

SUPPORTING INFORMATION

Synthesis and Structural Characterization of *Tris*(2-seleno-1-mesitylimidazolyl)hydroborato Complexes: A New Type of Strongly Electron Donating Tripodal Selenium Ligand

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EXPERIMENTAL SECTION

General Considerations

All manipulations were performed using Schlenk techniques under a nitrogen atmosphere unless otherwise specified. Solvents were purified and degassed by standard procedures. ^1H and ^{13}C NMR spectra were measured on Bruker 300 DRX, Bruker 400 DRX, and Bruker Avance 500 DMX spectrometers. ^1H and ^{13}C Chemical shifts are reported in ppm relative to SiMe_4 ($\delta = 0$) and were referenced internally with respect to the protio solvent impurity (δ 7.26 for CHCl_3 ; δ 7.16 for $\text{C}_6\text{D}_5\text{H}$, δ 1.94 for CHD_2CN). Coupling constants are given in hertz. Infrared spectra were recorded on Nicolet Avatar 370 DTGS spectrometer and are reported in cm^{-1} . Mass spectra were obtained on a Micromass Quadrupole-Time-of-Flight mass spectrometer using fast atom bombardment (FAB). 1-mesitylimidazole-2-selone was obtained using a method analogous to that for the methyl derivative (Guziec, L. J.; Guziec, F. S. Jr. *J. Org. Chem.* **1994**, *59*, 4691-4692) and “ $\text{Zn}(\text{SPh})_2$ ” was generated by reaction of Me_2Zn with PhSH .

X-ray structure determinations

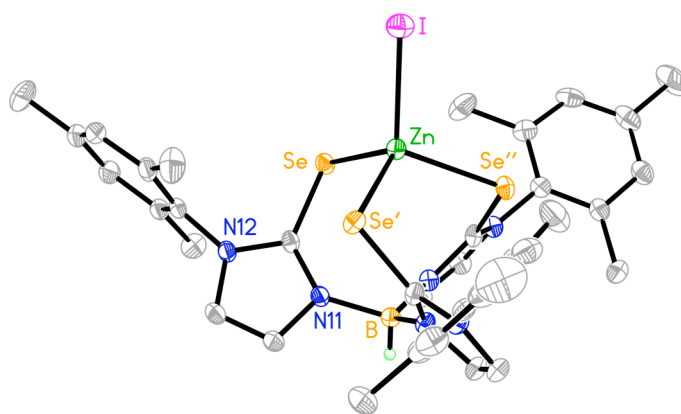
X-ray diffraction data were collected on a Bruker P4 diffractometer equipped with a SMART CCD detector; crystal data, data collection and refinement parameters are summarized in Table 2. The structures were solved using direct methods and standard difference map techniques, and were refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 5.10; Sheldrick, G. M. SHELXTL, An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data; University of Göttingen, Göttingen, Federal Republic of Germany, 1981). Hydrogen atoms on carbon are placed in idealized positions and thermal ellipsoid plots are illustrated at the 20% probability level.

Synthesis of [Tse^{Mes}]K

A mixture of 1-mesitylimidazole-2-selone (3.00 g, 11.3 mmol) and KBH₄ (0.24 g, 4.5 mmol) in toluene (35 mL) was refluxed under N₂ for 5 days, thereby depositing a light brown precipitate. The mixture was filtered and the precipitate was washed with pentane (3 × 15 mL) and dried *in vacuo* to give [Tse^{Mes}]K as a light brown powder (2.46 g, 77%). ¹H NMR (CD₃CN): 2.02 [s, 18 H, 6 Me of 3 mesityl], 2.31 [s, 9 H, 3 Me of 3 mesityl], 6.74 [d, ³J_{H-H} = 2, 3 H of 3 imidazole], 6.96 [s, 6 H, 6 CH of 3 mesityl], 7.08 [d, ³J_{H-H} = 2, 3 H of 3 imidazole]. Mass spectrum: *m/z* = 804.7 {M – K}⁻.

