SUPPORTING INFORMATION

„Synthesis, structure and reactivity of cyclopropenyl-1-ylidene stabilized S(II), Se(II) and Te(II) mono- and dications”

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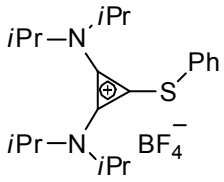
Experimental procedures:

General: All reactions were carried out in flame-dried glassware under Ar. All solvents were purified by distillation over the drying agents indicated and were transferred under Ar. IR: Nicolet FT-7199 spectrometer, wavenumbers in cm^{-1}. MS (EI): Finnigan MAT 8200 (70 eV), ESIMS: Finnigan MAT 95, accurate mass determinations: Bruker APEX III FT-MS (7 T magnet). NMR: Spectra were recorded on a Bruker AV 400 or DPX 300; ^{1}H and ^{13}C chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale. Column chromatography was performed on Merck 60 silica gel (40-63 µm). Thin-layer chromatography (TLC) analysis was performed using Merck silica gel 60 F254 TLC plates, and visualized by UV.

All commercially available compounds (ABCR, Acros, Aldrich, Fischer) were used as received. 2,3-bis(diisopropylamino)-1-chlorocyclopropenium tetrafluoroborate **1**,[1] 2,3-bis(diisopropylamino)-1-chlorocyclopropenium triflate **2**,[2] phenyl trimethylsilyl selenide,[3] phenyl trimethylsilyl telluride,[4] 2,3-bis(diisopropylamino)cyclopropenone[5] were prepared according to literature procedures.

Compound 3



Trimethyl(phenylthio)silane (235 µL, 1.24 mmol) was added to a stirred suspension of chlorocyclopropenium salt **1** (446 mg, 1.24 mmol) in dry THF (10 mL) and the resulting mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was evacuated and the product was purified by recrystallization from CH_2Cl_2/Et_2O to obtain **3** as a white solid (383 mg, 71%).

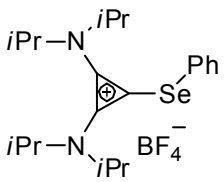
^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.16 (bs, 12H), 1.34 (bs, 12H), 3.46 (bs, 2H), 3.99 (bs, 2H), 7.47-7.55 (m, 3H), 7.60-7.66 (m, 2H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.3, 21.9, 51.5 (bs), 104.7, 127.4, 130.9, 131.4, 133.0, 134.6 ppm.

HRMS *calcd.* for $C_{21}H_{33}N_2S_1^+$: 345.235894; *found* 345.235863.

IR (neat) $\tilde{\nu}$ = 690, 750, 804, 891, 1019, 1032, 1043, 1089, 1140, 1160, 1209, 1349, 1377, 1417, 1440, 1462, 1479, 1573, 1883, 2941, 2986 cm^{-1}.

Compound 4



Phenyl trimethylsilyl selenide (610 mg, 2.66 mmol) was added to a stirred suspension of chlorocyclopropenium salt **1** (764 mg, 2.13 mmol) in dry THF (16 mL) and the resulting mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was evacuated and the residue purified by column

[1] R. Weiss, K. G. Wagner, C. Priesner, J. Macheleid, *J. Am. Chem. Soc.* 1985, **107**, 4491.
[2] Z. Yoshida, Y. Tawara, *J. Am. Chem. Soc.* 1971, **93**, 2573.
[3] N. Miyoshi, H. Ishii, K. Kondo, S. Murai, N. Sonoda, *Synthesis* 1979, 300.
[4] C. H. W. Jones, R. D. Sharma, *J. Organomet. Chem.* 1984, **268**, 113.
[5] Z. Yoshida, H. Konishi, Y. Tawara, H. Qgoshi, *J. Am. Chem. Soc.* 1973, **95**, 3043.

chromatography (CH_2Cl_2/MeOH, 94/6). Recrystallization from CH_2Cl_2/Et_2O afforded the title compound as a yellow solid (310 mg, 30%).

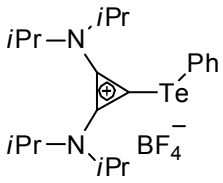
^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.17 (d, *J* = 5.2 Hz, 12H), 1.35 (d, *J* = 5.3 Hz, 12H), 3.56 (bs, 2H), 4.00 (bs, 2H), 7.45-7.56 (m, 3H), 7.70-7.74 (m, 2H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.3, 22.0, 51.5, 54.9, 96.5, 124.6, 131.0, 131.3, 136.3, 137.5 ppm.

HRMS *calcd.* for $C_{21}H_{33}N_2Se_1^+$: 393.181647; *found* 393.181621.

IR (neat) $\tilde{\nu}$ = 665, 691, 748, 890, 1018, 1032, 1047, 1093, 1140, 1155, 1208, 1351, 1374, 1391, 1411, 1456, 1478, 1577, 1878, 2939, 2985 cm^{-1}.

Compound 5



Phenyl trimethylsilyl telluride (392 mg, 1.41 mmol) was added to a stirred suspension of chlorocyclopropenium salt **1** (440 mg, 1.23 mmol) in dry THF (11 mL) and the resulting mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was removed and the residue washed with 4 x 2 mL Et_2O. After recrystallization from CH_2Cl_2/Et_2O compound **5** was obtained as a yellow solid (233 mg, 36%).

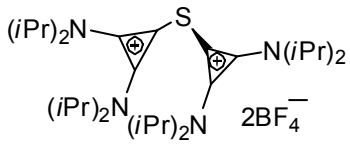
^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.16 (d, *J* = 6.6 Hz, 12H), 1.32 (d, *J* = 6.7 Hz, 12H), 3.66 (sept, *J* = 6.7 Hz, 2H), 3.98 (sept, *J* = 6.7 Hz, 2H), 7.36-7.43 (m, 2H), 7.48-7.54 (m, 1H), 7.95-78.00 (m, 2H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.3, 22.2, 51.4, 54.7, 76.1, 111.9, 130.8, 131.0, 141.5, 142.9 ppm.

HRMS *calcd.* for $C_{21}H_{33}N_2Te_1^+$: 443.170512; *found* 443.170115.

IR (neat) $\tilde{\nu}$ = 692, 742, 889, 1017, 1028, 1052, 1096, 1139, 1153, 1208, 1351, 1373, 1406, 1455, 1475, 1570, 1870, 2934, 2975 cm^{-1}.

Compound 6



Bis(trimethylsilyl)sulfide (77 µL, 0.41 mmol) was added to a stirred suspension of chlorocyclopropenium salt **1** (294 mg, 0.82 mmol) in dry THF (7 mL) and the reaction mixture was heated at 60 °C overnight. After cooling to room temperature, the precipitate was filtered off and washed with THF (3 × 9 mL), affording the desired compound as a white solid (236 mg, 85%).

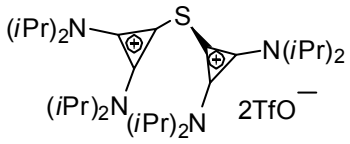
^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.31 (d, *J* = 6.9 Hz, 24H), 1.33 (d, *J* = 6.9 Hz, 24H), 3.86 (sept, *J* = 6.9 Hz, 4H), 4.06 (sept, *J* = 6.9 Hz, 4H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.4, 22.7, 51.7, 57.5, 92.7, 136.9 ppm.

HRMS *calcd*. for $C_{30}H_{56}BF_4N_4S^+$: 591.426501; *found* 591.427218.

IR (neat) $\tilde{\nu}$ = 893, 1045, 1350, 1562, 1873, 2979 cm^{-1}.

Compound 7



Bis(trimethylsilyl)sulfide (95 µL, 0.50 mmol) was added to a stirred suspension of chlorocyclopropenium salt **2** (425 mg, 1.01 mmol) in dry THF (10 mL) and the reaction mixture was heated at 60 °C overnight. After cooling to room temperature, the precipitate was filtered off and washed with THF (3 × 12 mL), affording the desired compound as a white solid (713 mg, 88%).

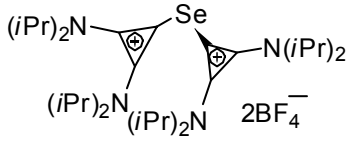
^{1}H NMR (300 MHz,CD_2Cl_2) δ = 1.39 (d, *J* = 5.2 Hz, 24H), 1.42 (d, *J* = 5.2 Hz, 24H), 3.95 (sept, *J* = 6.8 Hz, 4H), 4.14 (sept, *J* = 6.8 Hz, 4H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.1, 22.4, 51.4, 56.9, 92.9 ,121.8 (q, *J* = 321.4 Hz), 136.6 ppm.

HRMS *calcd*. for $C_{31}H_{56}N_4O_3F_3S_2^+$: 653.374049; *found* 653.374644.

IR (neat) $\tilde{\nu}$ = 1029, 1140, 1260, 1558, 1588, 1877, 2975 cm^{-1}.

Compound 8



Bis(trimethylsilyl)selenide (50 µL, 0.20 mmol) was added to a stirred suspension of chlorocyclopropenium salt **1** (143 mg, 0.40 mmol) in dry THF (4 mL) and the reaction mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was removed *in vacuo* and the residue was dissolved in DCM (10 mL). The resulting solution was filtered through the syringe filter and the filtrate concentrated *in vacuo*. The residue was washed with THF (2 × 8 mL), affording the desired compound as a white solid (96 mg, 66%).

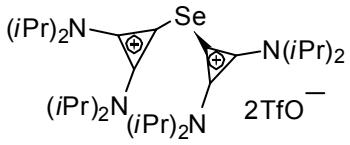
^{1}H NMR (300 MHz, CD_2Cl_2) δ = 1.31 (d, *J* = 6.9 Hz, 24H), 1.32 (d, *J* = 6.9 Hz, 24H), 3.90 (sept, *J* = 6.9 Hz, 4H), 4.04 (sept, *J* = 6.9 Hz, 4H) ppm.

^{13}C NMR (75 MHz, CD_2Cl_2) δ = 21.5, 22.6, 51.6, 57.2, 87.1, 139.9 ppm.

HRMS *calcd*. for $C_{30}H_{56}BF_4N_4Se^+$: 639.371658; *found* 639.372040.

IR (neat) $\tilde{\nu}$ = 680, 890, 1057, 1354, 1549, 1872, 2974 cm^{-1}.

Compound 9



Bis(trimethylsilyl)selenide (0.3 mL, 1.20 mmol) was added to a stirred suspension of chlorocyclopropenium salt **2** (1 g, 2.40 mmol) in dry THF (10 mL) and the reaction mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was removed *in vacuo* and the residue was dissolved in DCM (25 mL). The resulting solution was filtered through the syringe filter and the filtrate concentrated *in vacuo*. The residue was washed with THF (2 × 10 mL), affording the desired compound as a white solid (714 mg, 70%).

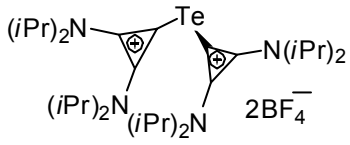
^{1}H NMR (300 MHz, CD_2Cl_2) δ = 1.39 (d, *J* = 6.8 Hz, 24H), 1.39 (d, *J* = 6.8 Hz, 24H), 3.99 (sept, *J* = 6.8 Hz, 4H), 4.11 (sept, *J* = 6.8 Hz, 4H) ppm.

^{13}C NMR (75 MHz, CD_2Cl_2) δ = 21.1, 22.2, 51.4, 56.4, 87.8, 121.3 (q, *J* = 321.4 Hz), 139.4 ppm.

HRMS *calcd*. for $C_{31}H_{56}F_3N_4O_3SSe^+$: 701.318486; *found* 701.320843.

IR (neat) $\tilde{\nu}$ = 800, 1028, 1139, 1258, 1558, 1872, 2973 cm^{-1}.

Compound 10



Bis(trimethylsilyl)telluride (50 µL, 0.17 mmol) was added to a stirred suspension of chlorocyclopropenium salt **42** (123 mg, 0.34 mmol) in dry THF (3 mL) and the reaction mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was removed *in vacuo* and the residue was dissolved in DCM (5 mL). The resulting solution was filtered through the syringe filter and the filtrate concentrated *in vacuo*. The residue was washed with THF (2 × 10 mL), affording the desired compound as a white solid (43 mg, 32%).

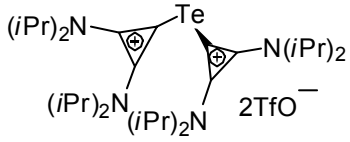
^{1}H NMR (300 MHz, CD_2Cl_2) δ = 1.38 (d, *J* = 7.0 Hz, 24H), 1.40 (d, *J* = 7.0 Hz, 24H), 4.10 (sept, *J* = 6.9 Hz, 4H), 4.11 (sept, *J* = 6.9 Hz, 4H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.3, 22.3, 51.3, 56.1, 71.4, 143.6 ppm.

HRMS *calcd*. for $C_{30}H_{56}BN_4F_4Te^+$: 689.360549; *found* 689.360863.

IR (neat) $\tilde{\nu}$ = 669, 889, 1013, 1063, 1141, 1354, 1539, 1575, 1863, 2973 cm^{-1}.

Compound 11



Freshly dried THF (6 mL) was added to a mixture of sodium (28 mg, 1.22 mmol) and naphthalene (156 mg, 1.22 mmol). A dark green solution was formed which was stirred at room temperature for 1h. Pulverized tellurium (78 mg, 0.61 mmol) was added to the reaction mixture which was stirred overnight. The chlorocyclopropenium salt **2** (512 mg, 1.22 mmol) was added to a white suspension of sodium telluride and the mixture was stirred for 24h. The solvent was removed *in vacuo* and the dark residue was washed with pentane (4 × 5 mL) to remove the naphthalene. The remaining residue was washed with DCM (4 × 2 mL) to dissolve the product. The filtrate was concentrated *in vacuo*, then washed with hot THF (~ 60 °C, 6 × 7 mL) affording the desired compound as a white solid (289 mg, 53%).

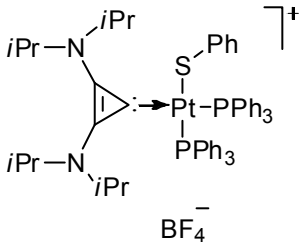
^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.30 (d, *J* = 6.9 Hz, 24H), 1.33 (d, *J* = 6.9 Hz, 24H), 4.03 (sept, *J* = 6.9 Hz, 4H), 4.04 (sept, *J* = 6.9 Hz, 4H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.4, 22.3, 51.4, 55.4, 74.3, 121.1 (q, *J* = 321.0 Hz), 143.4 ppm.

HRMS *calcd*. for $C_{31}H_{56}N_4O_3F_3STe^+$: 751.308665; *found* 751.309581.

IR (neat) $\tilde{\nu}$ = 1027, 1152, 1263, 1553, 1862, 2984 cm^{-1}.

Compound 12



A mixture of the compound **3** (52 mg, 0.12 mmol) and $Pt(PPh_3)_4$ (150 mg, 0.12 mmol) was evacuated for 10 minutes. Toluene (6 mL) was then added under Ar and the suspension was stirred at 100 °C overnight. After reaching room temperature, the solvent was removed *in vacuo* and the residue washed with Et_2O (4 x 2 mL). Recrystallization of the product from CH_2Cl_2/Et_2O gave compound **12** as a yellow solid (113 mg, 82%).

^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.06 (d, *J* = 6.9 Hz, 6H), 1.13 (d, *J* = 6.5 Hz, 6H), 1.14 (d, *J* = 6.5 Hz, 6H), 1.25 (d, *J* = 6.8 Hz, 6H), 3.71 (sept, *J* = 6.9 Hz, 2H), 4.15 (sept, *J* = 6.3 Hz, 2H), 6.93-6.98 (m, 2H), 6.99-7.05 (m, 3H), 7.18-7.27 (m, 15H), 7.36-7.49 (m, 15H) ppm.

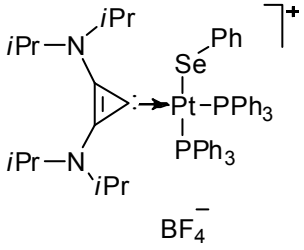
^{31}P NMR (162 MHz, CD_2Cl_2) δ = 16.5 (^{1}J(Pt-P) = 2898 Hz, ^{2}J(P-P) = 23.3 Hz), 20.1 (^{1}J(Pt-P) = 2360 Hz, ^{2}J(P-P) = 23.3 Hz) ppm.

^{13}C NMR (126 MHz, CD_2Cl_2) δ = 22.1, 22.2, 22.3, 22.7, 50.5, 51.4, 126.0, 128.3 (d, *J* = 10.6 Hz), 128.5, 128.9 (bs), 130.4 (d, *J* = 55.2 Hz), 130.9, 131.1, 131.1, 131.6, 131.8 (bs), 132.3 (d, *J* = 9.8 Hz), 134.6, 135.5 (d, *J* = 9.9 Hz), 144.4 ppm.

HRMS *calcd*. for $C_{57}H_{63}N_2P_2Pt_1S_1^+$: 1064.382988; *found*: 1064.382347.

IR (neat) $\tilde{\nu}$ = 691, 743, 999, 1050, 1093, 1156, 1185, 1212, 1334, 1372, 1435, 1455, 1492, 1574, 1858, 2977, 3055 cm^{-1}.

Compound 13



A mixture of the compound **4** (63 mg, 0.13 mmol) and $Pt(PPh_3)_4$ (162 mg, 0.13 mmol) was evacuated for 10 minutes. Toluene (6 mL) was then added under Ar and the suspension was stirred at 100 °C overnight. After reaching room temperature, the solvent was removed *in vacuo* and the residue washed with Et_2O (4 x 2 mL). Recrystallization of the product from CH_2Cl_2/Et_2O gave compound **13** as a yellow solid (103 mg, 66%).

^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.03 (d, *J* = 6.8 Hz, 6H), 1.12 (d, *J* = 4.3 Hz, 6H), 1.14 (d, *J* = 4.3 Hz, 6H), 1.25 (d, *J* = 6.8 Hz, 6H), 3.68 (sept, *J* = 6.6 Hz, 2H), 4.16 (sept, *J* = 6.9 Hz, 2H), 6.95-7.01 (m, 3H), 7.08-7.13 (m, 2H), 7.18-7.27 (m, 15H), 7.36-7.48 (m, 15H) ppm.

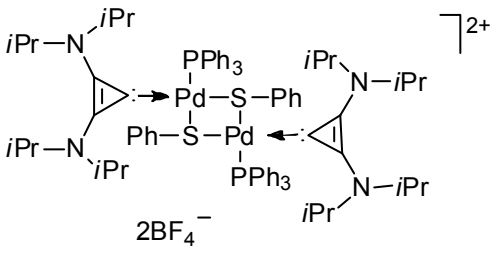
^{31}P NMR (162 MHz, CD_2Cl_2) δ = 14.4 (^{1}J(Pt-P) = 2910 Hz, ^{2}J(P-P) = 22.8 Hz), 18.2 (^{1}J(Pt-P) = 2345 Hz, ^{2}J(P-P) = 21.6 Hz) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 22.3, 22.4, 22.5, 22.8, 50.6, 51.4, 126.8, 128.2 (d, *J* = 10.5 Hz), 128.6, 128.9 (d, *J* = 10.3 Hz), 130.6 (d, *J* = 55.1 Hz), 131.2, 131.2, 131.8 (bs), 134.4 (bs), 135.6 (d, *J* = 10.1 Hz), 137.3, 144.3 ppm.

