e). Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and methyl propiolate (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, the mixture was purified by preparative recycling HPLC to provide methyl 3-dimethylcarbamoyl-2-phenyltelluroacrylate (**2e**) in 57% yield. After the *E/Z* ratio was determined by ¹H NMR (*E/Z* = 24/76), (*Z*)-**2e** was separated by preparative TLC eluted with *n*-hexane/Et₂O = 1/1. An attempt for isolation of (*E*)-**2e** failed, so the spectra data of (*E*)-**2e** were obtained from the *E/Z* mixture. (*Z*)-**2e**: ¹H NMR (400 MHz, CDCl₃) δ 3.07 (s, 3 H), 3.10 (s, 3 H), 3.11 (s, 3 H), 7.22-7.37 (m, 4 H), 7.83-7.87 (m, 2 H); ¹³C NMR (100 MHz, CDCl₃) δ 36.1, 37.1, 51.8, 119.7, 120.0, 128.2, 128.4, 140.3, 141.0, 166.1, 168.5; IR (NaCl) 3050, 2948, 1726, 1620 (C=O), 1433, 1401, 1242, 1158, 738, 695 cm⁻¹; MS (EI), *m/z* (relative intensity, %) 363 (M⁺, 87), 286 (100), 207 (14), 77 (25), 72 (34). HRMS calcd for C₁₃H₁₅NO₃Te: 363.0114. Found 363.0106. (*E*)-**2e**: ¹H NMR (400 MHz, CDCl₃) δ 2.86 (s, 3 H), 2.93 (s, 3 H), 3.72 (s, 3 H), 6.19 (s, 1 H), 7.22-7.46 (m, 3 H), 7.86-7.92 (m, 2 H); ¹³C NMR (100 MHz, CDCl₃) δ 34.8, 37.4, 52.9, 112.3, 119.3, 129.4, 129.9, 135.9, 141.1, 166.2, 166.6.

***N,N*-Dimethyl-3-phenyltellro-3-trimethylsilylacrylamide (2f).** Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and trimethylsilylacetylene (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, the mixture was purified by preparative recycling HPLC to provide *N,N*-dimethyl-3-phenyltellro-3-trimethylsilylacrylamide (**2f**) in 35% yield. Although the *E/Z* ratio was determined by ¹H NMR (*E/Z* = 61/39), an attempt for isolation of isomers by PTLC failed, so the following spectra and analytical data were obtained from the *E/Z* mixture. (*Z*)-**2f**: ¹H NMR (400 MHz, CDCl₃) δ -0.05 (s, 9 H), 3.05 (s, 3 H), 3.12 (s, 3 H), 7.19-7.42 (m, 3 H) 7.49 (s, 1 H), 7.99-8.02 (m, 2 H). NOE experiment: irradiation at methyl singlet at δ -0.05 resulted in a 14.0% enhancement of the signal at δ 7.49. (*E*)-**2f**: ¹H NMR (400 MHz, CDCl₃) δ 0.27 (s, 9 H), 2.72 (s, 3 H), 2.86 (s, 3 H), 6.62 (s, 1 H), 7.19-7.42 (m, 3 H), 7.79-7.82. *E/Z* mixture: ¹³C NMR (100 MHz, CDCl₃) δ 0.2 (*E*), 1.2 (*Z*),

29.8 (Z), 35.2 (E), 36.2 (Z), 37.3 (E), 113.4, 118.9, 126.3, 128.3, 128.8, 129.6, 136.7, 141.0, 142.2, 142.3, 153.5 (Z), 166.7 (E), 167.3 (Z); IR (NaCl) 2950, 1636, 1612, 1447, 1153, 842, 726, 698 cm^{-1} ; MS (EI), m/z (relative intensity, %) 377 (M^+ , 58), 362 (100), 300 (80), 232 (41), 170 (53), 72 (74). HRMS calcd for $C_{14}H_{21}NOSiTe$: 377.0455. Found 377.0448