Synthesis of [Tse^{Mes}]ZnI

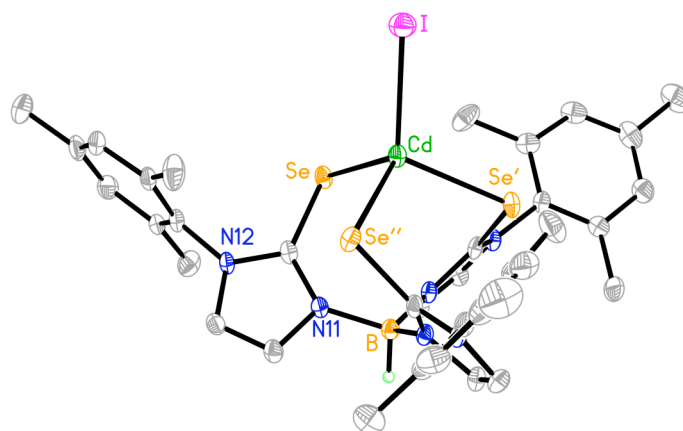
A solution of [Tse^{Mes}]K (50 mg, 0.059 mmol) in CH₂Cl₂ (10 mL) was added over a period of 10 minutes to a suspension of ZnI₂ (19 mg, 0.060 mmol) in CH₂Cl₂ (10 mL) resulting in the immediate deposition of a white precipitate. The mixture was stirred for 4 hours, allowed to settle for 15 minutes, and filtered. The volatile components were removed from the filtrate *in vacuo* to give [Tse^{Mes}]ZnI as a white powder (32 mg, 54%). Crystals of composition [Tse^{Mes}]ZnI•3CH₃CN suitable for X-ray diffraction were obtained from CH₃CN. ¹H NMR (C₆D₆): 1.82 [s, 9 H, 3 Me of 3 mesityl], 2.04 [s, 9 H, 3 Me of 3 mesityl], 2.14 [s, 9 H, 3 Me of 3 mesityl], 6.06 [d, ³J_{H-H} = 2, 3 H of 3 imidazole], 6.53 [s, 3 H, 3 CH of 3 mesityl], 6.74 [s, 3 H, 3 CH of 3 mesityl], 6.75 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole]. IR Data (KBr pellet, cm⁻¹): 3132 (w), 2966 (m), 2916 (m), 2856 (w), 2423 (w), 2346 (w), 2291 (w), 1608 (w), 1560 (w), 1485 (s), 1458 (w), 1437 (m), 1418 (s), 1358 (vs), 1317 (m), 1291 (m), 1260 (m), 1189 (vs), 1171 (s), 1130 (w), 1096 (m), 1032 (m), 967 (w), 934 (w), 851 (m), 800 (w), 760 (w), 734 (s), 684 (m), 584 (w), 553 (w), 500 (w). Mass spectrum: *m/z* = 994.9 {M – 1}⁺, 871.0 {M – I}⁺.