HRMS *calcd*. for $C_{57}H_{63}N_2P_2Pt_1Se_1^+$: 1112.329856; *found*: 1112.331737.

IR (neat) $\tilde{\nu}$ = 692, 742, 998, 1033, 1050, 1092, 1155, 1185, 1333, 1372, 1435, 1454, 1487, 1574, 1856, 2976, 3053 cm^{-1}.

Compound 14



A mixture of the compound **3** (48 mg, 0.11 mmol) and $Pd(PPh_3)_4$ (127 mg, 0.11 mmol) was evacuated for 10 minutes. Toluene (6 mL) was then added under Ar and the suspension was stirred at 100 °C overnight. After reaching room temperature, the solvent was removed *in vacuo* and the residue washed with Et_2O (4 x 2 mL). Recrystallization of the product from CH_2Cl_2/Et_2O gave compound **14** as a yellow solid (124 mg, 70%).

^{1}H NMR (400 MHz, CD_2Cl_2) δ = 0.98 (d, *J* = 6.8 Hz, 12H), 1.04 (d, *J* = 6.8 Hz, 12H), 1.13 (d, *J* = 6.6 Hz, 12H), 1.18 (d, *J* = 6.0 Hz, 12H), 3.70 (sept, *J* = 6.8 Hz, 4H), 3.97 (sept, *J* = 6.2 Hz, 4H), 6.88-6.98 (m, 4H), 7.09-7.13 (m, 2H), 7.17-7.31 (m, 28H), 7.44-7.50 (m, 6H) ppm.

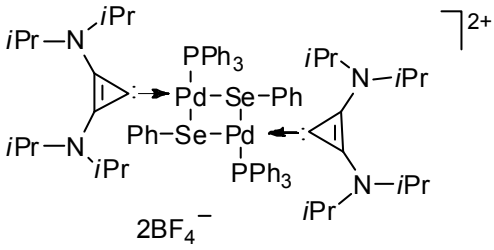
^{31}P NMR (162 MHz, CD_2Cl_2) δ = 25.8, 26.5 ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.7, 21.8, 22.3 (bs), 51.4 (bs), 128.3, 128.4, 128.7, 128.8, 129.1-129.4 (m), 132.3 (bs), 133.7, 134.2-134.5 (m), 146.8 ppm.

HRMS *calcd*. for $C_{78}H_{96}B_1F_4N_4P_2Pd_2S_2^+$: 1513.464329; *found*: 1513.468464.

IR (neat) $\tilde{\nu}$ = 691, 733, 740, 891, 998, 1032, 1049, 1092, 1140, 1153, 1184, 1322, 1349, 1366, 1436, 1454, 1480, 1498, 1577, 1852, 2935, 2973 cm^{-1}.

Compound 15



A mixture of the compound **4** (62 mg, 0.13 mmol) and $Pd(PPh_3)_4$ (150 mg, 0.13 mmol) was evacuated for 10 minutes. Toluene (6 mL) was then added under Ar and the suspension was stirred at 100 °C overnight. After reaching room temperature, the solvent was removed *in vacuo* and the residue washed with Et_2O (4 x 2 mL). Recrystallization of the product from CH_2Cl_2/Et_2O gave compound **15** as a yellow solid (150 mg, 68%).

^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.00 (d, *J* = 6.7 Hz, 12H), 1.07 (d, *J* = 6.8 Hz, 12H), 1.10 (d, *J* = 6.6 Hz, 12H), 1.17 (d, *J* = 6.0 Hz, 12H), 3.70 (sept, *J* = 6.8 Hz, 4H), 3.97 (sept, *J* = 6.8 Hz, 4H), 7.01-7.11 (m, 6H), 7.20-7.30 (m, 28H), 7.45-7.52 (m, 6H) ppm.

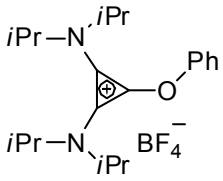
^{31}P NMR (162 MHz, CD_2Cl_2) δ = 23.4, 23.8 ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.8, 21.9, 22.4, 22.5, 50.9, 51.3, 127.8, 128.6, 128.9, 129.0, 129.1, 129.2-129.5 (m), 129.6, 132.3 (bs), 134.2-134.5 (m), 134.8 (bs), 147.4 ppm.

HRMS *calcd*. for $C_{78}H_{96}B_1F_4N_4P_2Pd_2Se_2^+$: 1609.359955; *found*: 1609.357749.

IR (neat) $\tilde{\nu}$ = 691, 738, 998, 1032, 1049, 1093, 1155, 1184, 1326, 1344, 1372, 1435, 1453, 1495, 1574, 1851, 2935, 2974 cm^{-1}.

Compound 16



Sodium phenoxide (356 mg, 3.07 mmol) was added to a stirred suspension of chlorocyclopropenium salt **1** (1 g, 2.79 mmol) in dry THF (21 mL) and the resulting mixture was heated at 60 °C overnight. After cooling to room temperature, the solvent was evaporated and the solid washed with 3 x 4 mL Et_2O. The residue was dissolved in CH_2Cl_2 (10 mL) and the NaCl was filtered off. Recrystallization of the dried filtrate from CH_2Cl_2/Et_2O gave the desired compound as white solid (120 mg, 28%).

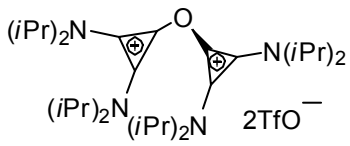
^{1}H NMR (400 MHz, CD_2Cl_2) δ = 1.26 (bs, 24H), 3.76 (bs, 4H), 7.27-7.31 (m, 2H), 7.32-7.38 (m, 1H), 7.47-7.53 (m, 2H) ppm.

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.6, 116.3, 119.3, 122.6, 127.5, 131.1, 154.7 ppm. Even after long acquisition time, the CH(iPr) signal was not observed.

HRMS *calcd.* for $C_{21}H_{33}N_2O_1^+$: 329.258741; *found* 329.258611.

IR (neat) $\tilde{\nu}$ = 691, 762, 875, 1023, 1033, 1045, 1089, 1143, 1161, 1188, 1211, 1349, 1378, 1454, 1575, 2986 cm^{-1}.

Compound 17



This compound was prepared following the procedure already described for the dimethylamino substituted analogue.[6] Triflic anhydride (65 µL, 0.39 mmol) was added dropwise to a cooled solution (0 °C) of 2,3-bis(diisopropylamino)cyclopropenone (200 mg, 0.79 mmol) in CH_2Cl_2 (2.5 mL) and the mixture was stirred at room temperature for 1h. Upon addition of Et_2O (15 mL) to the reaction mixture a white solid precipitated. After filtration, the desired product was obtained (280 mg, 90%).

^{1}H NMR (300 MHz, CD_2Cl_2) δ = 1.35 (d, *J* = 6.7 Hz, 24H), 1.40 (d, *J* = 6.7 Hz, 24H), 3.85 (sept, *J* = 6.6 Hz, 4H), 4.15 ppm (sept, *J* = 6.6 Hz, 4H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.2, 22.4, 50.9, 56.0, 110.1, 121.4 (q, *J* = 321.3 Hz), 125.5 ppm.

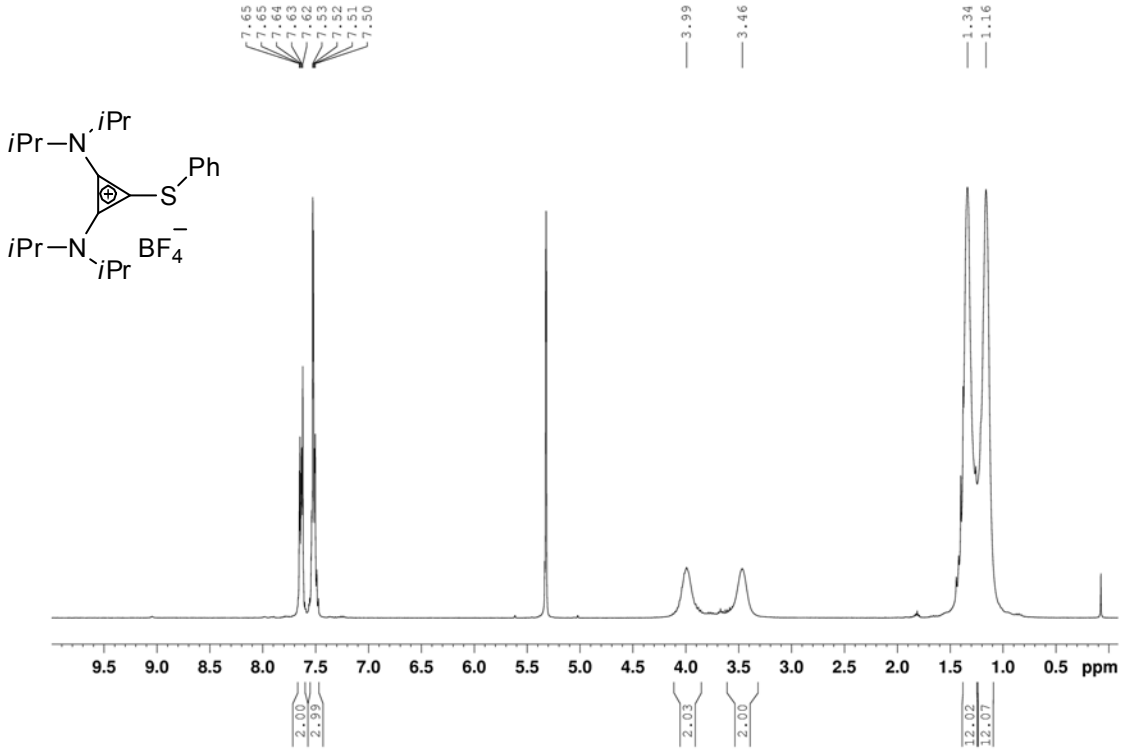
HRMS *calcd*. for $C_{31}H_{56}N_4O_4F_3S_1^+$: 637.396886; *found*: 637.397130.

IR (neat) $\tilde{\nu}$ = 752, 880, 1022, 1046, 1090, 1129, 1154, 1194, 1218, 1334, 1360, 1387, 1455, 1480, 2877, 2937, 2979 cm^{-1}.

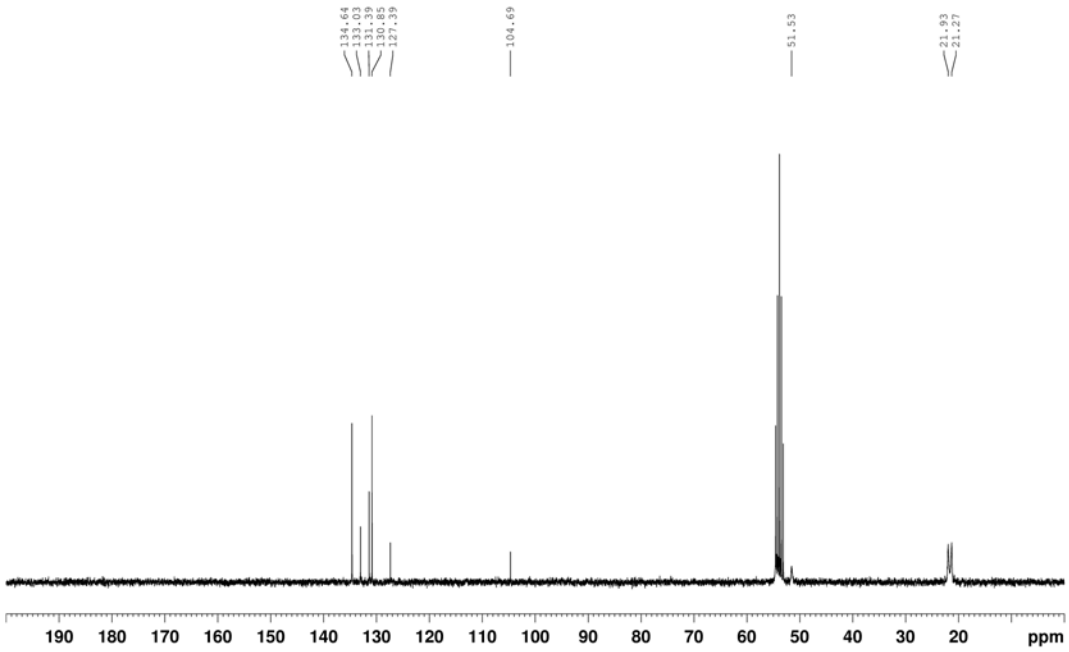
[6] G. Maas, P. J. Stang, *J. Org. Chem.* 1983, **48**, 3038.