***N,N*-Diethyl-3-phenyl-3-phenyltelluroacrylamide (2g).** Into a 3 mL Pyrex flask were placed carbamotelluroate **1b** (1 mmol) and phenylacetylene (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, excess phenylacetylene was removed *in vacuo* and the mixture was purified by preparative recycling HPLC to provide *N,N*-diethyl-3-phenyl-3-phenyltelluroacrylamide (**2g**) in 72% yield. After the *E/Z* ratio was determined by ^1H NMR (*E/Z* = 37/63), (*E*)- and (*Z*)-**2g** were separated by preparative TLC eluted with *n*-hexane/ Et_2O = 5/1. (*E*)-**2g**: ^1H NMR (400 MHz, CDCl_3) δ 0.81 (t, J = 7.2 Hz, 3 H), 0.87 (t, J = 7.1 Hz, 3 H), 3.06 (q, J = 7.2 Hz, 2 H), 3.20 (q, J = 7.1 Hz, 2 H), 6.07 (s, 1 H), 7.20-7.42 (m, 8 H), 7.86 (d, J = 6.8 Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 12.5, 14.1, 39.8, 42.4, 114.4, 127.6, 127.9, 128.0, 128.1, 128.8, 129.6, 129.7, 140.2, 140.3, 166.4; IR (NaCl) 2973, 2930, 1620 (C=O), 1433, 1274, 694 cm^{-1} ; MS (EI), m/z (relative intensity, %) 410 (M^+ , 100), 332 (9), 202 (6), 100 (11). Anal. Calcd for $C_{19}H_{21}NOTe$: C, 56.07; H, 5.20; N, 3.44. Found: C, 56.16; H, 4.95; N, 3.52. (*Z*)-**2g**: ^1H NMR (400 MHz, CDCl_3) δ 1.21 (t, J = 7.2 Hz, 3 H), 1.23 (t, J = 7.2 Hz, 3 H), 3.41 (q, J = 7.2 Hz, 2 H), 3.52 (q, J = 7.2 Hz, 2 H), 6.86-7.07 (m, 9 H), 7.39-7.42 (m, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 13.5, 14.9, 41.3, 42.2, 119.6, 121.4, 126.8, 126.9, 127.0, 127.8, 128.0, 140.0, 141.5, 152.3, 166.0; IR (NaCl) 3062, 2975, 1608 (C=O), 1432, 1252, 1145, 695 cm^{-1} ; MS (EI), m/z (relative intensity, %) 409 (M^+ , 100), 332 (47), 100 (20). Anal. Calcd for $C_{19}H_{21}NOTe$: C, 56.07; H, 5.20; N, 3.44. Found: C, 55.85; H, 5.15; N, 3.52.

***N,N*-Dimethyl-3-phenyl-3-butyltelluroacrylamide (2h).** Into a 20 mL flask were placed carbamotelluroate **1c** (0.5 mmol), phenylacetylene (1 mmol), AIBN (0.05 mmol) and benzene (0.5 mL) under Ar. The mixture was then heated under reflux for 2 h. After cooling to room temperature, excess phenylacetylene was removed *in vacuo* and the residue was purified by preparative recycling HPLC to provide *N,N*-dimethyl-3-phenyl-3-butyltelluroacrylamide (**2h**) in 43% yield accompanied with 3% of by-products (**6**), arising from the addition of 1-cyano-1-methylethyl and PhTe groups to phenylacetylene. After the *E/Z* ratio was determined by ¹H NMR (*E/Z* = 9/91), (*Z*)-**2h** was separated by preparative TLC eluted with *n*-hexane/Et₂O = 1/1. (*Z*)-**2h**: ¹H NMR (400 MHz, CDCl₃) δ 0.69 (t, 3 H, *J* = 7.3 Hz), 1.09 (sext, 2 H, *J* = 7.3 Hz), 1.37 (q, 2 H, *J* = 7.3 Hz), 1.91 (t, 2 H, *J* = 7.3 Hz), 3.05 (s, 6 H), 6.94 (s, 1 H), 7.21-7.30 (m, 3 H), 7.33-7.39 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 9.1, 13.3, 25.1, 33.2, 35.8, 37.0, 120.8, 127.2, 127.3, 127.5, 142.4, 149.1, 166.6; IR (NaCl) 2955, 2925, 1616 (C=O), 1489, 1396, 1147, 700 cm⁻¹; MS (EI), *m/z* (relative intensity, %) 361 (M⁺, 19), 304 (100), 191 (33), 105 (64), 72 (61). HRMS calcd for C₁₅H₂₁NOTe: 361.0685. Found 361.0679. An attempt for isolation of (*E*)-**2h** failed