Molecular structure of [Tse^{Mes}]ZnI

Synthesis of [Tse^{Mes}]CdI

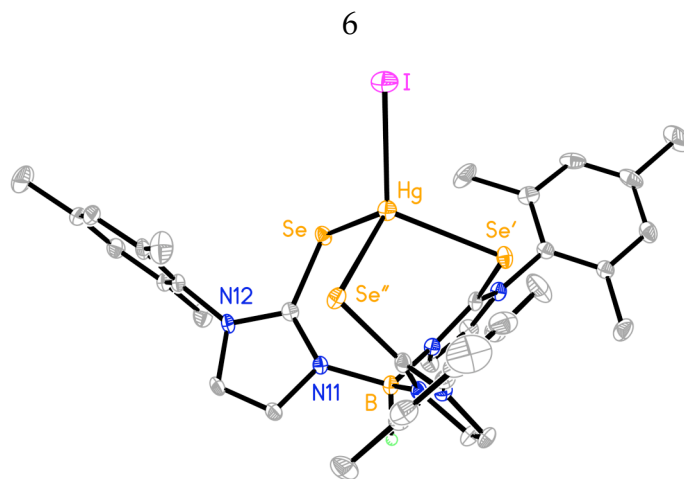
A solution of [Tse^{Mes}]K (50 mg, 0.059 mmol) in CH₂Cl₂ (10 mL) was added over a period of 10 minutes to a suspension of CdI₂ (22 mg, 0.060 mmol) in CH₂Cl₂ (10 mL) resulting in the immediate deposition of a white precipitate. The mixture was stirred for 3 hours, allowed to settle for 15 minutes and filtered. The volatile components were removed from the filtrate *in vacuo* to give [Tse^{Mes}]CdI as a white powder (31 mg, 50%). Crystals of composition [Tse^{Mes}]CdI·3CH₃CN suitable for X-ray diffraction were obtained from CH₃CN. Anal. Calcd. for C₃₆H₄₀BN₆Se₃CdI·CH₃CN: C, 42.1%; H, 4.0%; N, 9.0%. Found: C, 42.1%; H, 3.8%; 9.5%. ¹H NMR (C₆D₆): 1.85 [s, 9 H, 3 Me of 3 mesityl], 2.04 [s, 9 H, 3 Me of 3 mesityl], 2.09 [s, 9 H, 3 Me of 3 mesityl], 6.08 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole], 6.53 [s, 3 H, 3 CH of 3 mesityl], 6.68 [s, 3 H, 3 CH of 3 mesityl], 6.77 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole]. IR Data (KBr pellet, cm⁻¹): 3165 (m), 3134 (m), 3090 (w), 2946 (w), 2915 (m), 2855 (w), 2733 (w), 2406 (w), 2364 (w), 2344 (w), 2290 (w), 2251 (m), 1607 (w), 1562 (w), 1485 (m), 1435 (m), 1416 (m), 1354 (s), 1316 (m), 1290 (w), 1186 (vs), 1130 (m), 1096 (w), 1033 (m), 965 (w), 933 (w), 888 (w), 850 (s), 761 (w), 732 (m), 682 (m), 682 (w), 582 (w), 555 (w), 495 (w), 464 (w), 425 (w). Mass spectrum: *m/z* = 1042.8 {M - I}⁺, 916.8 {M - I}⁺.



Molecular structure of $[\text{Tse}^{\text{Mes}}]\text{CdI}$

Synthesis of $[\text{Tse}^{\text{Mes}}]\text{HgI}$

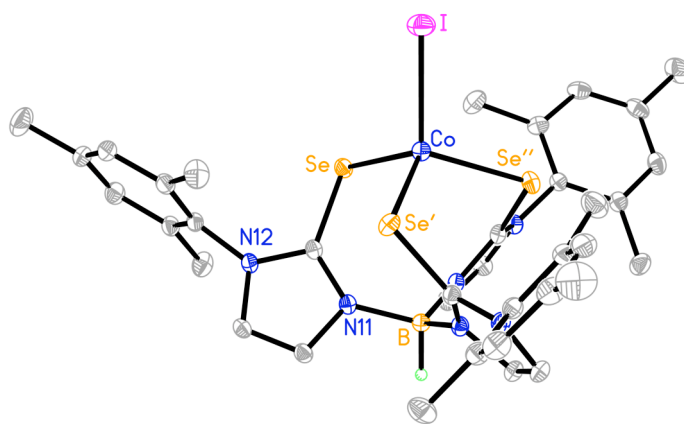
A solution of $[\text{Tse}^{\text{Mes}}]\text{K}$ (50 mg, 0.059 mmol) in CH_2Cl_2 (10 mL) was added over 10 minutes to a suspension of HgI_2 (27 mg, 0.059 mmol) in CH_2Cl_2 (10 mL) resulting in the immediate deposition of a white precipitate. The mixture was stirred for 3 hours, allowed to settle for 15 minutes, and filtered. The volatile components were removed from the filtrate *in vacuo* to give $[\text{Tse}^{\text{Mes}}]\text{HgI}$ as a white powder (35 mg, 52%). Crystals of composition $[\text{Tse}^{\text{Mes}}]\text{HgI} \cdot 3\text{CH}_3\text{OH}$ suitable for X-ray diffraction were obtained from CH_3OH . ^1H NMR (C_6D_6): 1.84 [s, 9 H, 3 Me of 3 mesityl], 2.04 [s, 9 H, 3 Me of 3 mesityl], 2.11 [s, 9 H, 3 Me of 3 mesityl], 6.06 [d, 3H, $^3J_{\text{H-H}} = 2$, 3 H of 3 imidazole], 6.54 [s, 3 H, 3 CH of 3 mesityl], 6.68 [s, 3 H, 3 CH of 3 mesityl], 6.80 [d, 3H, $^3J_{\text{H-H}} = 2$, 3 H of 3 imidazole]. IR Data (KBr pellet, cm^{-1}): 3163 (w), 3126 (w), 3093 (w), 2924 (s), 2855 (m), 2404 (w), 2233 (w), 2066 (m), 1606 (m), 1484 (m), 1460 (s), 1417 (m), 1376 (m), 1355 (m), 1315 (m), 1293 (w), 1188 (m), 1113 (w), 1033 (w), 966 (w), 934 (w), 848 (m), 783 (w), 765 (w), 747 (m), 683 (w), 582 (w). Mass spectrum: $m/z = 1131.3 \{M\}^+$, $1005.4 \{M - I\}^+$.