Selected NMR spectra

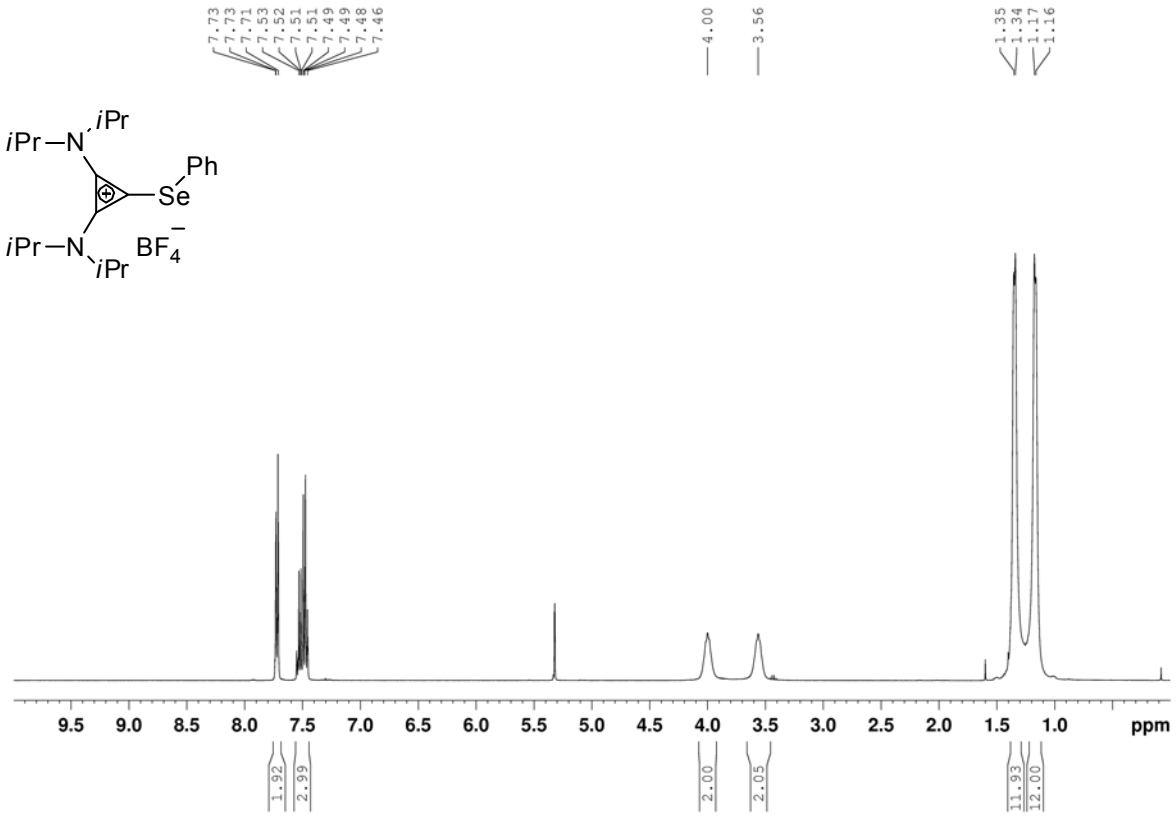
^{1}H NMR (400 MHz, CD_2Cl_2) **3**



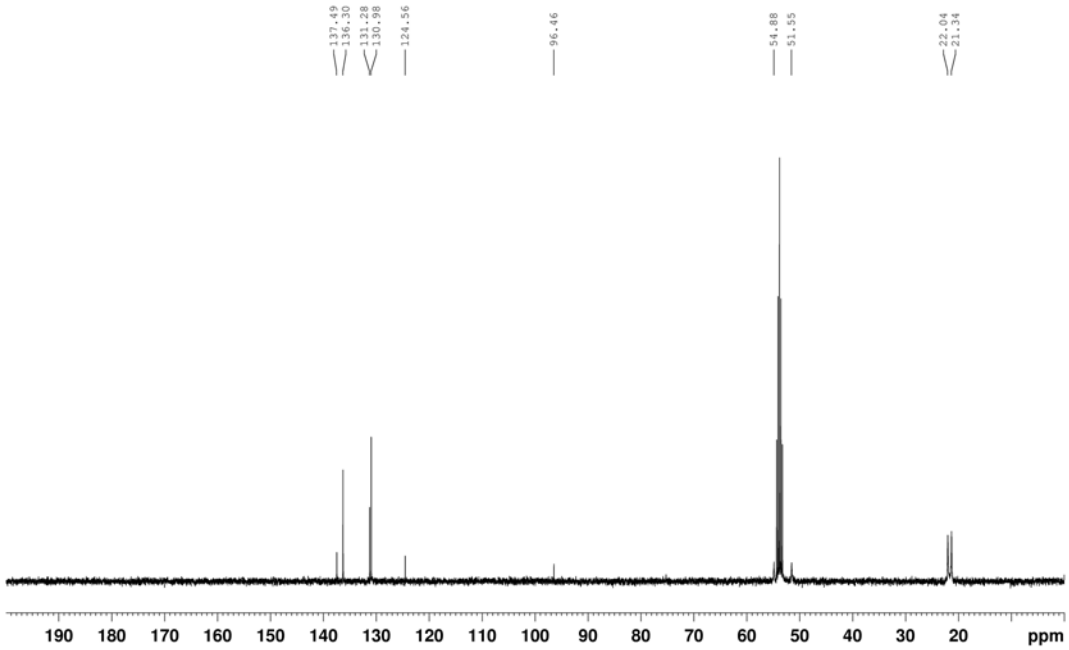
^{13}C NMR (101 MHz, CD_2Cl_2) **3**



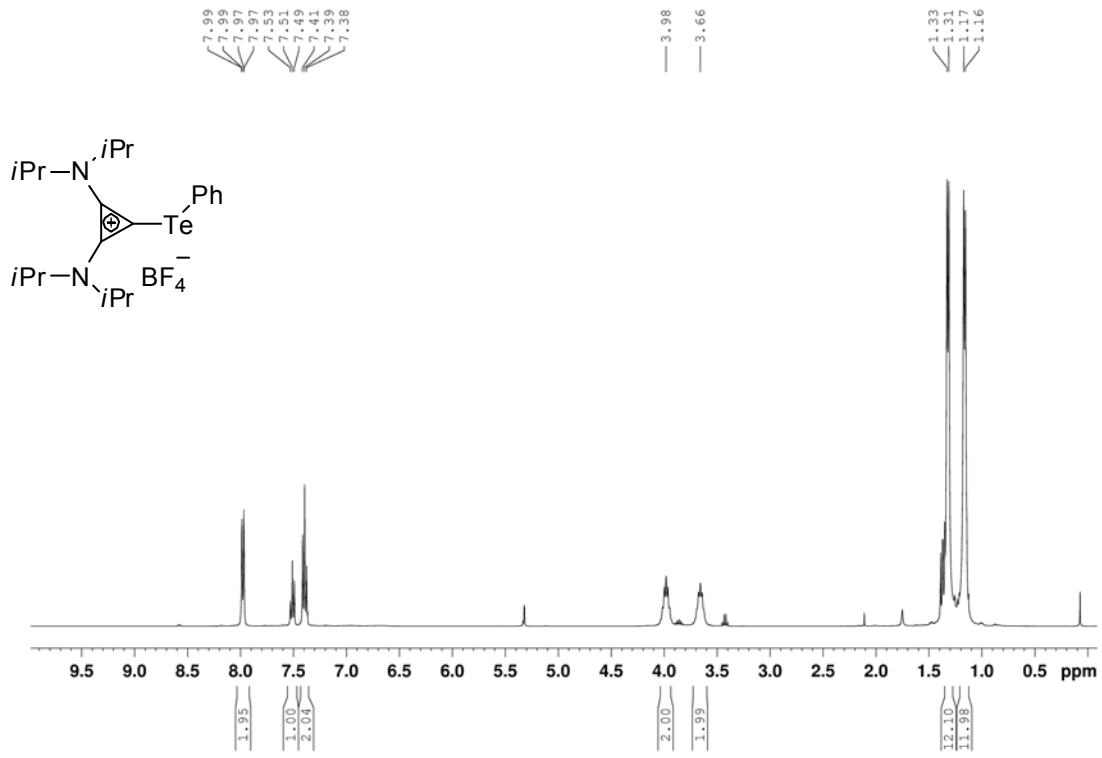
^{1}H NMR (400 MHz, CD_2Cl_2) **4**



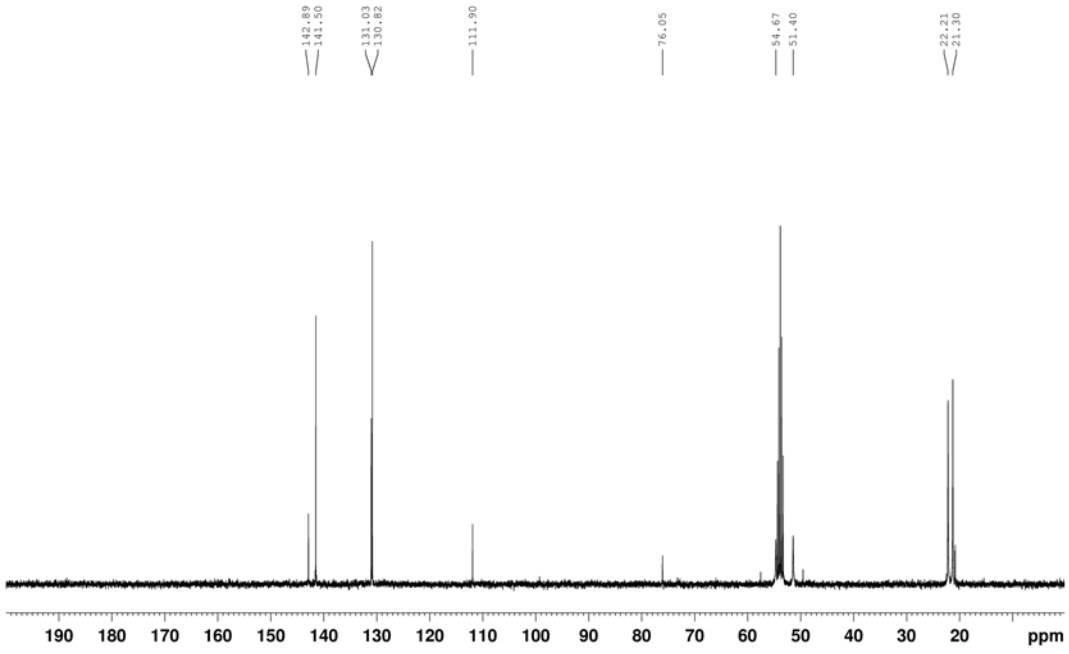
^{13}C NMR (101 MHz, CD_2Cl_2) **4**



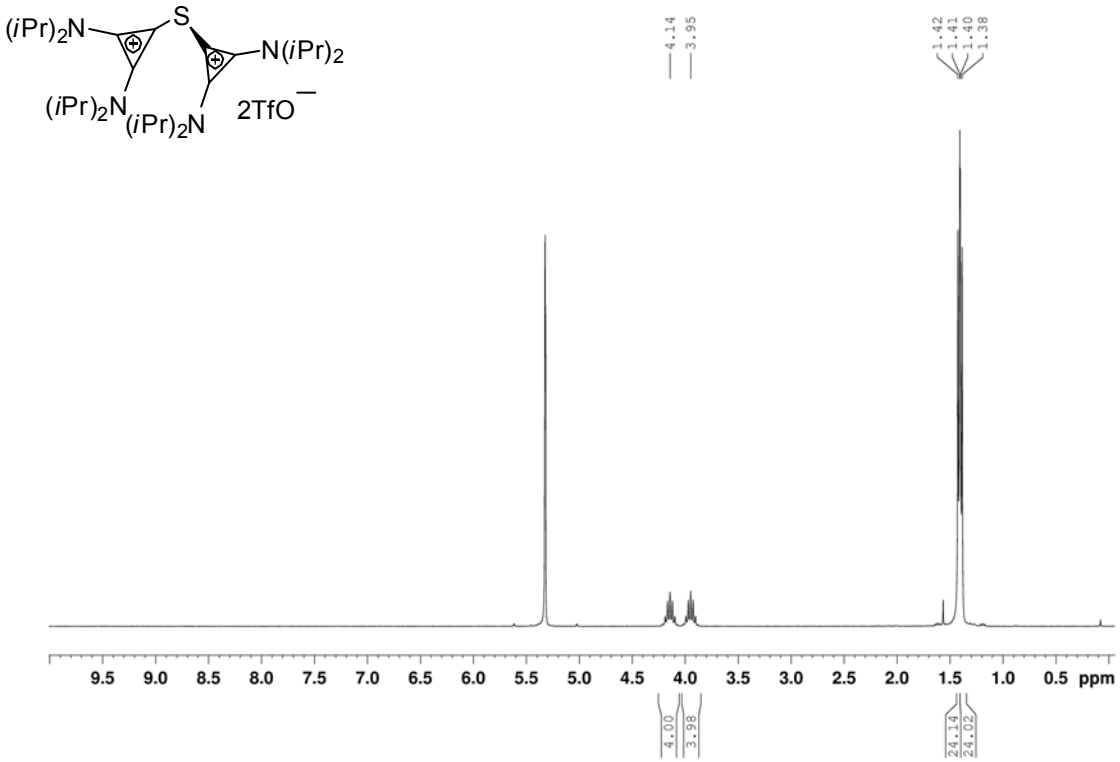
^{1}H NMR (400 MHz, CD_2Cl_2) **5**



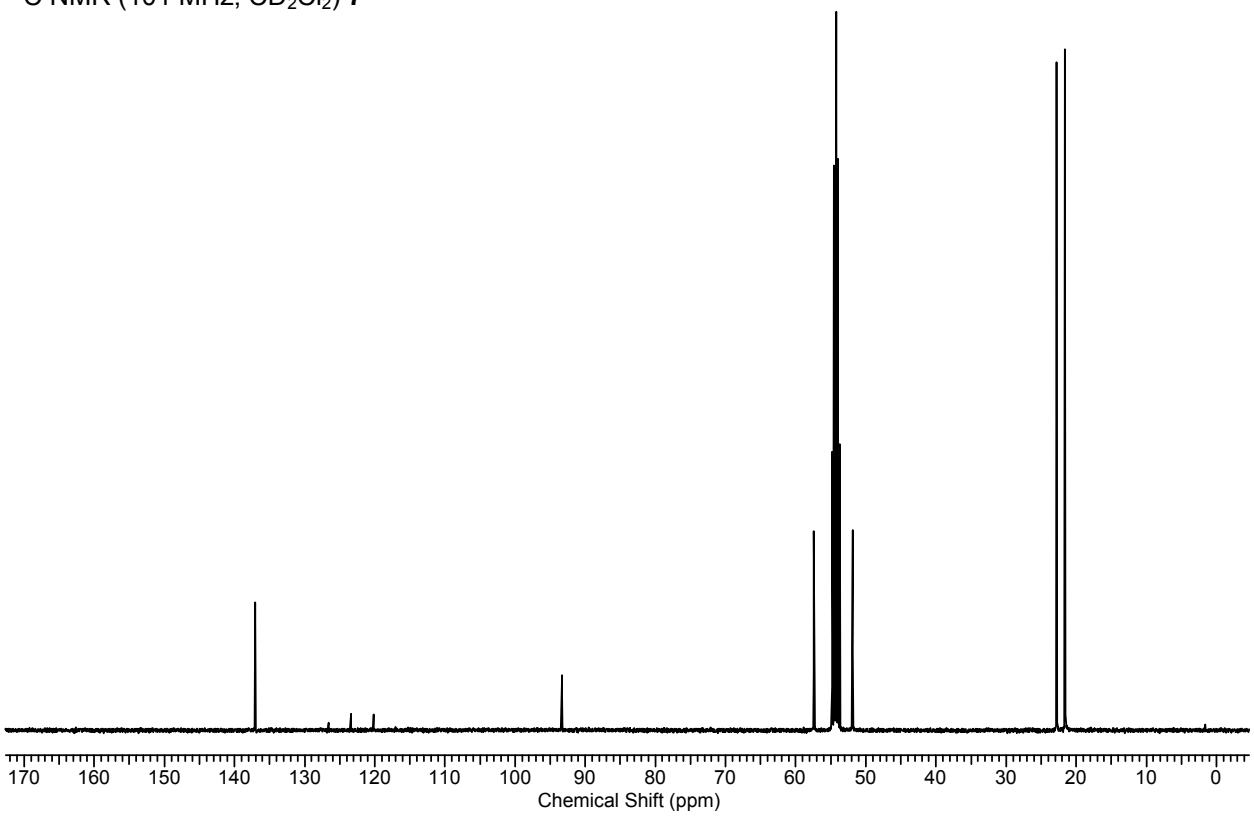
^{13}C NMR (101 MHz, CD_2Cl_2) **5**



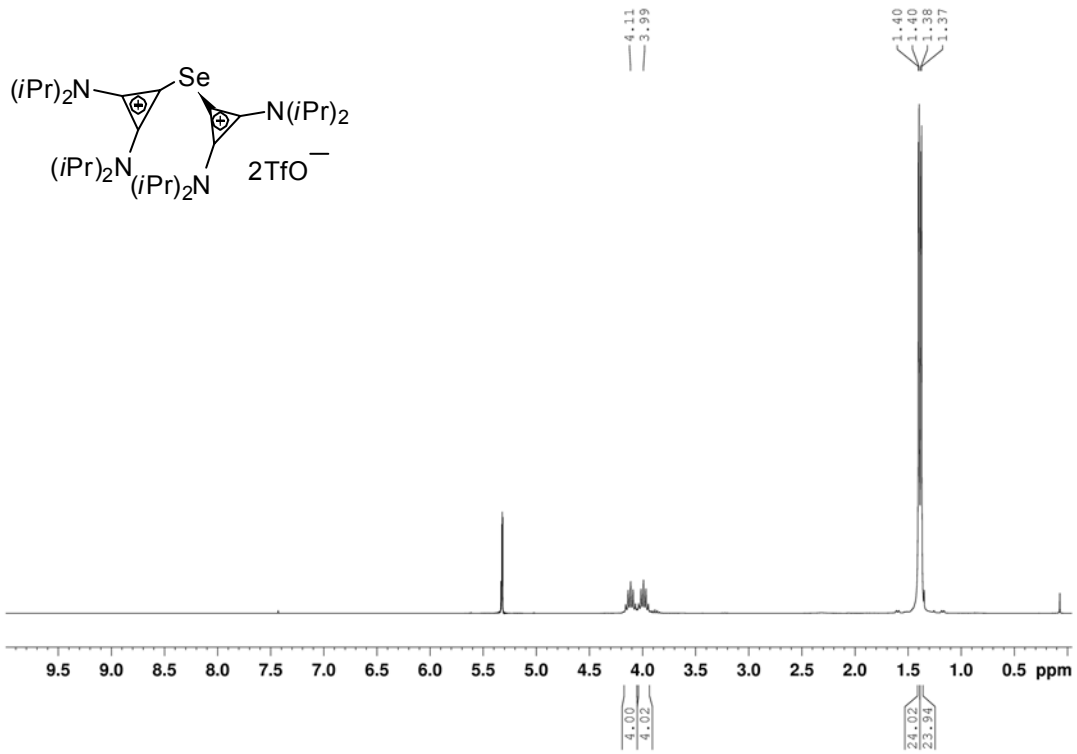
^{1}H NMR (300 MHz, CD_2Cl_2) **7**



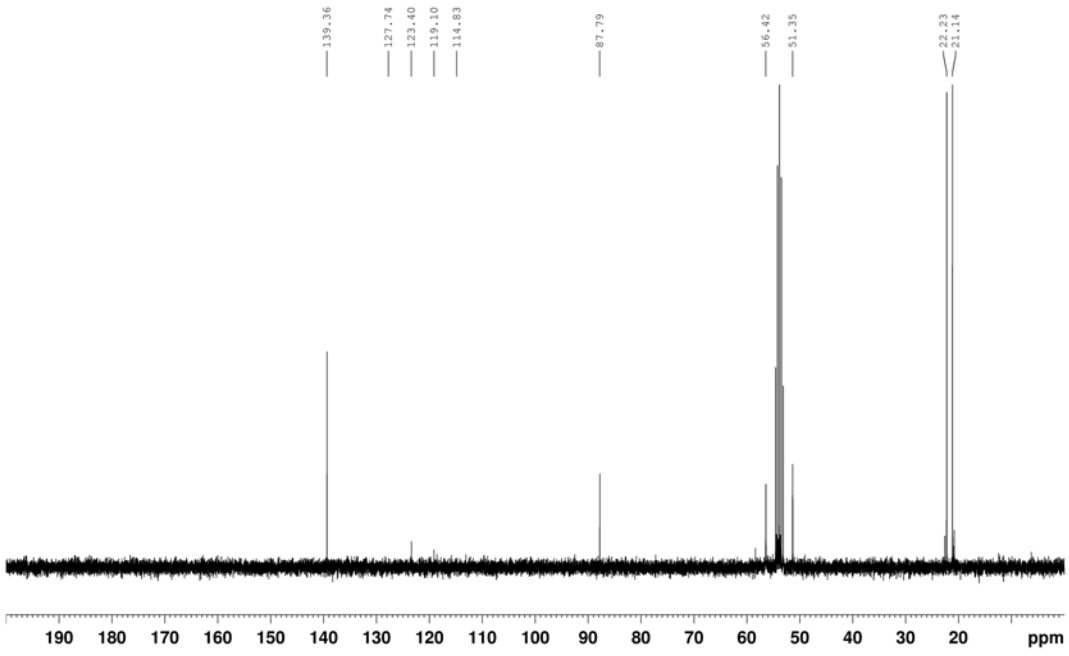
^{13}C NMR (101 MHz, CD_2Cl_2) **7**



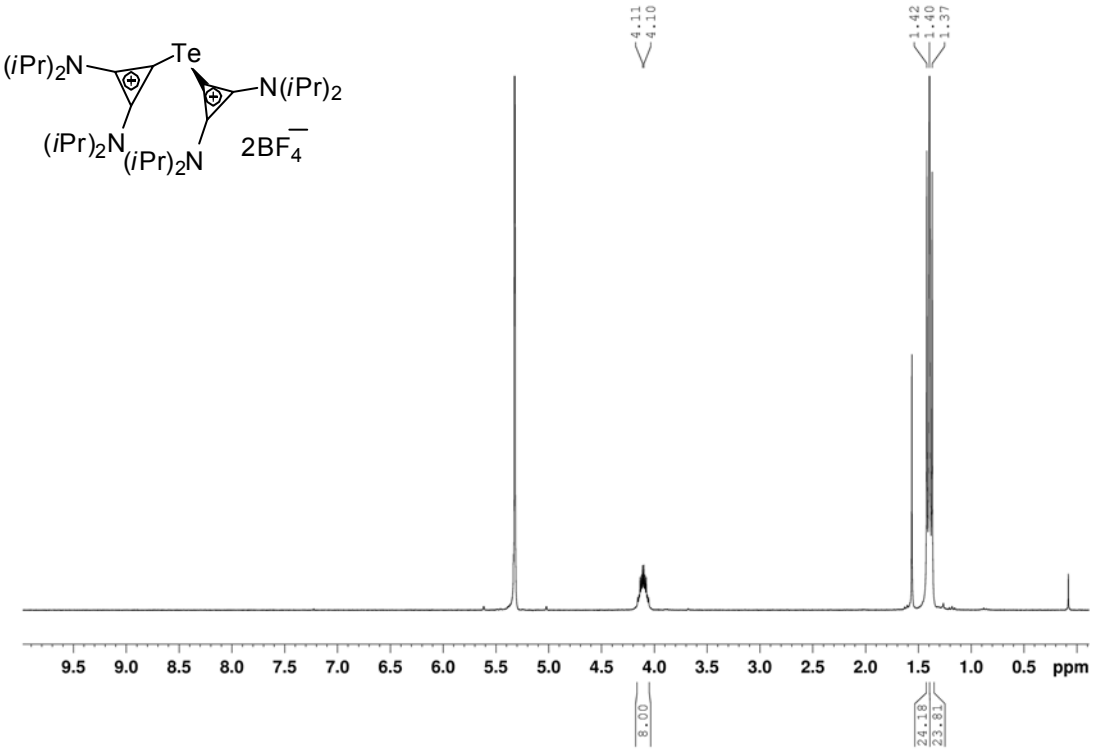
^{1}H NMR (300 MHz, CD_2Cl_2) **9**



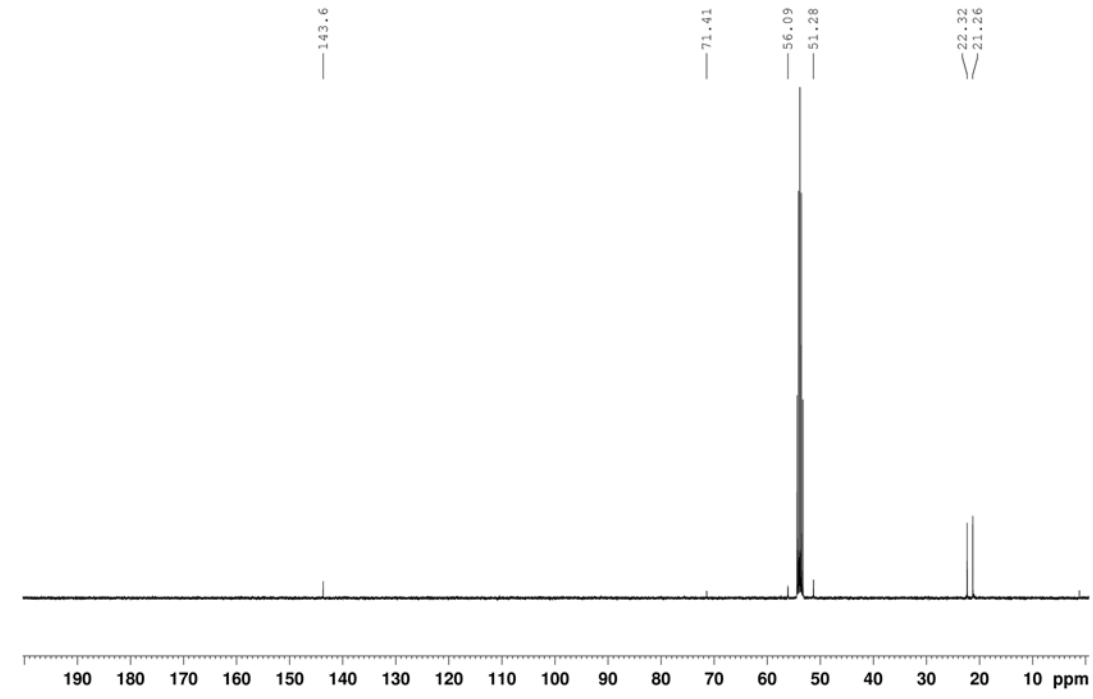
^{13}C NMR (75 MHz, CD_2Cl_2) **9**



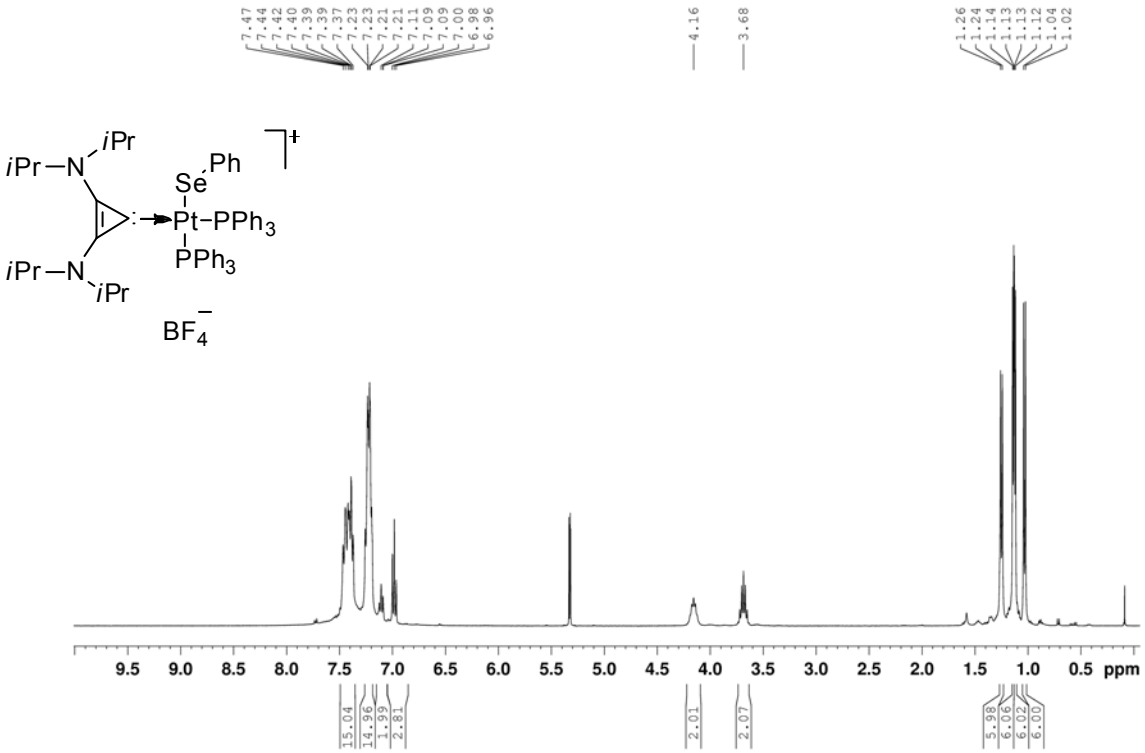
^{1}H NMR (300 MHz, CD_2Cl_2) **10**



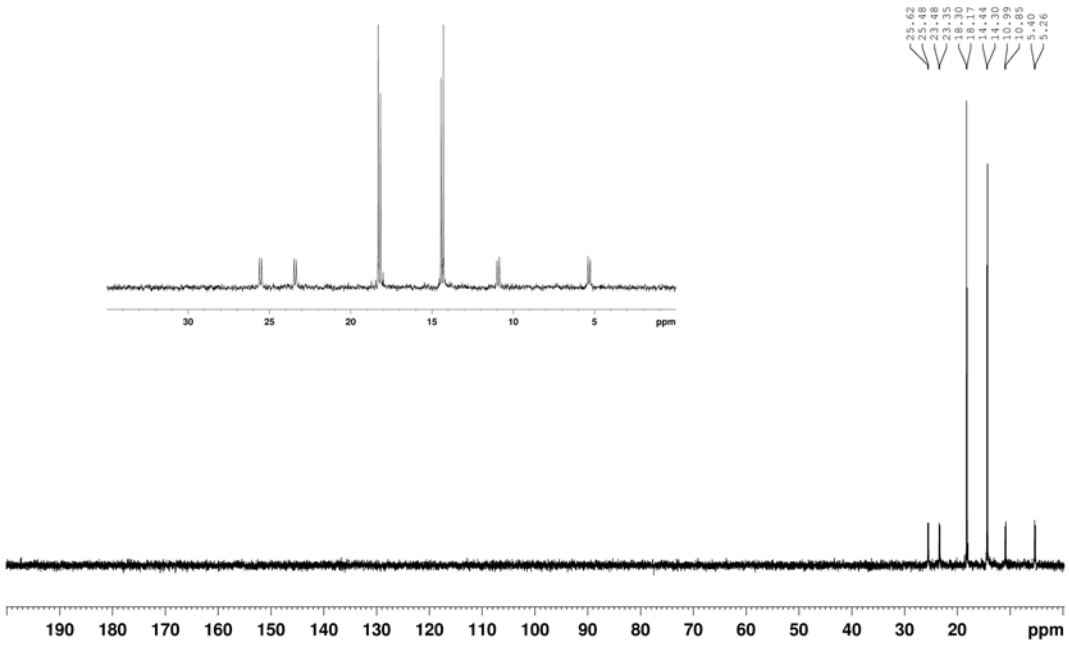
^{13}C NMR (75 MHz, CD_2Cl_2) **10**



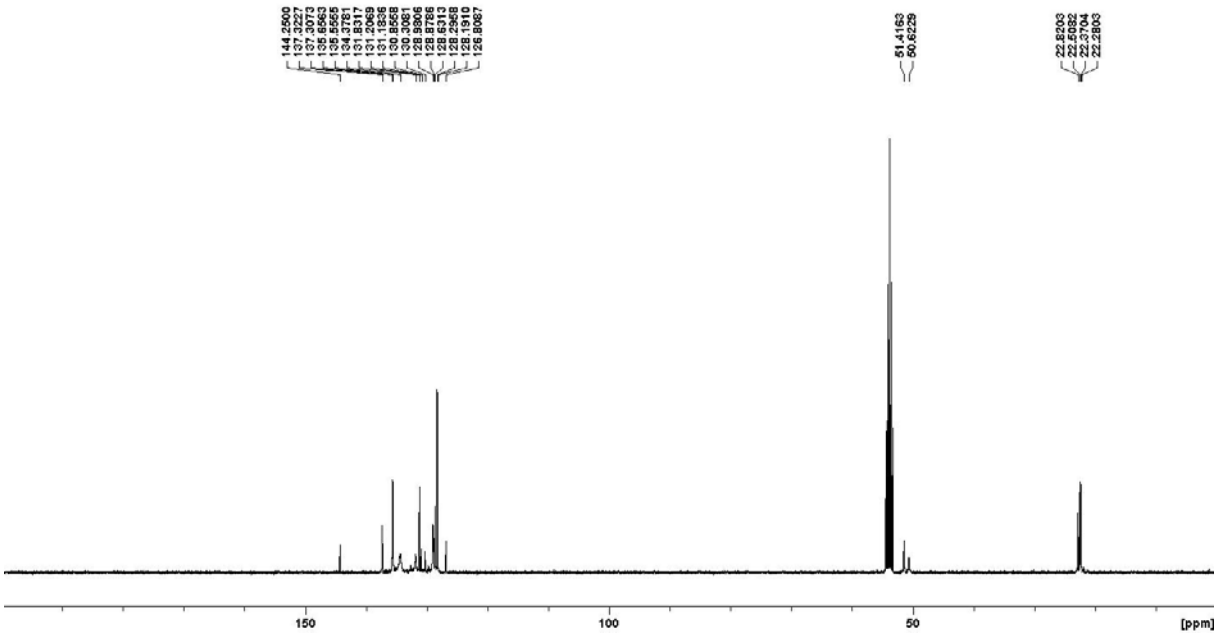
^{1}H NMR (400 MHz, CD_2Cl_2) **13**



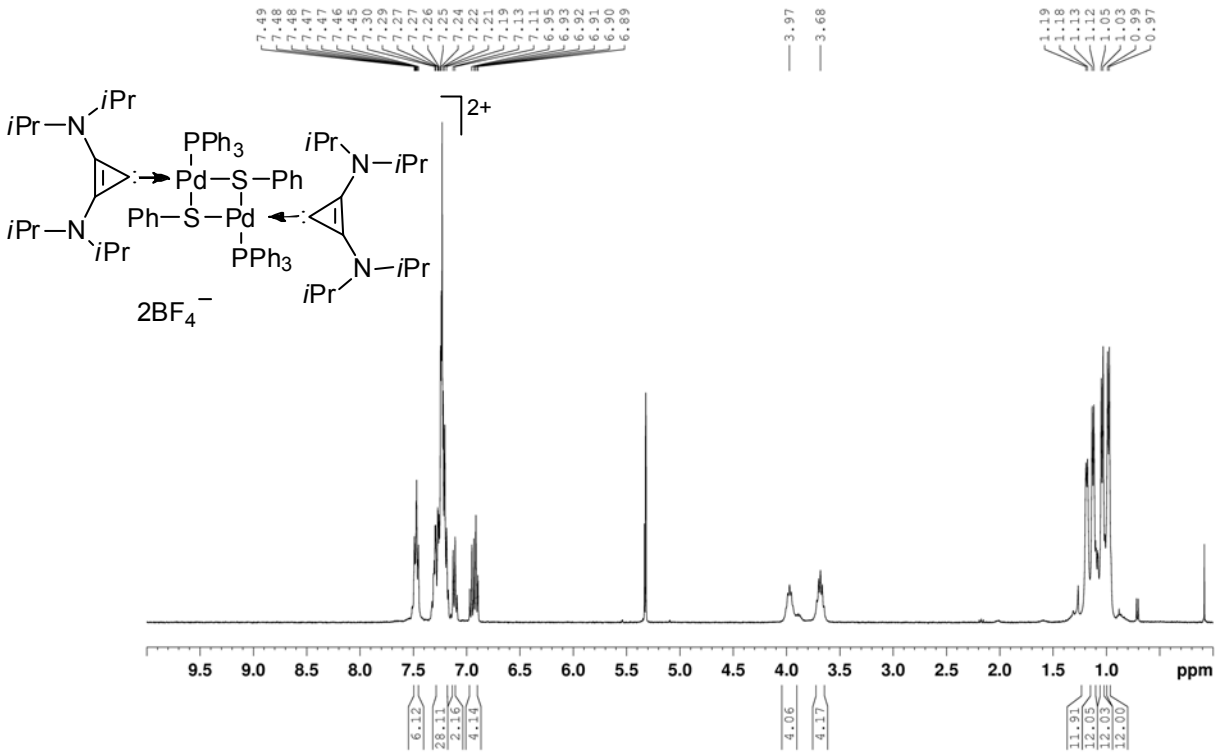
^{31}P NMR (162 MHz, CD_2Cl_2)**13**



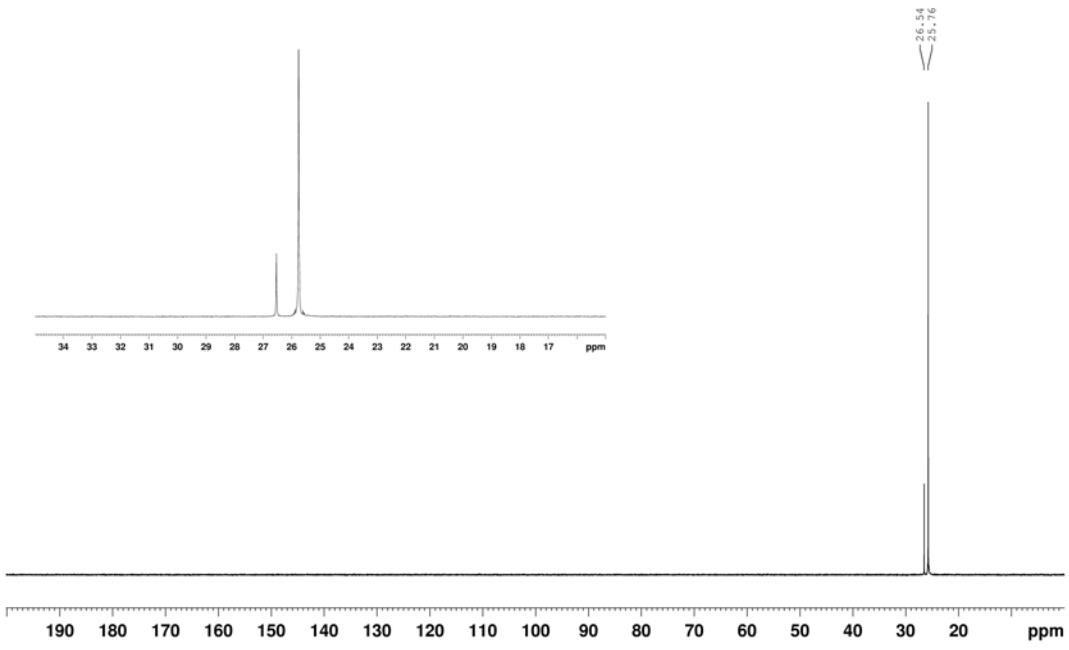
^{13}C NMR (100 MHz, CD_2Cl_2) **13**



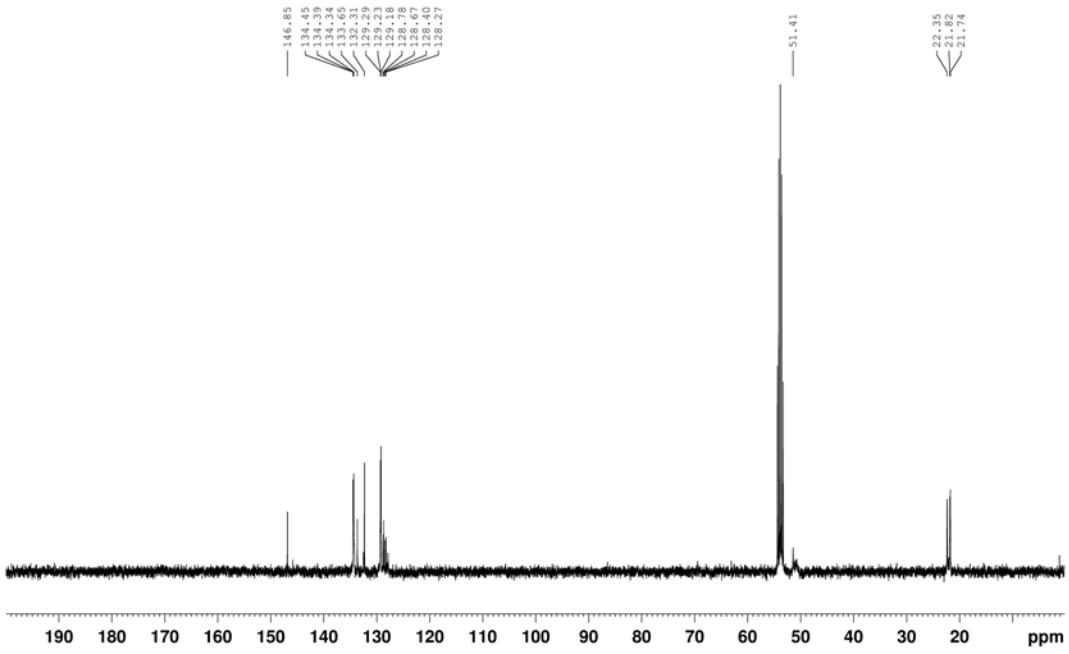
^{1}H NMR (400 MHz, CD_2Cl_2) **14**



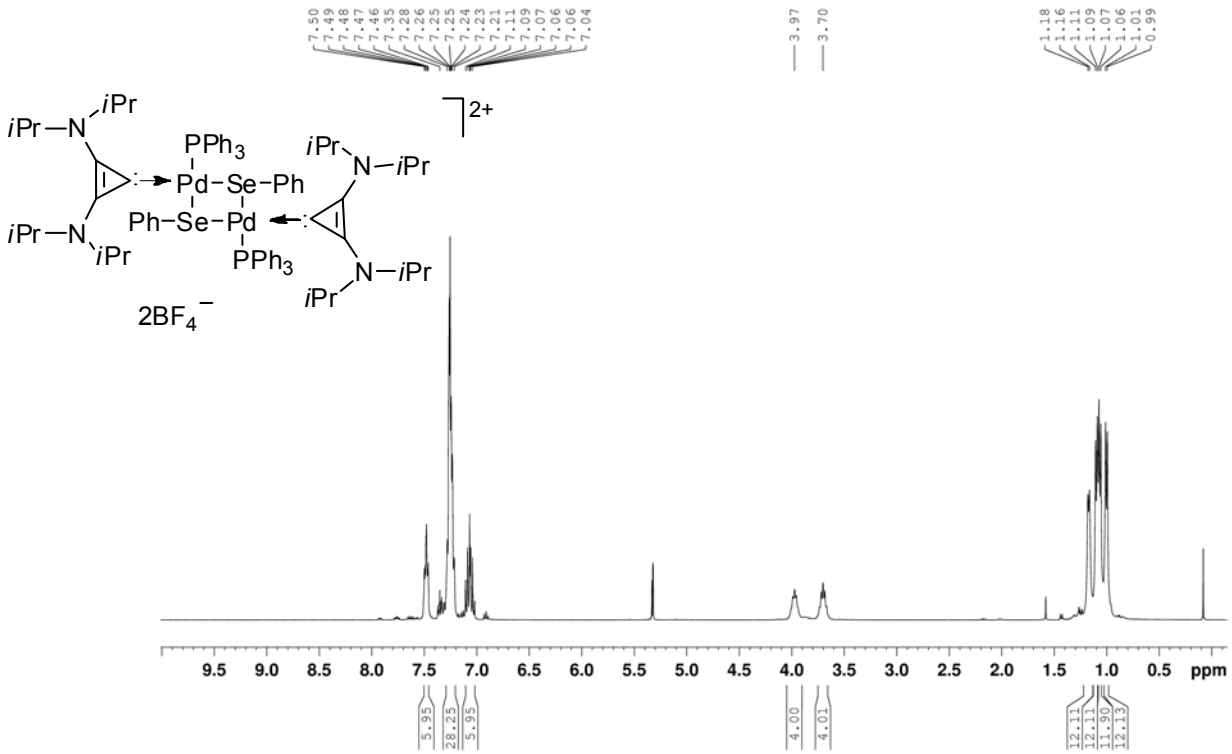