Dimethyl 2-dimethylcarbamoyl-3-phenyltellurobut-2-enedioate (2i). Into a 3 mL Pyrex flask were placed carbamotelluroate **1a** (1 mmol) and dimethyl acetylenedicarboxylate (2 mmol) under Ar. The mixture was then irradiated in a water bath kept at 60°C using a 500W tungsten lamp with a distance of 10 cm for 24 h. After cooling to room temperature, the mixture was purified by preparative recycling HPLC to provide dimethyl 2-dimethylcarbamoyl-3-phenyltellurobut-2-enedioate (**2i**) in 77% yield. After the *E/Z* ratio was determined by ¹H NMR (*E/Z* = 38/62), (*E*)- and (*Z*)-**2i** were separated by preparative TLC eluted with Et₂O. (*Z*)-**2i**: ¹H NMR (400 MHz, CDCl₃) δ 2.93 (s, 3 H), 2.97 (s, 3 H), 3.03 (s, 3 H), 3.87 (s, 3 H), 7.23-7.42 (m, 3 H), 7.81-7.89 (m, 2 H); ¹³C NMR (100 MHz, CDCl₃) δ 35.0, 38.3, 51.9, 53.4, 117.5, 128.8, 141.1, 143.0, 165.2, 165.4, 166.2; IR (NaCl) 3005, 2951, 1724, 1681, 1644, 1434, 1284, 1250, 1026, 751 cm⁻¹; MS (EI), *m/z* (relative intensity, %) 421 (M⁺, 100), 344 (92), 72 (70). HRMS calcd for C₁₅H₁₇NO₅Te: 421.0169. Found 421.0177. (*E*)-**2i**: ¹H NMR (400 MHz, CDCl₃) δ 2.99 (s, 3 H), 3.10 (s, 3 H), 3.18 (s, 3 H), 3.74 (s, 3 H), 7.26-7.46 (m, 3 H), 7.85-7.90

(m, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 35.7, 38.0, 51.8, 52.6, 114.0, 128.9, 129.5, 141.6, 160.9, 165.9, 166.5; IR (NaCl) 3052, 2951, 1732, 1709, 1633, 1434, 1245, 1201, 1015, 746 cm^{-1} ; MS (EI), m/z (relative intensity, %) 421 (M^+ , 100), 344 (71), 207 (21), 72 (71). HRMS calcd for $\text{C}_{15}\text{H}_{17}\text{NO}_5\text{Te}$: 421.0169. Found 421.0171