Molecular structure of [Tse^{Mes}]HgI

Synthesis of [Tse^{Mes}]CoI

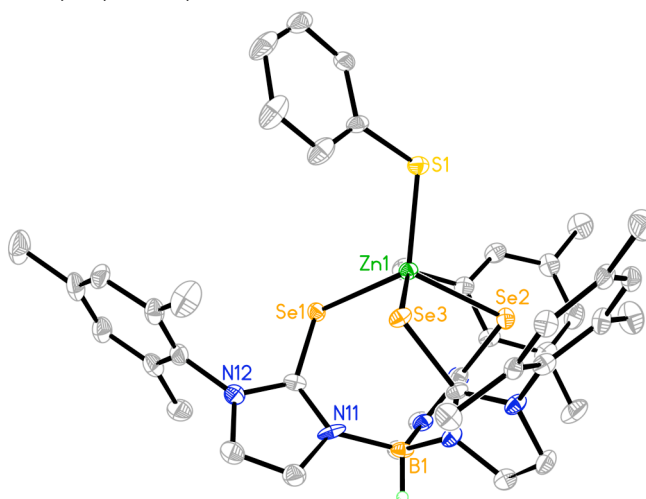
A solution of [Tse^{Mes}]K (50 mg, 0.059 mmol) in CH₂Cl₂ (10 mL) was added over a period of 10 minutes to a suspension of CoI₂ (19 mg, 0.061 mmol) in CH₂Cl₂ (10 mL) resulting in the immediate formation of a white precipitate in a green solution. The mixture was stirred for 4 hours and allowed to settle for 15 minutes. The mixture was filtered and the volatile components were removed *in vacuo* to give [Tse^{Mes}]CoI as a green powder (37 mg, 63%). Crystals of composition [Tse^{Mes}]CoI·3CH₃CN suitable for X-ray diffraction were obtained from CH₃CN. ¹H NMR (C₆D₆): -0.92 [br, 9 H, 3 Me of 3 mesityl], 2.15 [s, 9 H, 3 Me of 3 mesityl], 2.25 [s, 18 H, 3 Me of 3 mesityl], 3.29 [br, 3 H of 3 imidazole], 4.05 [br, 3 H of 3 imidazole], 6.27 [s, 3 H, 3 CH of 3 mesityl], 6.38 [s, 3 H, 3 CH of 3 mesityl] (assignments tentative due to the paramagnetic nature of the complex). IR Data (KBr pellet, cm⁻¹): 3169 (m), 3142 (m), 3098 (w), 3010 (w), 2972 (w), 2940 (w), 2915 (m), 2855 (w), 2407 (m), 2291 (w), 2254 (m), 1773 (w), 1753 (w), 1608 (m), 1562 (m), 1487 (s), 1437 (m), 1417 (s), 1359 (s), 1316 (m), 1291 (m), 1262 (m), 1187 (vs), 1135 (w), 1094 (w), 1032 (m), 966 (w), 934 (m), 920 (w), 887 (w), 849 (s), 801 (w), 783 (w), 756 (s), 734 (m), 686 (m), 585 (m), 573 (w), 498 (w), 473 (w), 464 (w), 426 (w). Mass spectrum: *m/z* = 990.9{M}⁺, 864.0 {M - I}⁺.