^{31}P NMR (162 MHz, CD_2Cl_2) **14**



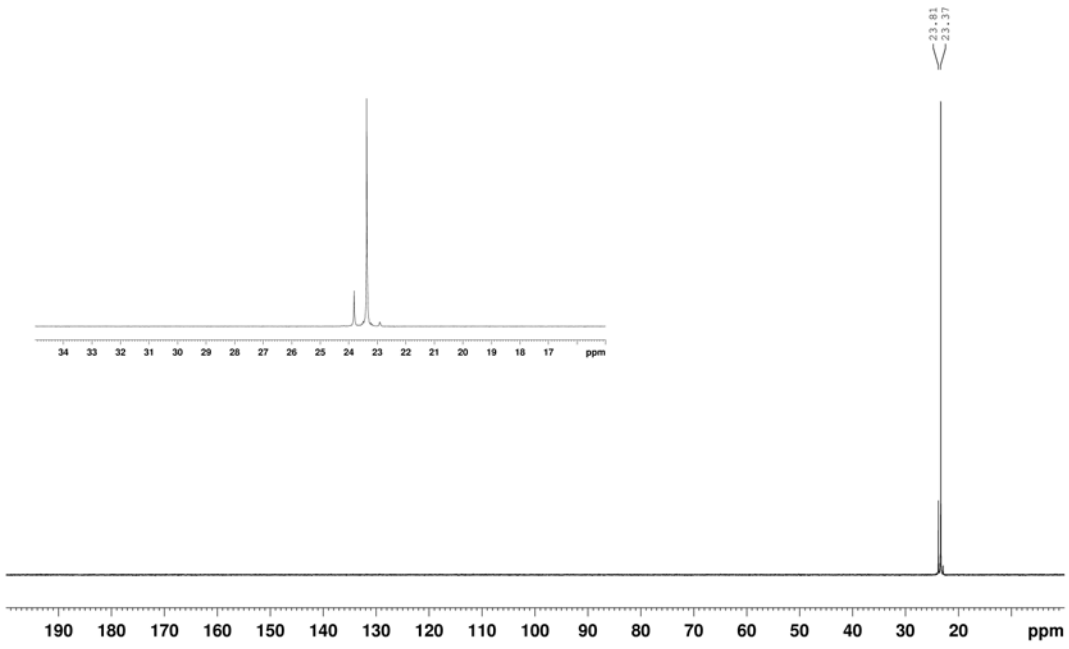
^{13}C NMR (100 MHz, CD_2Cl_2) **14**



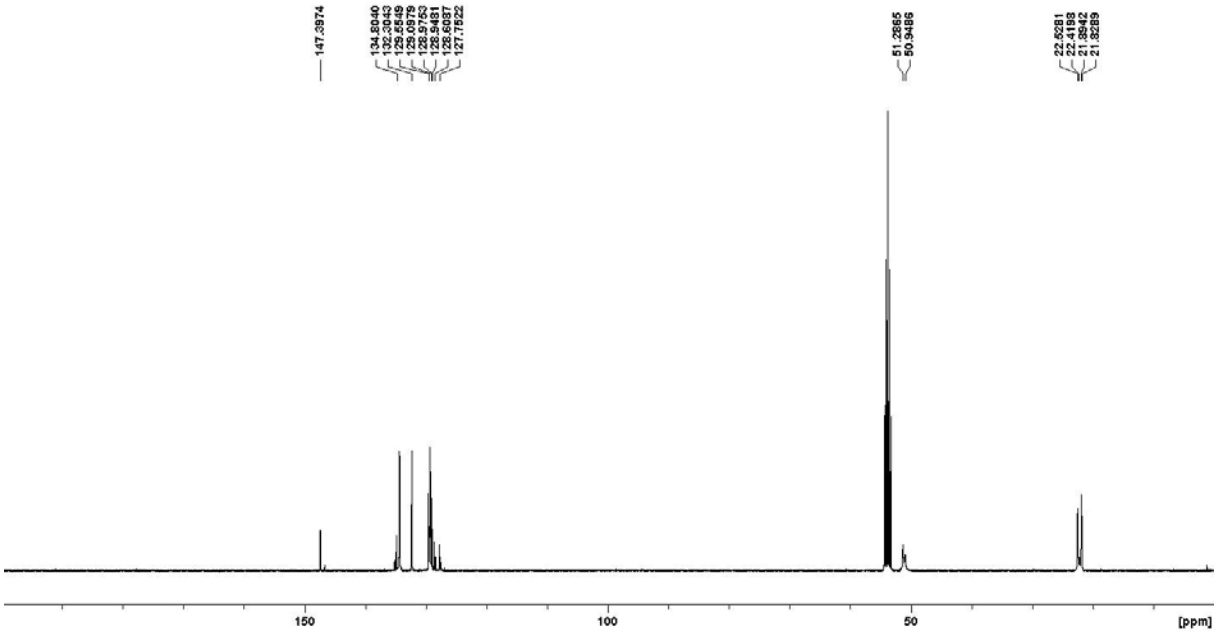
^{1}H NMR (400 MHz, CD_2Cl_2) **15**



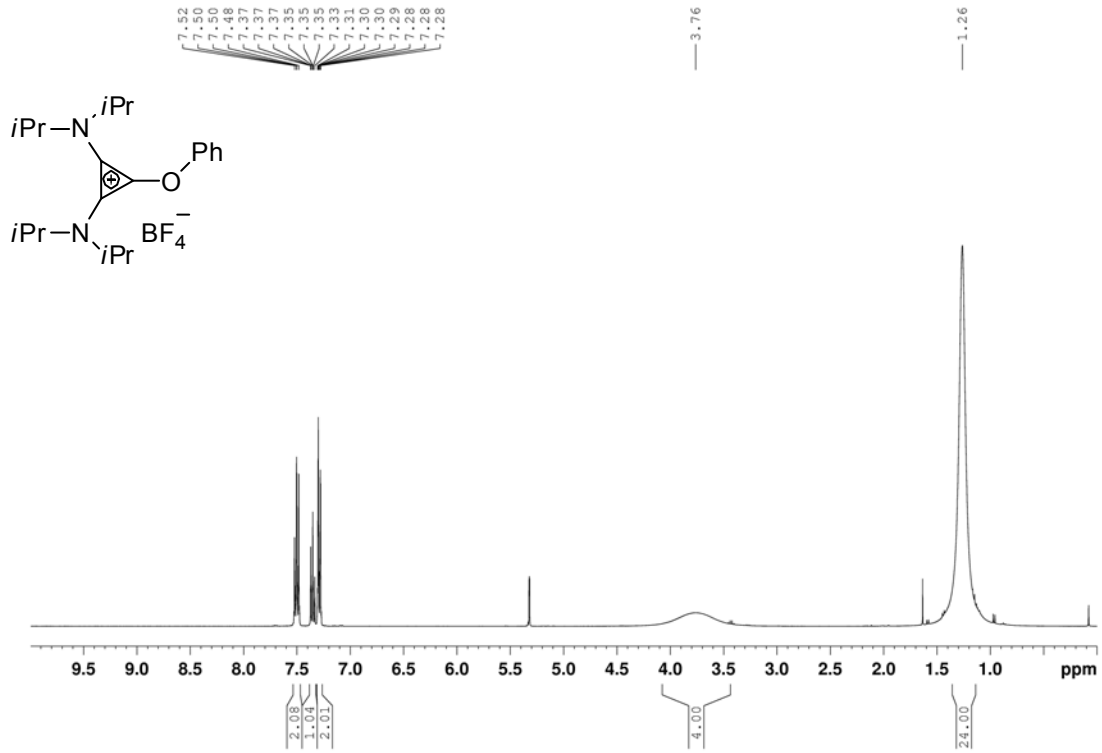
^{31}P NMR (162 MHz, CD_2Cl_2)**15**



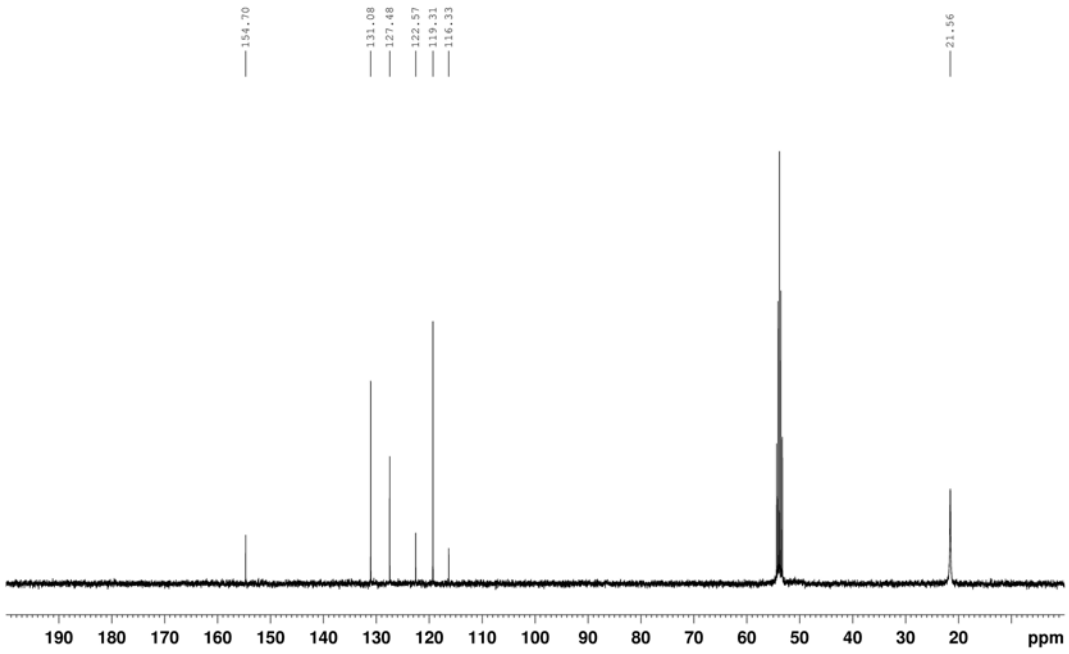
^{13}C NMR (100 MHz, CD_2Cl_2) **15**



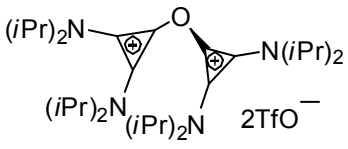
^{1}H NMR (400 MHz, CD_2Cl_2) **16**



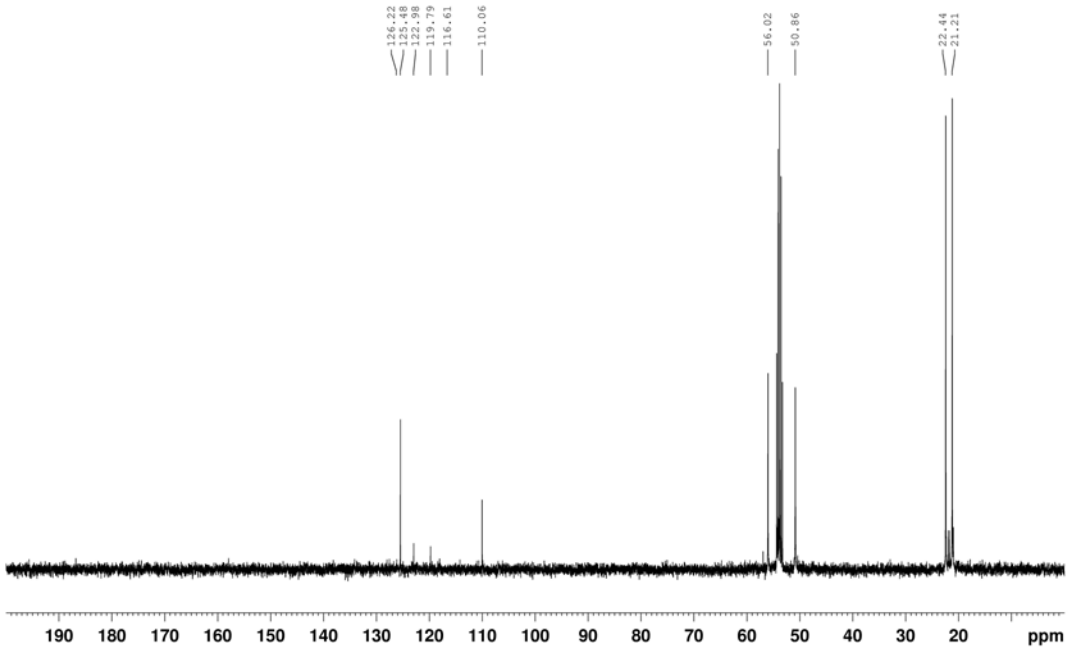
^{13}C NMR (101 MHz, CD_2Cl_2)



^{1}H NMR (300 MHz, CD_2Cl_2) **17**

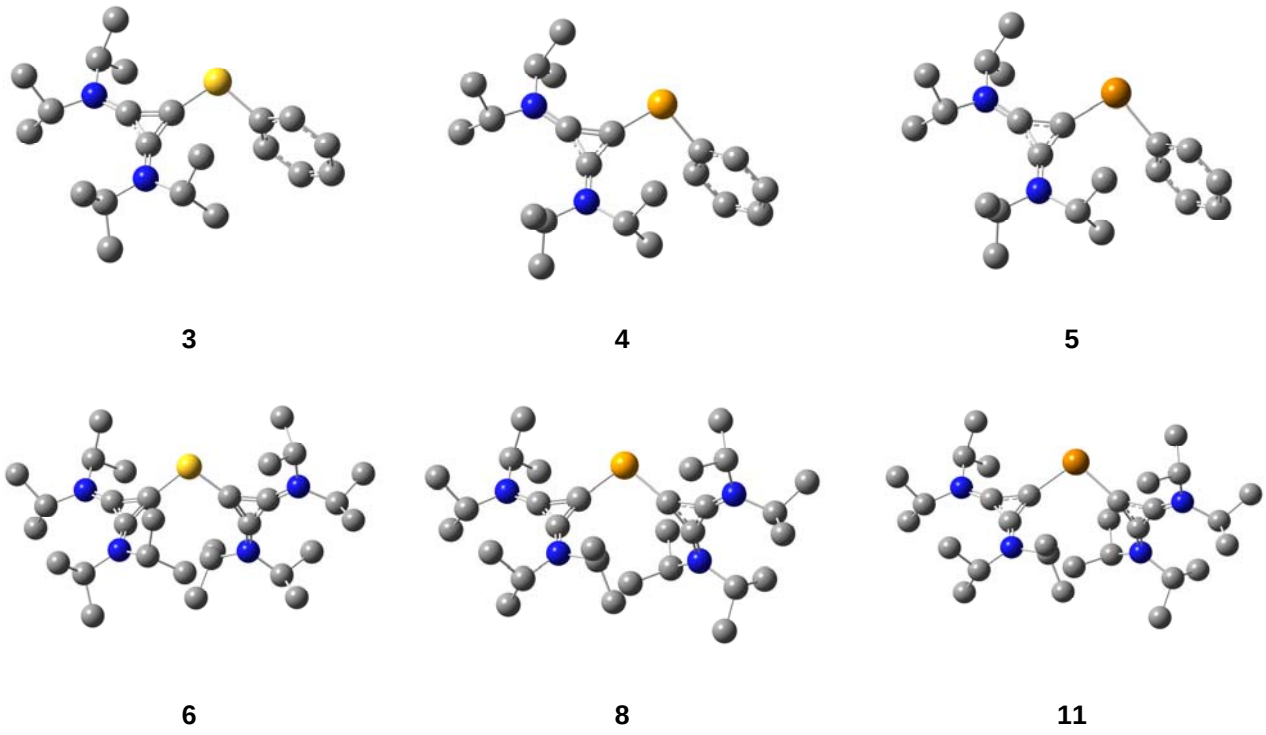


^{13}C NMR (100 MHz, CD_2Cl_2) **17**



Computational methods

Quantum-chemical calculations were carried out using the Gaussian 09 package.[7] Geometry optimizations were performed at the hybrid DFT B3LYP level.[8,9] The chalcogen centre in the compounds **3-6**, **8** and **11** was described with the LANL2DZ basis set,[10] while the 6-31G* basis set has been used for C, N and H atoms. Molecular orbital analyses were carried out using the NBO program[11] for natural bond order and charge analysis.



3 **4** **5**

6 **8** **11**

Figure S1. Optimized structures of compounds **3-6**, **8** and **11**. Hydrogen atoms are omitted for clarity.

[7]Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

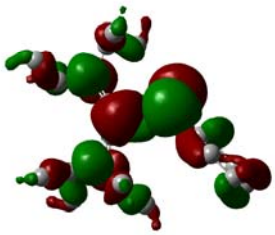