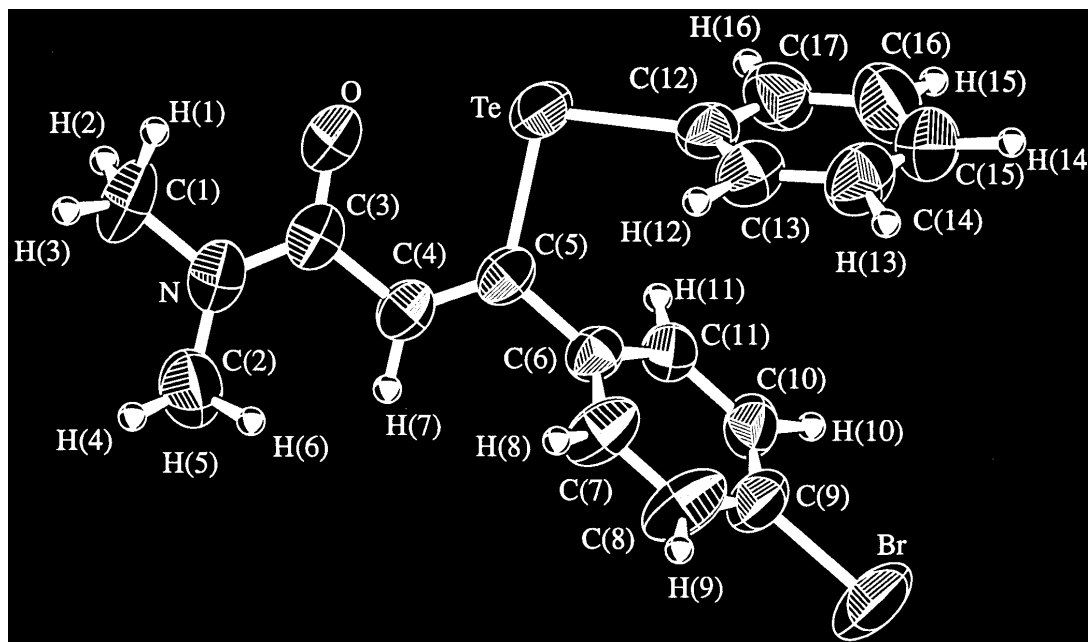


Figure S1. ORTEP Drawing of (Z)-2b

Table S1. Positional Parameters and B(eq) for (Z)-2b

atom	x	y	z	B(eq)
Te	0.90656(2)	0.52990(3)	0.22476(2)	0.06892(9)
Br	0.49085(5)	-0.04227(9)	0.12848(5)	0.1266(3)
O	1.0540(2)	0.5053(4)	0.3867(2)	0.0774(9)
N	1.1068(3)	0.3254(4)	0.4974(2)	0.068(1)
C(1)	1.2031(4)	0.4092(8)	0.5360(4)	0.085(2)
C(2)	1.0910(5)	0.1909(7)	0.5457(4)	0.086(2)
C(3)	1.0381(3)	0.3841(5)	0.4224(3)	0.061(1)
C(4)	0.9424(3)	0.3011(5)	0.3802(3)	0.056(1)
C(5)	0.8771(3)	0.3409(4)	0.2985(2)	0.0527(10)
C(6)	0.7825(3)	0.2502(4)	0.2572(2)	0.0515(9)
C(7)	0.7892(4)	0.0950(5)	0.2415(4)	0.078(1)
C(8)	0.7018(5)	0.0098(6)	0.2032(5)	0.093(2)
C(9)	0.6093(4)	0.0785(6)	0.1822(3)	0.073(1)

C(10)	0.6008(3)	0.2308(5)	0.1988(3)	0.065(1)
C(11)	0.6876(3)	0.3171(5)	0.2358(2)	0.056(1)
C(12)	0.7827(4)	0.4884(5)	0.1025(3)	0.064(1)
C(13)	0.7813(4)	0.3623(5)	0.0458(3)	0.069(1)
C(14)	0.7024(4)	0.3440(7)	-0.0352(3)	0.082(2)
C(15)	0.6260(5)	0.4470(7)	-0.0609(4)	0.092(2)
C(16)	0.6247(5)	0.5708(7)	-0.0066(4)	0.099(2)
C(17)	0.7024(4)	0.5916(6)	0.0752(3)	0.079(1)
H(1)	1.224(5)	0.466(7)	0.487(5)	0.12(2)
H(2)	1.196(5)	0.493(7)	0.566(5)	0.12(2)
H(3)	1.258(6)	0.342(8)	0.554(4)	0.13(2)
H(4)	1.141(5)	0.155(7)	0.580(4)	0.12(2)
H(5)	1.052(5)	0.218(7)	0.579(4)	0.12(2)
H(6)	1.060(5)	0.089(8)	0.496(4)	0.13(2)
H(7)	0.933(3)	0.219(5)	0.412(3)	0.07(1)
H(8)	0.845(5)	0.052(6)	0.251(4)	0.10(2)
H(9)	0.712(4)	-0.090(7)	0.202(4)	0.11(2)
H(10)	0.533(4)	0.287(6)	0.187(3)	0.11(2)
H(11)	0.686(3)	0.420(5)	0.253(3)	0.07(1)
H(12)	0.833(4)	0.287(6)	0.066(3)	0.09(2)
H(13)	0.698(4)	0.251(7)	-0.075(3)	0.10(2)
H(14)	0.573(5)	0.440(6)	-0.119(4)	0.10(2)
H(15)	0.576(4)	0.632(6)	-0.021(3)	0.09(2)
H(16)	0.704(4)	0.674(7)	0.118(4)	0.11(2)