Molecular structure of [Tse^{Mes}]CoI

Synthesis of [Tse^{Mes}]ZnSPh

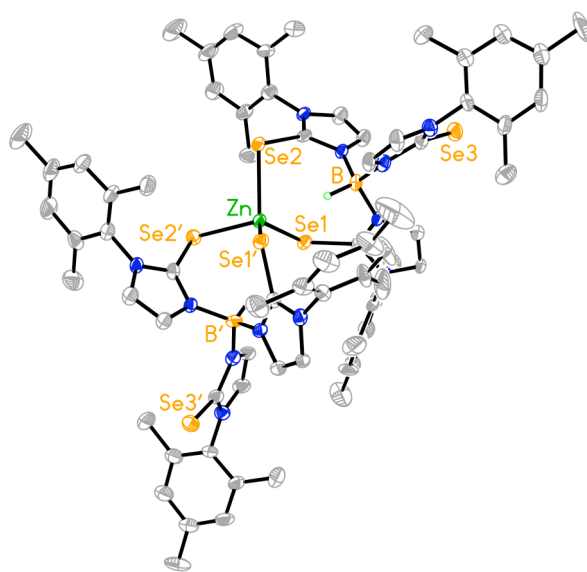
A mixture of [Tse^{Mes}]K (20 mg, 0.024 mmol) and "Zn(SPh)₂" (20 mg, 0.070 mmol) were treated with CD₃CN (1 mL), thereby demonstrating the rapid formation of [Tse^{Mes}]ZnSPh. The mixture was filtered and the solution was allowed to evaporate to deposit colorless crystals that were isolated and dried *in vacuo* (6 mg, 26 % yield). ¹H NMR (CD₃CN): 1.91 [s, 9 H, 3 Me of 3 mesityl], 1.99 [s, 9 H, 3 Me of 3 mesityl], 2.31 [s, 9 H, 3 Me of 3 mesityl], 6.77-6.90 [m, 3 H, 1 para and 2 meta H's of SPh], 7.00 [s, 3 H, 3 CH of 3 mesityl], 7.01 [s, 3 H, 3 CH of 3 mesityl], 7.06 [d, J_{H-H} = 7, 2 ortho H's of SPh], 7.14 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole], 7.35 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole]. Mass spectrum: *m/z* = 870.9 {M – SPh}⁺. Anal. Calcd. for C₄₂H₄₅BN₆SSe₃Zn: C, 51.5%; H, 4.6%; N, 8.6%. Found: C, 51.5%; H, 4.6%; 8.5%.



Molecular structure of [Tse^{Mes}]ZnSPh

Synthesis of [Tse^{Mes}]₂Zn

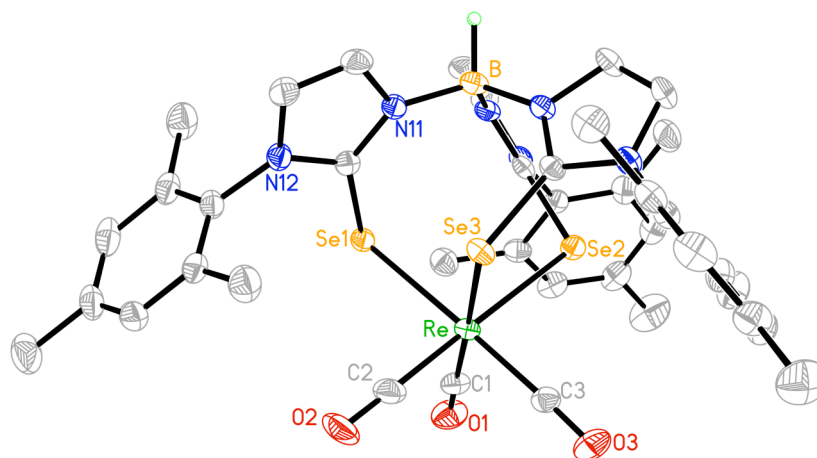
A solution of [Tse^{Mes}]⁺K⁻ (15 mg, 0.018 mmol) in MeCN (0.7 mL) was treated with ZnI₂ (2 mg, 0.006 mmol). The mixture was shaken vigorously and filtered. The solution was allowed to evaporate slowly to deposit [Tse^{Mes}]₂Zn as colorless crystals after 2 days, which were isolated and dried *in vacuo* (4 mg, 38% yield). ¹H NMR (C₆D₆ at 70°C): 1.99 [s, 36H, 12 *o*-Me of 6 mesityl], 2.08 [s, 18H, 6 *p*-Me of 6 mesityl], 6.26 [d, J_{H-H} = 1.4 Hz, 6H of 6 imidazole), 6.72 [s, 12H of 6 aryl rings], 8.67 [br, 6H of 6 imidazole]. Mass spectrum: *m/z* = 1674.0 {M}⁺. Anal. Calcd. for C₇₂H₈₀B₂N₁₂Se₆Zn: C, 51.7%; H, 4.8%; N, 10.0%. Found: C, 51.5%; H, 4.6%; N, 9.8%.