[8](a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785. (b) A. D. Becke, *Phys. Rev. A* 1988, **38**, 3098. (c) A. D. Becke, *J. Chem. Phys.* 1993, **98,** 1372. (d) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648.

[9](a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* 1971, **54**, 724. (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys*. 1972, **56**, 2257. (c) P. C. Hariharan, J. Pople, *Theor. Chim. Acta*. 1973, **28**, 213.

[10](a) P. J. Hay, W. R. Wadt, *J. Chem. Phys*. 1985, **82**, 270. (b) W. R. Wadt, P. J. Hay, *J. Chem. Phys*. 1985, **82**, 284. (c) P. J. Hay, W. R. Wadt, *J. Chem. Phys*. 1985, **82**, 299.

[11] NBO Version 3.1, E. D. Glendening, A. E. Reed, J. E. Carpenter, and F. Weinhold.

3



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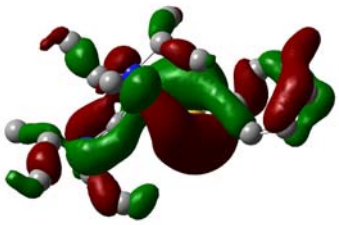
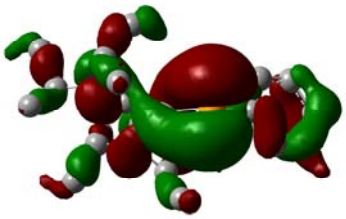


HOMO-3

4

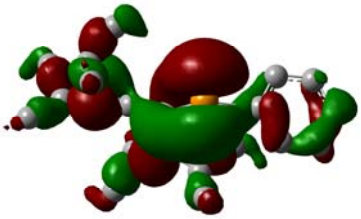
HOMO



HOMO-3

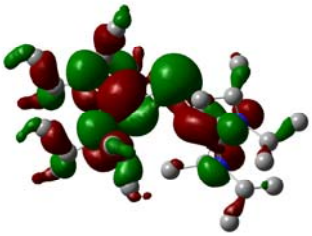
5

HOMO

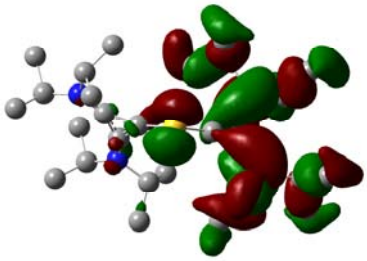


HOMO-3

6

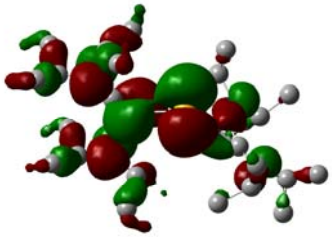


HOMO

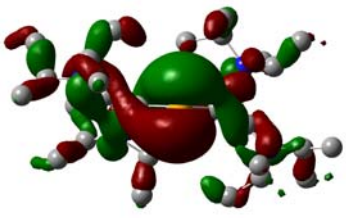


HOMO-3

8

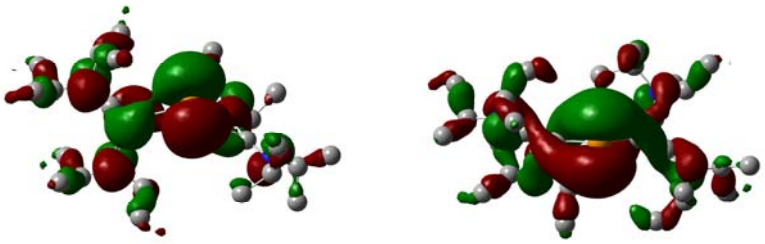


HOMO



HOMO-2

11



HOMO HOMO-2

Figure S2. Highest occupied molecular orbitals of **3-6**, **8** and **11**. Hydrogen atoms are omitted for clarity.