Table S2. Unisotropic Displacement Parameters for (Z)-2b

	U11	U22	U33	U12	U13	U23
Te	0.0716(2)	0.0723(2)	0.0615(2)	-0.0295(1)	0.0198(1)	-0.0049(1)
Br	0.0899(4)	0.1495(6)	0.1302(5)	-0.0724(4)	0.0219(4)	-0.0151(4)
O	0.058(2)	0.086(2)	0.079(2)	-0.022(1)	0.009(1)	-0.001(2)
N	0.055(2)	0.072(2)	0.070(2)	0.003(2)	0.009(2)	-0.013(2)
C(1)	0.049(3)	0.096(3)	0.094(3)	-0.007(3)	0.002(2)	-0.032(3)
C(2)	0.080(4)	0.088(4)	0.075(3)	0.009(3)	0.005(3)	0.001(3)
C(3)	0.051(2)	0.070(3)	0.062(2)	-0.004(2)	0.018(2)	-0.013(2)
C(4)	0.046(2)	0.060(2)	0.064(2)	-0.004(2)	0.020(2)	-0.004(2)
C(5)	0.046(2)	0.056(2)	0.061(2)	-0.006(2)	0.023(2)	-0.011(2)
C(6)	0.049(2)	0.059(2)	0.052(2)	-0.008(2)	0.024(2)	-0.004(2)
C(7)	0.057(3)	0.065(2)	0.118(4)	-0.008(2)	0.037(3)	-0.023(3)
C(8)	0.088(4)	0.067(3)	0.134(5)	-0.028(3)	0.047(3)	-0.036(3)
C(9)	0.060(3)	0.093(3)	0.067(2)	-0.030(2)	0.020(2)	-0.005(2)
C(10)	0.045(2)	0.088(3)	0.057(2)	-0.006(2)	0.011(2)	0.007(2)
C(11)	0.053(2)	0.061(2)	0.053(2)	-0.002(2)	0.015(2)	0.003(2)
C(12)	0.075(3)	0.067(2)	0.052(2)	-0.021(2)	0.025(2)	-0.002(2)

C(13)	0.076(3)	0.071(3)	0.067(2)	-0.011(2)	0.031(2)	-0.015(2)
C(14)	0.091(4)	0.088(3)	0.067(2)	-0.019(3)	0.026(2)	-0.021(2)
C(15)	0.095(4)	0.100(4)	0.065(3)	-0.022(3)	0.007(3)	0.000(3)
C(16)	0.112(5)	0.083(3)	0.082(3)	0.016(3)	0.005(3)	0.011(3)
C(17)	0.106(4)	0.060(2)	0.067(2)	0.000(2)	0.020(3)	0.000(2)

Table S3. Bond Lengths for (Z)-**2b**

atom	atom	distance	atom	atom	distance
Te	C(5)	2.106(4)	Te	C(12)	2.128(4)
Br	C(9)	1.901(4)	O	C(3)	1.237(5)
N	C(1)	1.470(6)	N	C(2)	1.436(7)
N	C(3)	1.336(5)	C(3)	C(4)	1.467(5)
C(4)	C(5)	1.335(5)	C(5)	C(6)	1.487(5)
C(6)	C(7)	1.373(6)	C(6)	C(11)	1.382(5)
C(7)	C(8)	1.382(7)	C(8)	C(9)	1.360(8)
C(9)	C(10)	1.355(7)	C(10)	C(11)	1.378(5)
C(12)	C(13)	1.393(6)	C(12)	C(17)	1.386(7)
C(13)	C(14)	1.375(6)	C(14)	C(15)	1.347(8)
C(15)	C(16)	1.361(8)	C(16)	C(17)	1.378(7)