Table S1. Selected bond lengths (Å) and angles (°) in the experimental and theoretical structures of compounds **3-5**.

Compound	Ch–C(cyclopropyl)	C –C(phenyl)	C(cyclopropyl)–Ch–C(phenyl)
3 experiment	1.73	1.78	103
3 calculation	1.78	1.85	105
4 experiment	1.88	1.93	99
4 calculation	1.92	1.97	102
5 experiment	2.07	2.12	95
5 calculation	2.10	2.14	101

Table S2. Selected bond lengths (Å) and angles (°) in the experimental and theoretical structures of compounds **6, 8 and 11**.

Compound	Ch–C(cyclopropyl1)	Ch–C(cyclopropyl2)	C(cyclopropyl1)–Ch –C(cyclopropyl2)
6 experiment	1.73	1.74	100
6 calculation	1.80	1.80	105
8 experiment	1.88	1.88	97
8 calculation	1.92	1.92	103
11 experiment	2.08	2.09	95
11 calculation	2.10	2.10	100

Table S3. Representative natural bond orders and natural charge (*e*) on the chalcogen atom in compounds **3-5**.

Compound	Ch–C(cyclopropyl)	Ch –C(phenyl)	Natural charge
3	1.039	1.016	0.39
4	0.979	0.980	0.52
5	0.884	0.932	0.72

Table S4. Representative natural bond orders and natural charge (*e*) on the chalcogen atom in compounds **6**, **8** and **11**.

Compound	Ch–C(cyclopropyl1)	Ch –C(cyclopropyl2)	Natural charge
6	1.041	1.016	0.47
8	0.967	0.987	0.61
11	0.890	0.891	0.83

Table S15. The optimized geometries (Cartesian coordinates in Å) and energies (a.u.) of compounds **3-6**, **8** and **11**.

Compound **3** E = -939.44323884 Nimag = 0				Compound **4** E = -938.56348598 Nimag = 0			
16	1.676781	-0.475723	-1.524079	34	1.691346	-0.460885	-1.503335
7	-1.073529	1.997917	0.002251	7	-1.882293	-1.646538	0.138066
7	-1.739714	-1.640825	0.141070	7	-1.255658	1.994559	0.026520
6	0.237145	-0.152155	-0.612163	6	0.068808	-0.132719	-0.617522
6	-0.699426	0.763024	-0.184316	6	-1.120090	-0.631704	-0.138573
6	-0.956041	-0.636269	-0.127293	6	-0.876635	0.771831	-0.181001
6	-2.450916	2.323975	0.437844	6	-1.384025	-3.022407	-0.137254
1	-2.906139	1.479529	0.636337	1	-2.090503	-3.652185	0.114286
6	-2.436108	3.150286	1.718209	6	-1.102424	-3.207809	-1.619322
1	-1.924489	2.691799	2.388815	1	-0.370695	-2.642861	-1.879304
1	-3.335454	3.272370	2.030110	1	-1.883151	-2.974322	-2.126006
1	-2.039050	4.006668	1.541397	1	-0.873221	-4.124275	-1.789303
6	-3.207659	2.997784	-0.714346	6	-0.166223	-3.320899	0.722779
1	-2.829752	3.864110	-0.881402	1	-0.380452	-3.164972	1.645890
1	-4.133874	3.092073	-0.477194	1	0.557959	-2.74772	0.462906
1	-3.133968	2.458241	-1.504390	1	0.092097	-4.237388	0.603655
6	-0.136168	3.111013	-0.331869	6	-3.259422	-1.469253	0.677645
1	-0.606764	3.953687	-0.163122	1	-3.421184	-0.505341	0.754837
6	1.076205	3.074399	0.581360	6	-4.296367	-2.029831	-0.289384
1	0.787067	3.027811	1.495846	1	-4.216101	-2.985758	-0.325947
1	1.598686	3.868840	0.451556	1	-4.149869	-1.661716	-1.163929
1	1.609456	2.303808	0.374573	1	-5.176696	-1.793714	0.012771
6	0.240602	3.083025	-1.804464	6	-3.371607	-2.060107	2.070318
1	0.691753	2.259235	-2.003629	1	-2.645007	-1.743714	2.611833
1	0.821548	3.822239	-2.000799	1	-3.335488	-3.017458	2.015271
1	-0.553601	3.149264	-2.339470	1	-4.204699	-1.792758	2.464744
6	-1.277493	-3.020951	-0.164779	6	-2.596176	2.312651	0.594350
1	-2.008414	-3.637204	0.052747	1	-2.983626	1.477443	0.929211
6	-0.966108	-3.170315	-1.646080	6	-2.468314	3.263119	1.770637
1	-1.697174	-2.825986	-2.162909	1	-2.190812	4.126659	1.455885
1	-0.837884	-4.098016	-1.853585	1	-1.817547	2.921844	2.387909
1	-0.167141	-2.680710	-1.856041	1	-3.317518	3.342051	2.211123
6	-0.094609	-3.369772	0.722039	6	-3.504079	2.834266	-0.497049
1	0.644149	-2.794813	0.511021	1	-3.491295	2.227178	-1.24097
1	0.158683	-4.283615	0.572698	1	-3.197377	3.697256	-0.782669
1	-0.338554	-3.252071	1.642703	1	-4.399874	2.909159	-0.159823
6	-3.173168	-1.515208	0.477349	6	-0.393669	3.125655	-0.418585
1	-3.358306	-0.561854	0.614151	1	-0.895029	3.955908	-0.277375
6	-3.407219	-2.221321	1.815415	6	-0.093466	3.012968	-1.90822
1	-4.238347	-1.923541	2.192235	1	-0.915367	2.920734	-2.394298
1	-2.689489	-2.013154	2.416312	1	0.460888	2.244048	-2.064845
1	-3.441122	-3.170135	1.674188	1	0.365457	3.802918	-2.20207
6	-4.129275	-2.005346	-0.512119	6	0.863496	3.191108	0.444767
1	-3.998139	-1.540958	-1.341287	1	1.404697	2.414761	0.281419
1	-5.022963	-1.852429	-0.196149	1	0.613405	3.218176	1.370818
1	-3.995873	-2.946156	-0.647350	1	1.361011	3.981038	0.224774
6	2.963807	-0.419450	-0.297887	6	2.881783	-0.291352	0.008176
6	4.259252	-0.575343	-0.808775	6	2.459645	-0.383208	1.322679
1	4.391514	-0.710912	-1.719570	1	1.557337	-0.492103	1.519302
6	5.350523	-0.525435	0.063404	6	3.399922	-0.311915	2.348845
1	6.212665	-0.642763	-0.262980	1	3.123199	-0.373069	3.233879

6	5.146011	-0.301217	1.411260	6	4.736339	-0.150603	2.057668
1	5.874912	-0.244971	1.985680	1	5.359978	-0.106151	2.746565
6	3.859652	-0.159786	1.917986	6	5.154387	-0.054445	0.736207
1	3.732030	-0.018537	2.828853	1	6.058328	0.049793	0.540528
6	2.752544	-0.229400	1.057444	6	4.227701	-0.113008	-0.288352
1	1.888927	-0.149157	1.393374	1	4.503540	-0.03354	-1.172628

Compound **5** E = -937.38846869 Nimag = 0				Compound **6** E = -1405.41332186 Nimag = 0			
52	1.697493	-0.547829	-1.423126	6	1.386502	-0.214543	-0.937319
7	-2.092532	-1.607524	0.283727	6	2.705729	-0.096716	-0.562833
7	-1.455596	2.029517	0.024536	6	1.820621	-0.960291	0.130068
6	-0.106102	-0.129672	-0.495923	6	3.976792	1.592596	-1.721809
6	-1.312218	-0.602908	-0.020122	1	4.943861	1.834569	-1.801383
6	-1.069625	0.787935	-0.121002	6	3.489467	1.201139	-3.112742
6	-1.581642	-2.990299	0.099446	1	3.945988	0.384808	-3.399887
1	-2.292549	-3.60675	0.374896	1	3.686226	1.923837	-3.743862
6	-0.384927	-3.240343	1.002171	1	2.522012	1.042506	-3.087995
1	0.313791	-2.618515	0.787207	6	3.248414	2.802874	-1.160635
1	-0.066411	-4.136682	0.870380	1	2.287197	2.616736	-1.123964
1	-0.645423	-3.124785	1.918592	1	3.410616	3.579952	-1.737416
6	-1.267328	-3.274927	-1.36065	1	3.577852	2.994315	-0.256655
1	-2.021595	-3.031316	-1.904201	6	5.097682	-0.005934	-0.048582
1	-1.082435	-4.209702	-1.471626	1	4.810678	-0.687362	0.624426
1	-0.501262	-2.762075	-1.62852	6	6.050350	-0.696726	-1.018406
6	-3.490154	-1.405106	0.742805	1	6.342176	-0.055836	-1.70019
1	-3.657892	-0.439626	0.758937	1	5.590179	-1.447827	-1.449758
6	-3.655775	-1.921203	2.163660	1	6.829887	-1.029857	-0.527664
1	-3.607996	-2.879657	2.162921	6	5.765274	1.134906	0.711296
1	-4.507568	-1.643621	2.507987	1	6.552009	0.793446	1.187836
1	-2.956059	-1.566243	2.716513	1	5.130521	1.514128	1.355263
6	-4.482429	-2.024718	-0.229037	1	6.043009	1.829816	0.077912
1	-4.326360	-1.676757	-1.110644	6	2.388164	-2.176392	2.186646
1	-5.376934	-1.810026	0.046379	1	1.844578	-2.691554	2.849830
1	-4.370603	-2.978024	-0.236047	6	3.480872	-3.108717	1.683181
6	-2.810377	2.368271	0.517433	1	3.966801	-2.676006	0.950799
1	-3.206541	1.553488	0.890220	1	3.078226	-3.941106	1.360010
6	-2.734264	3.403470	1.635709	1	4.101757	-3.309076	2.414223
1	-2.098863	3.115614	2.294449	6	2.907123	-0.939263	2.899980
1	-3.598296	3.497448	2.044262	1	3.448883	-1.210015	3.670605
1	-2.458918	4.247483	1.271415	1	2.151133	-0.398171	3.206548
6	-3.676621	2.817227	-0.637958	1	3.457491	-0.413447	2.282472
1	-3.363716	3.665578	-0.961086	6	0.106600	-2.369756	1.011281
1	-4.586241	2.903359	-0.341607	1	-0.289784	-2.098581	0.134843
1	-3.630435	2.168451	-1.343635	6	0.146498	-3.895070	1.042425
6	-0.564063	3.128806	-0.449283	1	0.745153	-4.220007	0.339192
1	-1.051731	3.971416	-0.336921	1	-0.754869	-4.247947	0.893240
6	0.679981	3.199009	0.429579	1	0.474467	-4.194177	1.915859
1	0.417897	3.230397	1.352965	6	-0.769376	-1.779504	2.107437
1	1.180351	3.988527	0.212483	1	-0.430151	-2.058322	2.983374
1	1.222782	2.422712	0.277023	1	-1.689862	-2.098621	1.997055
6	-0.247356	2.978776	-1.924399	1	-0.752594	-0.801272	2.048588
1	0.295631	2.197682	-2.057003	6	-1.223489	0.300398	-0.954289
1	0.228203	3.755293	-2.230433	6	-2.514704	-0.087037	-0.669
1	-1.064582	2.887872	-2.419957	6	-1.907331	0.998637	0.019385

6	2.875981	-0.195635	0.299222
6	2.351399	-0.246564	1.592993
1	1.444056	-0.401921	1.725223
6	3.199009	-0.06289	2.685947
1	2.851181	-0.094159	3.547519
6	4.545331	0.164606	2.502810
1	5.103471	0.277205	3.237831
6	5.066132	0.226522	1.216398
1	5.973184	0.389076	1.092214
6	4.235361	0.045550	0.108327
1	4.587251	0.085938	-0.751767

6	-0.827915	2.927278	0.982872
1	-1.097597	3.651169	1.617056
6	0.420623	2.259996	1.547582
1	0.228649	1.914363	2.444294
1	1.147607	2.915951	1.598778
1	0.688607	1.521946	0.963571
6	-0.612454	3.563987	-0.382463
1	0.063871	4.269375	-0.310528
1	-1.456450	3.949992	-0.699087
1	-0.306345	2.882513	-1.016212
6	-3.153001	2.171237	1.755545
1	-3.751592	1.378288	1.638471
6	-2.766430	2.236147	3.222468
1	-2.269450	1.427476	3.465769
1	-3.575715	2.299629	3.771913
1	-2.205022	3.023049	3.377840
6	-3.915060	3.391628	1.280305
1	-3.357682	4.190745	1.394579
1	-4.736237	3.489010	1.806109
1	-4.143254	3.284248	0.333815
6	-3.536641	-1.954064	-1.848695
1	-4.472812	-2.294396	-1.943407
6	-2.687802	-3.098531	-1.326819
1	-1.745424	-2.832361	-1.330045
1	-2.807699	-3.884436	-1.901423
1	-2.961218	-3.318784	-0.412423
6	-3.084893	-1.478804	-3.218734
1	-2.140063	-1.218589	-3.179129
1	-3.625398	-0.706485	-3.491172
1	-3.197839	-2.201801	-3.869676
6	-4.858337	-0.482501	-0.207253
1	-4.666154	0.226874	0.470969
6	-5.452055	-1.662442	0.530373
1	-5.712014	-2.352489	-0.114525
1	-6.241128	-1.368858	1.031979
1	-4.787685	-2.027704	1.150016
6	-5.814905	0.113691	-1.226469
1	-5.388126	0.876915	-1.667949
1	-6.631531	0.413541	-0.772614
1	-6.043050	-0.563796	-1.895515
7	3.879057	0.454599	-0.761033
7	1.480105	-1.801568	1.072947
7	-1.952316	1.949575	0.909423
7	-3.567371	-0.829995	-0.867188
16	0.130818	0.223879	-2.043287

Compound **8** E = -1404.53777393 Nimag = 0			
34	-0.126335	-0.288619	-2.044281
7	3.641703	0.831741	-0.743942
7	2.018197	-1.90783	1.094423
7	-3.938785	-0.463167	-0.583435
7	-1.522331	1.860937	1.134460
6	1.308924	-0.320213	-0.823261
6	1.982106	-0.985457	0.174389

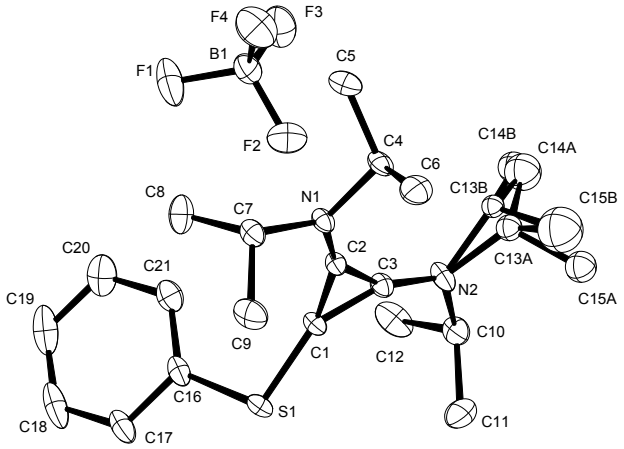
Compound **11** E = -1403.36911738 Nimag = 0			
6	1.536151	-0.361246	-0.701818
6	2.044032	-0.952451	0.426606
6	2.838442	-0.05085	-0.326487
6	5.161529	0.370816	0.289253
1	4.919788	-0.260055	0.999517
6	5.630915	1.655387	0.959563
1	6.351051	1.458156	1.560944

6	2.592687	0.082339	-0.535548	1	4.902764	2.046358	1.448707
6	3.597844	1.931261	-1.7529	1	5.933878	2.271789	0.290710
1	4.506854	2.285865	-1.837724	6	6.246672	-0.283279	-0.548657
6	2.716124	3.063114	-1.271842	1	6.468820	0.288863	-1.288007
1	1.798535	2.780795	-1.286841	1	5.930374	-1.126154	-0.879957
1	2.827679	3.823514	-1.84888	1	7.026565	-0.423347	-0.007356
1	2.963884	3.302329	-0.375971	6	4.030306	1.598410	-1.641009
6	3.184244	1.417871	-3.115159	1	4.927751	1.991698	-1.606436
1	3.725913	0.661563	-3.349447	6	3.037657	2.726943	-1.417716
1	3.302719	2.111740	-3.768598	1	2.142664	2.381025	-1.468857
1	2.260783	1.154519	-3.091353	1	3.159409	3.399105	-2.090599
6	4.934611	0.506347	-0.080469	1	3.181773	3.114192	-0.550127
1	4.749170	-0.163558	0.609072	6	3.881040	0.942212	-3.001726
6	5.535218	1.708115	0.609790	1	4.488690	0.201382	-3.068717
1	5.812539	2.348938	-0.048039	1	4.079835	1.581619	-3.688949
1	6.293645	1.433181	1.128379	1	2.980643	0.627618	-3.10727
1	4.879918	2.104914	1.188234	6	2.801713	-1.999573	2.512648
6	5.882505	-0.123087	-1.080822	1	2.369674	-2.584758	3.169287
1	5.458445	-0.880819	-1.49126	6	3.139997	-0.703182	3.234888
1	6.680336	-0.40969	-0.629917	1	3.776203	-0.880994	3.929784
1	6.110293	0.520841	-1.754153	1	2.340878	-0.333093	3.619184
6	3.209180	-2.095243	1.960022	1	3.512049	-0.076158	2.609377
1	3.803907	-1.330437	1.809171	6	3.999239	-2.765656	1.967509
6	2.807591	-2.076146	3.424814	1	4.388591	-2.276699	1.239235
1	2.334800	-1.262226	3.616415	1	3.713960	-3.627029	1.655108
1	3.593649	-2.125777	3.973904	1	4.651609	-2.878427	2.662885
1	2.239079	-2.82562	3.611160	6	0.489877	-2.442936	1.463545
6	3.965082	-3.342647	1.555451	1	-0.013583	-2.157252	0.672509
1	3.412655	-4.114051	1.700821	6	0.661922	-3.948975	1.389657
1	4.762413	-3.417531	2.082711	1	1.194369	-4.17339	0.623304
1	4.198615	-3.286568	0.626210	1	-0.199893	-4.365065	1.313219
6	0.885672	-2.872066	1.204363	1	1.098891	-4.262313	2.185804
1	1.137109	-3.548115	1.867437	6	-0.307153	-2.042133	2.689279
6	0.680509	-3.582975	-0.12057	1	0.139867	-2.355394	3.477385
1	0.018702	-4.270431	-0.01654	1	-1.182843	-2.430898	2.641377
1	1.507882	-3.977126	-0.404211	1	-0.381238	-1.086413	2.723055
1	0.384692	-2.950087	-0.779776	6	-1.493738	0.227619	-0.749594
6	-0.362404	-2.176516	1.713370	6	-2.820276	-0.034739	-0.424242
1	-0.179109	-1.775527	2.565817	6	-2.150207	1.064254	0.150493
1	-1.070809	-2.818807	1.807160	6	-0.889970	2.859164	1.174795
1	-0.626730	-1.497207	1.090137	1	-1.083004	3.558341	1.832399
6	-1.462928	0.219992	-0.828142	6	0.189229	1.961948	1.768476
6	-2.772426	0.106054	-0.425054	1	0.437179	1.291375	1.127892
6	-1.875562	0.990752	0.224205	1	-0.148054	1.538417	2.561171
6	-4.042630	-1.625971	-1.513766	1	0.959169	2.489954	1.992535
1	-4.986564	-1.886475	-1.55264	6	-0.443301	3.546767	-0.101825
6	-3.270947	-2.805865	-0.949299	1	0.349805	4.058335	0.071984
1	-3.431395	-3.581447	-1.491657	1	-1.139966	4.131852	-0.411517
1	-3.561671	-2.977108	-0.051095	1	-0.257442	2.884979	-0.773241
1	-2.333144	-2.603441	-0.949041	6	-3.357585	2.454646	1.744789
6	-3.616306	-1.261177	-2.925283	1	-4.071837	1.837639	1.484241
1	-4.089765	-0.476535	-3.210125	6	-3.125665	2.276770	3.231876
1	-3.817933	-1.988374	-3.517717	1	-2.833991	1.378220	3.406935
1	-2.672619	-1.089323	-2.939687	1	-3.943773	2.446778	3.705691
6	-5.157108	0.006085	0.128157	1	-2.452001	2.895644	3.526895
1	-4.877471	0.704462	0.756010	6	-3.811088	3.856199	1.372596
6	-6.135581	0.638194	-0.852259	1	-3.133966	4.488423	1.621293
1	-5.700272	1.353898	-1.321118	1	-4.626551	4.062628	1.835511
1	-6.892028	0.983762	-0.371487	1	-3.961674	3.902846	0.425468
1	-6.431032	-0.02265	-1.48129	6	-3.861693	-2.091426	-1.209122
6	-5.790098	-1.108975	0.943923	1	-4.687786	-2.561111	-0.970719
1	-6.056744	-1.82133	0.358582	6	-2.706525	-2.920413	-0.684792

1	-6.560135	-0.77081	1.406990	1	-1.876113	-2.544607	-0.990907
1	-5.152627	-1.440576	1.581540	1	-2.786138	-3.820835	-1.006309
6	-0.148340	2.422267	1.035623	1	-2.722522	-2.919571	0.273698
1	0.223300	2.136392	0.175005	6	-3.843479	-1.94759	-2.729451
6	0.747334	1.856485	2.126572	1	-3.043611	-1.491835	-2.998797
1	0.428311	2.147374	2.984843	1	-4.611400	-1.4423	-3.011601
1	1.644941	2.168559	1.996885	1	-3.867531	-2.816656	-3.132982
1	0.733388	0.896641	2.087798	6	-5.167749	-0.309369	0.104334
6	-0.184503	3.942626	1.031233	1	-5.060516	0.644659	0.311843
1	-0.775568	4.247241	0.337680	6	-6.358922	-0.428465	-0.842007
1	0.697908	4.283759	0.870426	1	-6.108289	-0.112103	-1.711933
1	-0.498969	4.258310	1.882165	1	-7.088089	0.097509	-0.505926
6	-2.410247	2.260344	2.256636	1	-6.629572	-1.347814	-0.900993
1	-1.865859	2.785029	2.881078	6	-5.349389	-1.022629	1.412235
6	-3.515807	3.172329	1.755536	1	-5.504087	-1.957249	1.249628
1	-3.130584	3.978296	1.405533	1	-6.103194	-0.651417	1.877881
1	-4.106960	3.388154	2.480774	1	-4.560250	-0.918329	1.947943
1	-4.008986	2.727375	1.062037	7	3.943780	0.607572	-0.530781
6	-2.906258	1.041079	3.013623	7	1.808247	-1.756733	1.436064
1	-3.479428	0.521720	2.445385	7	-2.141848	2.086200	0.968093
1	-3.395800	1.322825	3.789578	7	-3.904843	-0.755674	-0.553557
1	-2.156873	0.507466	3.284670	52	0.013527	-0.228366	-2.119741

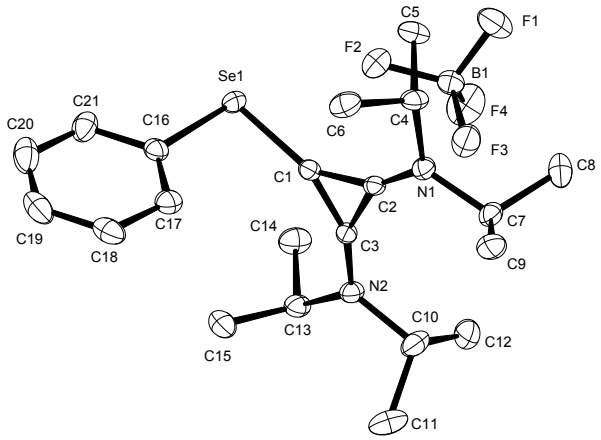
X-ray Structures

Compound **3**



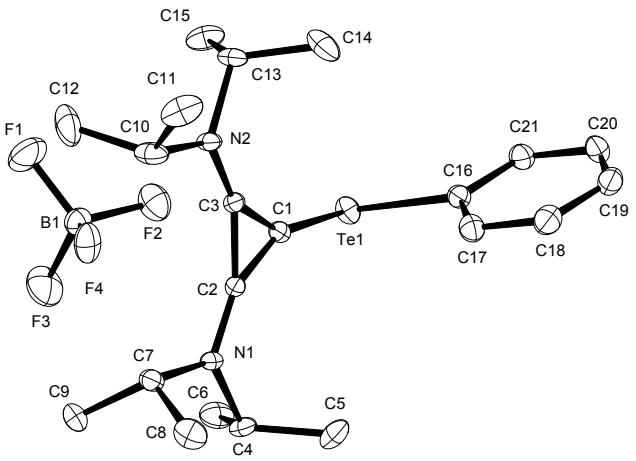
Empirical formula	$C_{21}H_{33}N_2S^+ \cdot BF_4^-$	
Color	colourless	
Formula weight	432.36 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**Cc, (no. 9)**	
Unit cell dimensions	a = 11.7908(7) Å	α= 90°.
	b = 15.1239(6) Å	β= 100.497(4)°.
	c = 13.0853(3) Å	γ = 90°.
Volume	2294.36(17) Å^3	
Z	4	
Density (calculated)	1.252 Mg · m^{-3}	
Absorption coefficient	0.182 mm^{-1}	
F(000)	920 e	
Crystal size	0.19 x 0.18 x 0.12 mm^3	
θ range for data collection	2.69 to 33.06°.	
Index ranges	-18 ≤ h ≤ 18, -23≤k ≤ 23, -20 ≤ l ≤11	
Reflections collected	16328	
Independent reflections	7171 [R_{int} = 0.0408]	
Reflections with I>2σ(I)	6135	
Completeness to θ= 27.50°	99.5 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.98 and 0.97	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7171 / 2 / 269	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2σ(I)]	R_1 = 0.0427	wR^2 = 0.0964
R indices (all data)	R_1 = 0.0566	wR^2 = 0.1067
Absolute structure parameter	0.02(6)	
Largest diff. peak and hole	0.604 and -0.418 e · Å^{-3}	

Compound **4**



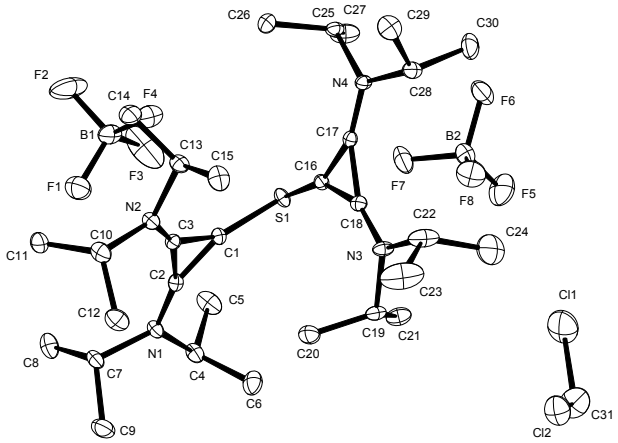
Empirical formula	$C_{21}H_{33}BF_4N_2Se$	
Color	colourless	
Formula weight	479.26 g · mol^{-1}	
Temperature	100 K	
Wavelength	1.54184 Å	
Crystal system	ORTHORHOMBIC	
Space group	**$Pca2_1$, (no. 29)**	
Unit cell dimensions	a = 15.4330(4) Å	α= 90°.
	b = 11.7351(3) Å	β= 90°.
	c = 12.8692(3) Å	γ = 90°.
Volume	2330.71(10) Å^3	
Z	4	
Density (calculated)	1.366 Mg · m^{-3}	
Absorption coefficient	2.538 mm^{-1}	
F(000)	992 e	
Crystal size	0.42 x 0.40 x 0.03 mm^3	
θ range for data collection	3.77 to 66.64°.	
Index ranges	-18 ≤ h ≤18, -13≤k ≤13, -13 ≤l ≤15	
Reflections collected	46405	
Independent reflections	3882 [R_{int} = 0.0686]	
Reflections with I>2σI)	3731	
Completeness to □ = 66.64°	99.5 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.93 and 0.42	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3882 / 1 / 270	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2σI)]	R_1 = 0.0275	wR^2 = 0.0638
R indices (all data)	R_1 = 0.0293	wR^2 = 0.0649
Absolute structure parameter	0.005(14)	
Largest diff. peak and hole	0.385 and -0.287 e · Å^{-3}	

Compound **5**



Empirical formula	$C_{21}H_{33}BF_4N_2Te$	
Color	yellow	
Formula weight	527.91 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	ORTHORHOMBIC	
Space group	**$Pca2_1$, (no. 29)**	
Unit cell dimensions	a = 15.5383(11) Å	α= 90°.
	b = 11.8089(6) Å	β= 90°.
	c = 12.9170(2) Å	γ = 90°.
Volume	2370.1(2) Å^3	
Z	4	
Density (calculated)	1.480 Mg · m^{-3}	
Absorption coefficient	1.295 mm^{-1}	
F(000)	1064 e	
Crystal size	0.29 x 0.22 x 0.12 mm^3	
Θ range for data collection	2.68 to 33.12°.	
Index ranges	-23 ≤ h ≤23, -18≤k ≤18, -19 ≤l ≤19	
Reflections collected	40015	
Independent reflections	8977 [R_{int} = 0.0431]	
Reflections with I>2σI)	8431	
Completeness to θ= 27.50°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.86 and 0.74	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8977 / 1 / 270	
Goodness-of-fit on F^2	1.149	
Final R indices [I>2σI)]	R_1 = 0.0243	wR^2 = 0.0621
R indices (all data)	R_1 = 0.0289	wR^2 = 0.0688
Absolute structure parameter	0.029(12)	
Largest diff. peak and hole	0.679 and -1.646 e · Å^{-3}	

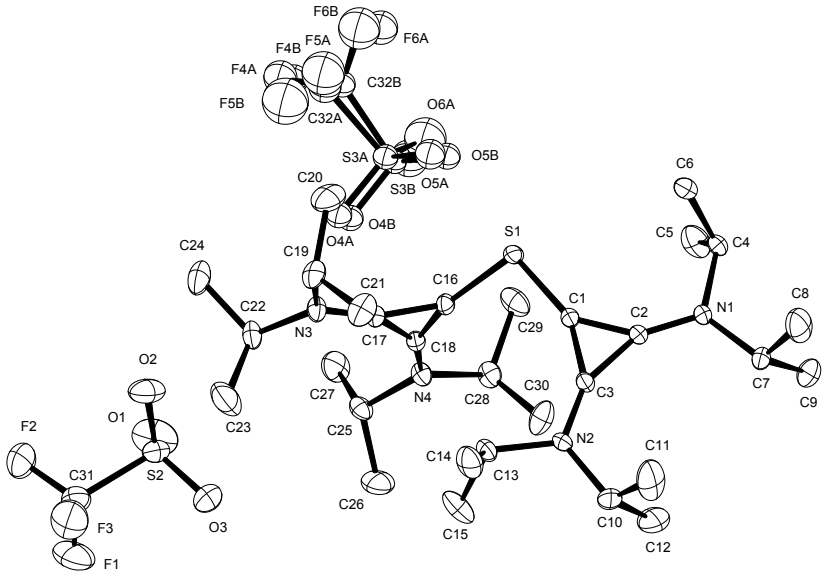
Compound **6**



Empirical formula	$C_{31}H_{58}B_2Cl_2F_8N_4S$	
Color	colourless	
Formula weight	763.39 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	ORTHORHOMBIC	
Space group	**Pbca, (no. 61)**	
Unit cell dimensions	a = 15.9281(17) Å	α= 90°.
	b = 16.791(3) Å	β= 90°.
	c = 29.680(2) Å	γ = 90°.
Volume	7937.7(18) Å^3	
Z	8	
Density (calculated)	1.278 Mg · m^{-3}	
Absorption coefficient	0.281 mm^{-1}	
F(000)	3232 e	
Crystal size	0.32 x 0.16 x 0.16 mm^3	
θ range for data collection	2.71 to 33.10°.	
Index ranges	-24 ≤h ≤24, -25≤ k ≤ 24, -44 ≤l ≤ 45	
Reflections collected	186573	
Independent reflections	15030 [R_{int} = 0.0649]	
Reflections with I>2σ(I)	9521	
Completeness to θ = 30.00°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.98 and 0.97	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15030 / 0 / 449	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2σ(I)]	R_1 = 0.0464	wR^2 = 0.1007
R indices (all data)	R_1 = 0.0959	wR^2 = 0.1178

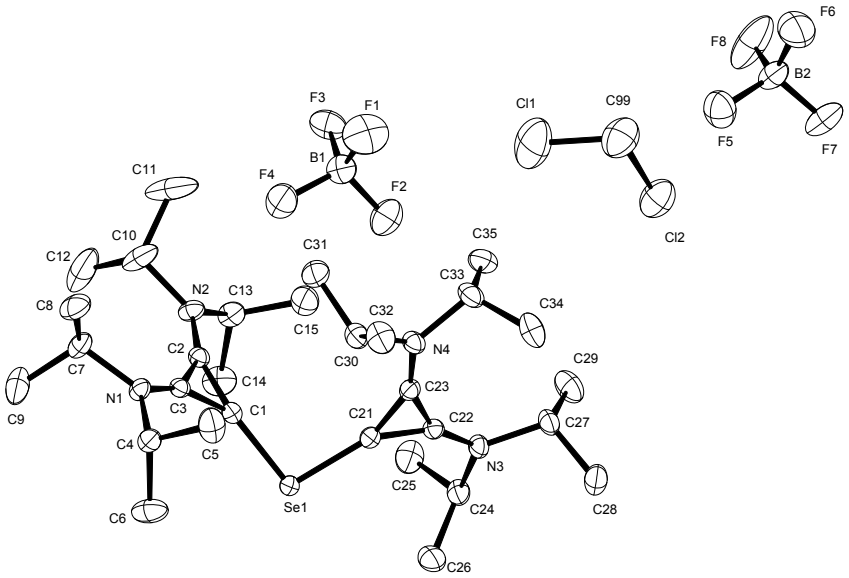
Largest diff. peak and hole 1.036 and -1.045 e · Å^{-3}

Compound **7**



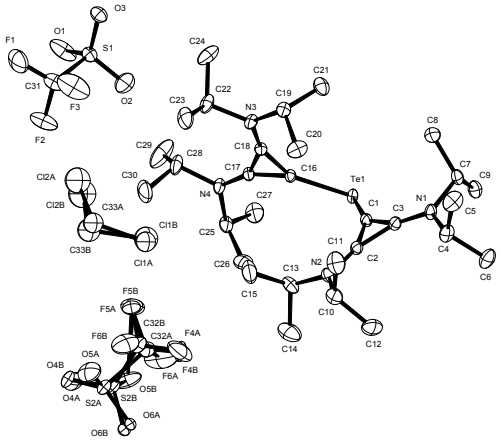
Empirical formula	$C_{32}H_{56}F_6N_4O_6S_3$	
Color	colourless	
Formula weight	802.99 g · mol^{-1}	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system	ORTHORHOMBIC	
Space group	**$P2_12_12_1$, (no. 19)**	
Unit cell dimensions	a = 10.1055(15) Å	α= 90°.
	b = 16.1466(18) Å	β= 90°.
	c = 25.670(3) Å	γ = 90°.
Volume	4188.6(9) Å^3	
Z	4	
Density (calculated)	1.273 Mg · m^{-3}	
Absorption coefficient	0.247 mm^{-1}	
F(000)	1704 e	
Crystal size	0.299 x 0.244 x 0.170 mm^3	
Θ range for data collection	2.64 to 33.09°.	
Index ranges	-15 ≤ h ≤ 15, -24≤ k ≤ 24, -39 ≤ l ≤ 39	
Reflections collected	114197	
Independent reflections	15887 [R_{int} = 0.0386]	
Reflections with I>2σ(I)	13682	
Completeness to Θ = 27.50°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.96 and 0.94	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15887 / 0 / 468	
Goodness-of-fit on F^2	1.080	
Final R indices [I>2σ(I)]	R_1 = 0.0557	wR^2 = 0.1273
R indices (all data)	R_1 = 0.0697	wR^2 = 0.1369
Absolute structure parameter	0.05(5)	
Largest diff. peak and hole	0.929 and -0.729 e · Å^{-3}	

Compound **8**



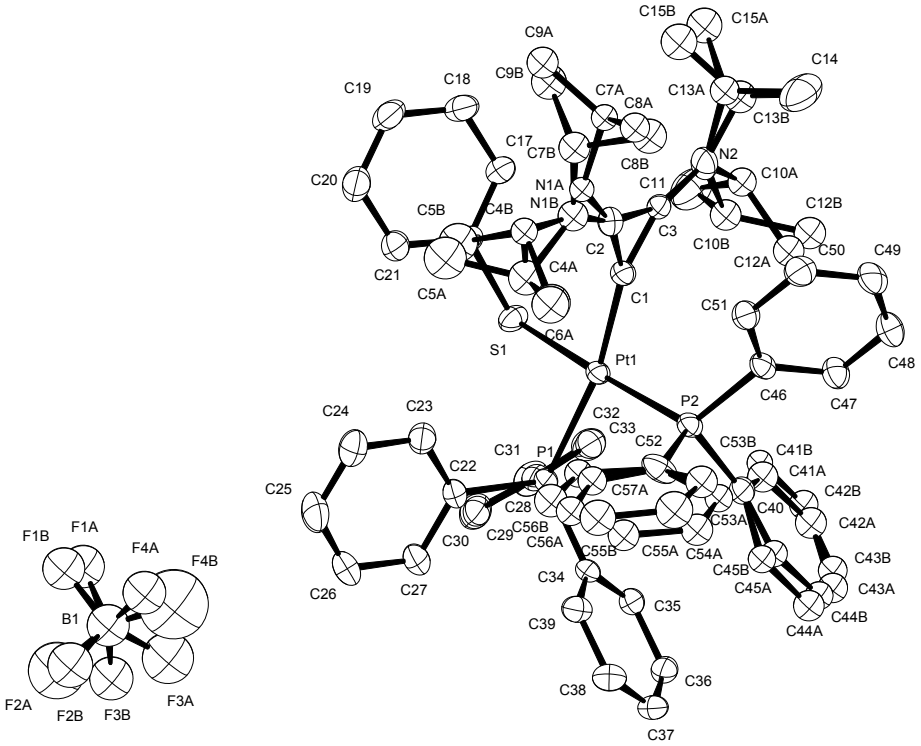
Empirical formula	$C_{31}H_{58}B_2Cl_2F_8N_4Se$	
Color	colorless	
Formula weight	810.29 g · mol^{-1}	
Temperature	130 K	
Wavelength	1.54184 Å	
Crystal system	ORTHORHOMBIC	
Space group	**Pbca, (no. 61)**	
Unit cell dimensions	a = 16.0030(6) Å	α= 90°.
	b = 16.9693(7) Å	β= 90°.
	c = 29.6752(12) Å	γ = 90°.
Volume	8058.6(6) Å^3	
Z	8	
Density (calculated)	1.336 Mg · m^{-3}	
Absorption coefficient	3.034 mm^{-1}	
F(000)	3376 e	
Crystal size	0.24 x 0.23 x 0.21 mm^3	
θ range for data collection	2.98 to 67.28°.	
Index ranges	-18 ≤ h ≤ 18, -20≤ k ≤ 20, -35 ≤ l ≤ 33	
Reflections collected	175830	
Independent reflections	7176 [R_{int} = 0.0501]	
Reflections with I>2σ(I)	6719	
Completeness to θ = 67.28°	99.3 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.74 and 0.63	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7176 / 0 / 449	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2σ(I)]	R_1 = 0.0301	wR^2 = 0.0747
R indices (all data)	R_1 = 0.0318	wR^2 = 0.0756
Largest diff. peak and hole	0.711 and -0.765 e · Å^{-3}	