Table S4. Bond Angles for (Z)-**2b**

atom	atom	atom	angle
C(5)	Te	C(12)	95.7(1)
C(1)	N	C(2)	117.7(4)
C(1)	N	C(3)	117.7(4)
C(2)	N	C(3)	124.5(4)
O	C(3)	N	121.6(4)
O	C(3)	C(4)	119.2(4)
N	C(3)	C(4)	119.2(4)
C(3)	C(4)	C(5)	122.2(4)
Te	C(5)	C(4)	120.9(3)
Te	C(5)	C(6)	118.8(2)
C(4)	C(5)	C(6)	120.3(3)
C(5)	C(6)	C(7)	119.3(4)
C(5)	C(6)	C(11)	121.9(3)
C(7)	C(6)	C(11)	118.8(4)
C(6)	C(7)	C(8)	119.8(5)
C(7)	C(8)	C(9)	120.3(5)
Br	C(9)	C(8)	119.0(4)
Br	C(9)	C(10)	120.0(4)
C(8)	C(9)	C(10)	121.0(4)

C(9)	C(10)	C(11)	119.1(4)
C(6)	C(11)	C(10)	121.1(4)
Te	C(12)	C(13)	121.8(4)
Te	C(12)	C(17)	120.1(3)
C(13)	C(12)	C(17)	118.1(4)
C(12)	C(13)	C(14)	120.0(5)
C(13)	C(14)	C(15)	120.8(5)
C(14)	C(15)	C(16)	120.5(5)
C(15)	C(16)	C(17)	119.9(6)
C(12)	C(17)	C(16)	120.6(5)

Table S5. Torsion Angles for (Z)-**2b**

atom	atom	atom	atom	angle
Te	C(5)	C(4)	C(3)	-0.9(5)
Te	C(5)	C(6)	C(7)	121.0(4)
Te	C(5)	C(6)	C(11)	-60.4(4)
Te	C(12)	C(13)	C(14)	-176.5(3)
Te	C(12)	C(17)	C(16)	176.2(4)
Br	C(9)	C(8)	C(7)	179.4(4)
Br	C(9)	C(10)	C(11)	-178.5(3)
O	C(3)	N	C(1)	-0.6(6)
O	C(3)	N	C(2)	175.9(5)
O	C(3)	C(4)	C(5)	8.5(6)
N	C(3)	C(4)	C(5)	-170.3(4)
C(1)	N	C(3)	C(4)	178.1(4)
C(2)	N	C(3)	C(4)	-5.4(6)
C(3)	C(4)	C(5)	C(6)	178.1(3)
C(4)	C(5)	Te	C(12)	172.0(3)
C(4)	C(5)	C(6)	C(7)	58.0(5)
C(4)	C(5)	C(6)	C(11)	120.6(4)
C(5)	Te	C(12)	C(13)	-69.9(3)
C(5)	Te	C(12)	C(17)	112.8(3)
C(5)	C(6)	C(7)	C(8)	180.0
C(5)	C(6)	C(11)	C(10)	-179.1(3)
C(6)	C(5)	Te	C(12)	-7.0(3)
C(6)	C(7)	C(8)	C(9)	-0.9(9)
C(6)	C(11)	C(10)	C(9)	-0.9(6)
C(7)	C(6)	C(11)	C(10)	-0.5(6)
C(7)	C(8)	C(9)	C(10)	-0.4(9)
C(8)	C(7)	C(6)	C(11)	1.3(7)
C(8)	C(9)	C(10)	C(11)	1.3(7)
C(12)	C(13)	C(14)	C(15)	0.1(7)
C(12)	C(17)	C(16)	C(15)	0.7(9)

C(13)	C(12)	C(17)	C(16)	-1.2(7)
C(13)	C(14)	C(15)	C(16)	-0.7(8)
C(14)	C(13)	C(12)	C(17)	0.8(6)
C(14)	C(15)	C(16)	C(17)	0.2(9)

References

- S1) Hihiro, T.; Mogami, T.; Kambe, N.; Fujiwara, S.; Sonoda, N. *Synth. Commun.* **1990**, 20, 703-711.
- S2) Negishi, E.; Kotori, M.; Xu, C. *J. Org. Chem.* **1997**, 62, 8957-8960.