Compound **11**



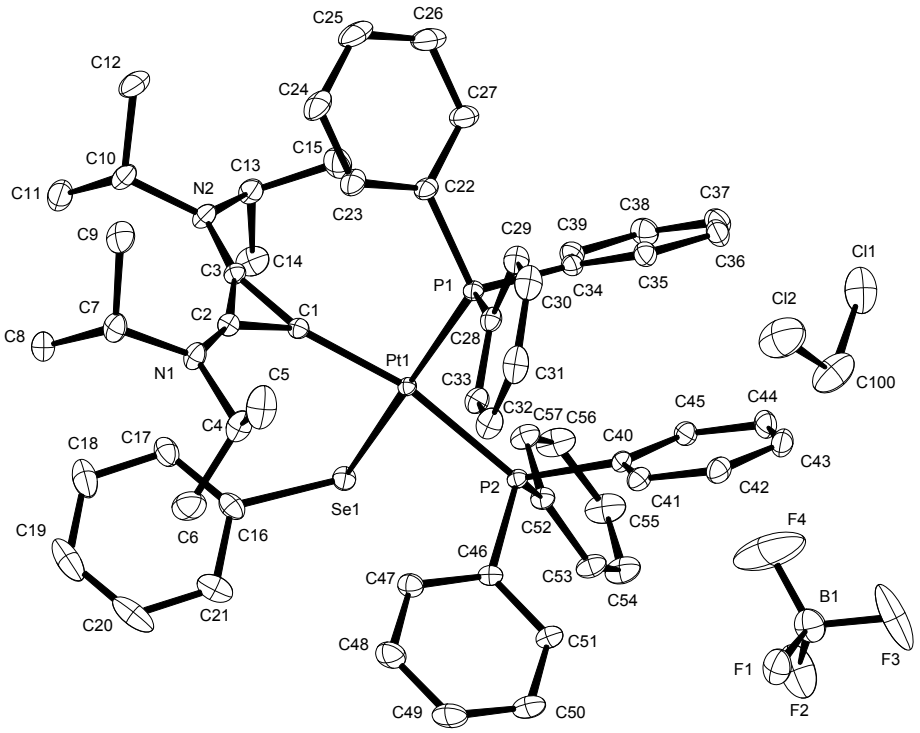
Empirical formula	$C_{33}H_{58}Cl_2F_6N_4O_6S_2Te$	
Color	colorless	
Formula weight	983.45 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	ORTHORHOMBIC	
Space group	**Pbca, (no. 61)**	
Unit cell dimensions	a = 15.536(2) Å	α= 90°.
	b = 18.1269(15) Å	β= 90°.
	c = 32.831(4) Å	γ = 90°.
Volume	9246.1(18) Å^3	
Z	8	
Density (calculated)	1.413 Mg · m^{-3}	
Absorption coefficient	0.915 mm^{-1}	
F(000)	4032 e	
Crystal size	0.29 x 0.19 x 0.06 mm^3	
θ range for data collection	2.62 to 33.11°.	
Index ranges	-23 ≤ h ≤ 23, -27≤ k ≤ 27, -50 ≤ l ≤ 50	
Reflections collected	164134	
Independent reflections	17563 [R_{int} = 0.0530]	
Reflections with I>2σ(I)	13988	
Completeness to θ = 27.50°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.95 and 0.88	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17563 / 0 / 572	
Goodness-of-fit on F^2	1.151	
Final R indices [I>2σ(I)]	R_1 = 0.0559	wR^2 = 0.1227
R indices (all data)	R_1 = 0.0741	wR^2 = 0.1299
Largest diff. peak and hole	2.381 and -2.058 e · Å^{-3}	

Compound **12**



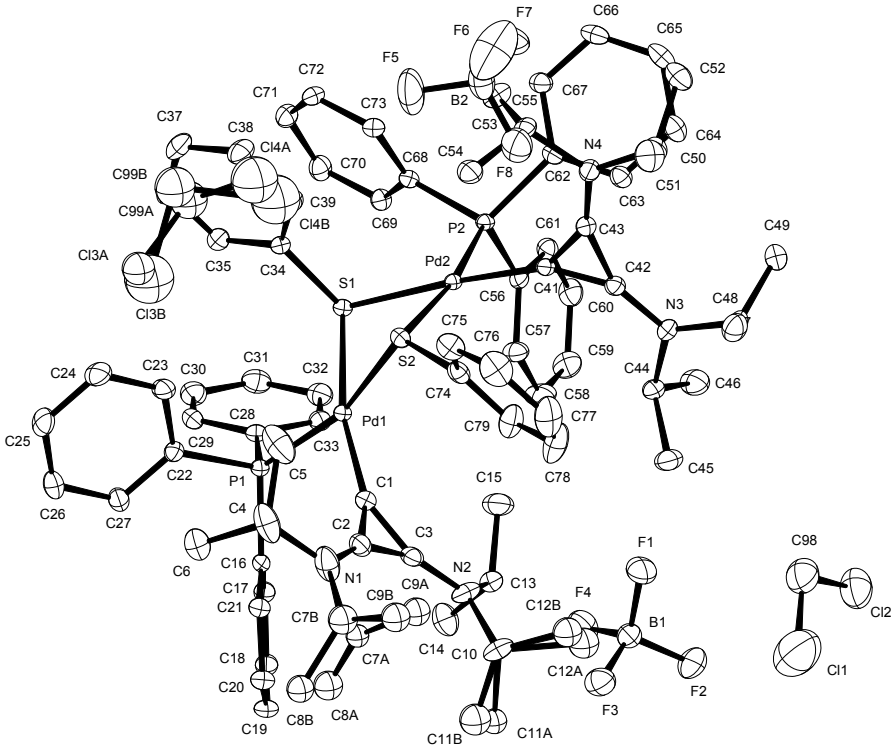
Empirical formula	$C_{57}H_{63}BF_4N_2P_2PtS$	
Color	colourless	
Formula weight	1151.99 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 17.3202(18) Å	α= 90°.
	b = 15.5062(9) Å	β= 94.972(5)°.
	c = 21.7660(16) Å	γ = 90°.
Volume	5823.7(8) Å^3	
Z	4	
Density (calculated)	1.314 Mg · m^{-3}	
Absorption coefficient	2.548 mm^{-1}	
F(000)	2336 e	
Crystal size	0.16 x 0.16 x 0.09 mm^3	
θ range for data collection	2.65 to 34.97°.	
Index ranges	-27 ≤ h ≤ 27, -24≤ k ≤ 24, -35 ≤ l ≤ 34	
Reflections collected	187089	
Independent reflections	25535 [R_{int} = 0.0492]	
Reflections with I>2σ(I)	20849	
Completeness to θ = 27.50°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.66 and 0.46	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	25535 / 129 / 597	
Goodness-of-fit on F^2	1.121	
Final R indices [I>2σ(I)]	R_1 = 0.0428	wR^2 = 0.1081
R indices (all data)	R_1 = 0.0570	wR^2 = 0.1146
Largest diff. peak and hole	2.237 and -1.510 e · Å^{-3}	

Compound **13**



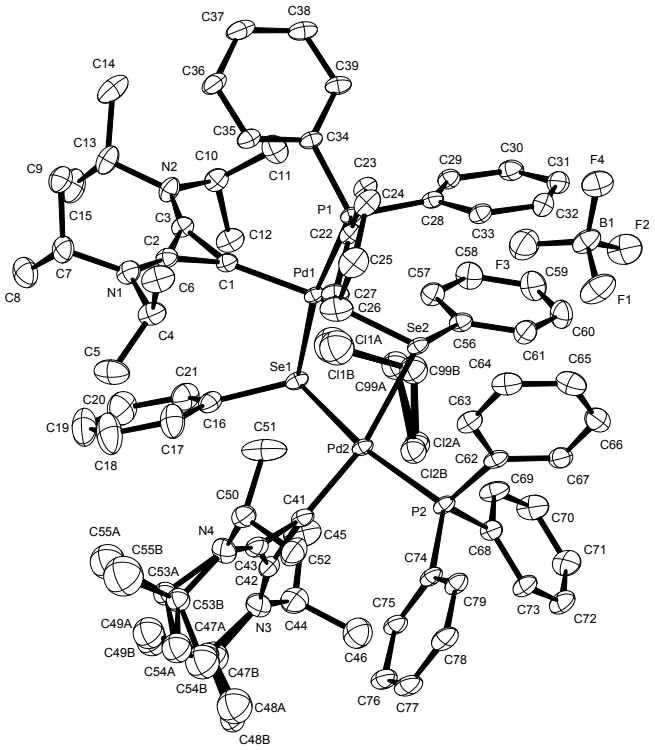
Empirical formula	$C_{57}H_{63}BF_4N_2P_2PtSe \cdot CH_2Cl_2$	
Color	yellow	
Formula weight	1283.82 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	**P$\bar{1}$, (no. 2)**	
Unit cell dimensions	a = 10.4351(12) Å	α= 76.054(4)°.
	b = 16.4154(16) Å	β= 89.013(4)°.
	c = 16.7476(3) Å	γ = 84.580(5)°.
Volume	2771.7(4) Å^3	
Z	2	
Density (calculated)	1.538 Mg · m^{-3}	
Absorption coefficient	3.395 mm^{-1}	
F(000)	1288 e	
Crystal size	0.22 x 0.12 x 0.09 mm^3	
θ range for data collection	2.71 to 35.98°.	
Index ranges	-17 ≤ h ≤ 17, -27≤k ≤ 27, -27 ≤ l ≤ 27	
Reflections collected	96395	
Independent reflections	26166 [R_{int} = 0.0457]	
Reflections with I>2σ(I)	24079	
Completeness to θ = 27.50°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.69 and 0.52	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26166 / 0 / 648	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2σ(I)]	R_1 = 0.0235	wR^2 = 0.0567
R indices (all data)	R_1 = 0.0281	wR^2 = 0.0587
Largest diff. peak and hole	0.933 and -2.392 e · Å^{-3}	

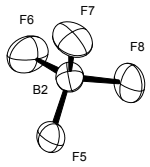
Compound **14**



Empirical formula	$C_{80}H_{99.50}B_2Cl_4F_8N_4P_2Pd_2S_2$	
Color	yellow	
Formula weight	1771.42 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 20.585(3) Å	α= 90°.
	b = 14.897(2) Å	β= 100.800(3)°.
	c = 27.925(4) Å	γ = 90°.
Volume	8412(2) Å^3	
Z	4	
Density (calculated)	1.399 Mg · m^{-3}	
Absorption coefficient	0.704 mm^{-1}	
F(000)	3646 e	
Crystal size	0.24 x 0.19 x 0.11 mm^3	
Θ range for data collection	1.48 to 29.57°.	
Index ranges	-28 ≤h ≤ 28, -20≤ k ≤ 20, -38 ≤ l ≤ 38	
Reflections collected	154609	
Independent reflections	23605 [R_{int} = 0.0486]	
Reflections with I>2σ(I)	19915	
Completeness to θ = 27.50°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.94 and 0.85	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23605 / 0 / 948	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2σ(I)]	R_1 = 0.0421	wR^2 = 0.1042
R indices (all data)	R_1 = 0.0538	wR^2 = 0.1153
Largest diff. peak and hole	2.476 and -2.399 e · Å^{-3}	

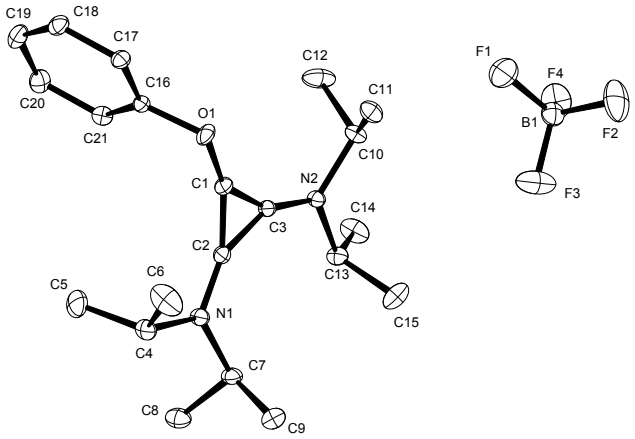
Compound **15**





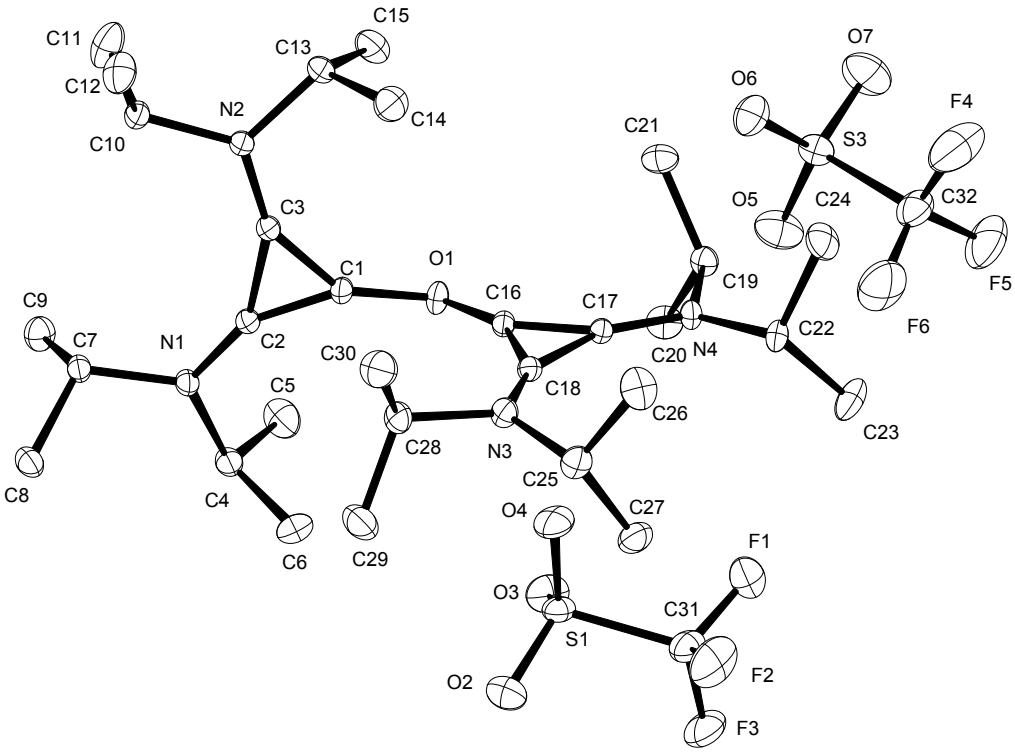
Empirical formula	$C_{78.50}H_{92}B_2ClF_8N_4P_2Pd_2Se_2$	
Color	yellow	
Formula weight	1733.29 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 20.978(3) Å	α= 90°.
	b = 14.8026(18) Å	β= 101.328(2)°.
	c = 28.165(3) Å	γ = 90°.
Volume	8575.7(18) Å^3	
Z	4	
Density (calculated)	1.342 Mg · m^{-3}	
Absorption coefficient	1.395 mm^{-1}	
F(000)	3520 e	
Crystal size	0.222 x 0.211 x 0.044 mm^3	
θ range for data collection	0.99 to 35.24°.	
Index ranges	-33 ≤ h ≤ 33, -23≤ k ≤ 23, -45 ≤ l ≤ 45	
Reflections collected	306663	
Independent reflections	38183 [R_{int} = 0.0562]	
Reflections with I>2σ(I)	27463	
Completeness to θ = 27.50°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.93 and 0.72	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	38183 / 0 / 920	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2σ(I)]	R_1 = 0.0484	wR^2 = 0.1384
R indices (all data)	R_1 = 0.0715	wR^2 = 0.1487
Largest diff. peak and hole	3.363 and -1.192 e · Å^{-3}	

Compound **16**



Empirical formula	$C_{21}H_{33}BF_4N_2O$	
Color	colourless	
Formula weight	416.30 g · mol^{-1}	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**Cc, (no. 9)**	
Unit cell dimensions	a = 11.5251(6) Å	α= 90°.
	b = 14.7912(5) Å	β= 98.893(3)°.
	c = 13.2009(5) Å	γ= 90°.
Volume	2223.31(16) $Å^3$	
Z	4	
Density (calculated)	1.244 Mg · m^{-3}	
Absorption coefficient	0.098 mm^{-1}	
F(000)	888 e	
Crystal size	0.37 x 0.26 x 0.18 mm^3	
θ range for data collection	2.90 to 33.07°.	
Index ranges	-17 ≤ h ≤ 17, -22≤ k ≤ 22, -20 ≤ l ≤ 20	
Reflections collected	22940	
Independent reflections	7941 [R_{int} = 0.0220]	
Reflections with I>2σ(I)	7359	
Completeness to θ = 27.50°	99.7 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.75 and 0.68	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7941 / 2 / 270	
Goodness-of-fit on F^2	1.129	
Final R indices [I>2σ(I)]	R_1 = 0.0340	wR^2 = 0.0912
R indices (all data)	R_1 = 0.0393	wR^2 = 0.0943
Absolute structure parameter	0.1(3)	
Largest diff. peak and hole	0.310 and -0.316 e · $Å^{-3}$	

Compound 17:



Empirical formula	$C_{32}H_{56}F_6N_4O_7S_2$	
Color	colourless	
Formula weight	786.93 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 13.6299(11) Å	α= 90°.
	b = 15.6457(13) Å	β= 101.772(2)°.
	c = 18.9753(15) Å	γ = 90°.
Volume	3961.4(6) Å^3	
Z	4	
Density (calculated)	1.319 Mg · m^{-3}	
Absorption coefficient	0.210 mm^{-1}	
F(000)	1672 e	
Crystal size	0.28 x 0.17 x 0.11 mm^3	
θ range for data collection	1.70 to 35.69°.	
Index ranges	-22 ≤ h ≤ 22, -25≤ k ≤ 25, -31 ≤ l ≤ 31	
Reflections collected	282313	
Independent reflections	18327 [R_{int} = 0.0388]	
Reflections with I>2σ(I)	15258	
Completeness to θ = 27.50°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.98 and 0.95	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18327 / 0 / 476	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2σ(I)]	R_1 = 0.0372	wR^2 = 0.1023
R indices (all data)	R_1 = 0.0481	wR^2 = 0.1103
Largest diff. peak and hole	0.739 and -0.568 e · Å^{-3}	