Molecular structure of [Tse^{Mes}]₂Zn

Synthesis of [Tse^{Mes}]Re(CO)₃

A mixture of [Tse^{Mes}]K (30 mg, 0.036 mmol) and Re(CO)₅Br (15 mg, 0.037 mmol) were treated with benzene (2 mL) and heated at 60 °C for 12 hours. The resulting pale yellow solution was filtered and allowed to form colorless crystals by slow evaporation, which were isolated and dried *in vacuo* (4 mg, 10 % yield). ¹H NMR (CD₃CN): 1.90 [s, 9 H, 3 Me of 3 mesityl], 2.10 [s, 9 H, 3 Me of 3 mesityl], 2.32 [s, 9 H, 3 Me of 3 mesityl], 7.01 [br s, 6 CH of 3 mesityl], 7.09 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole], 7.32 [d, 3H, ³J_{H-H} = 2, 3 H of 3 imidazole]. IR (KBr pellet, cm⁻¹): 3166 (w), 3137 (w), 2917 (w), 2857 (m), 2431 (w), 2370 (w), 1999 (s, ν_{CO}), 1886 (s, ν_{CO}), 1608 (w), 1561 (w), 1485 (w), 1439 (w), 1357 (m), 1317 (m), 1293 (w), 1190 (s), 1127 (m), 1033 (m), 934 (w), 849 (w), 763 (w), 736 (m), 682 (w), 630 (w), 582 (w), 509 (w). Mass spectrum: *m/z* = 1075.9 {M}⁺.

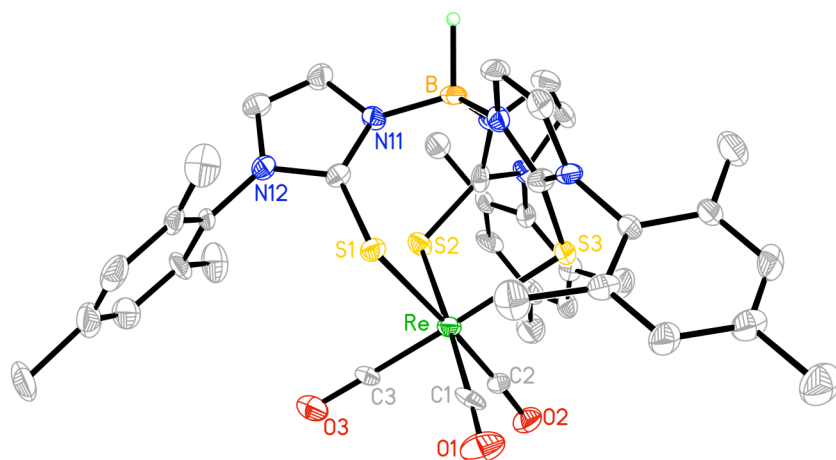


Molecular structure of [Tse^{Mes}]Re(CO)₃

Synthesis of [Tm^{Mes}]Re(CO)₃

A mixture of [Tm^{Mes}]Li (10 mg, 0.015 mmol) and Re(CO)₅Br (4 mg, 0.010 mmol) were treated with benzene (2 mL) and heated at 60 °C for 12 hours. The resulting solution was filtered and allowed to form colorless crystals by slow evaporation (4 mg, 43 % yield). ¹H NMR (CD₃CN): 1.95 [s, 9 H, 3 Me of 3 mesityl], 2.08 [s, 9 H, 3 Me of 3 mesityl], 2.32 [s, 9 H, 3 Me of 3 mesityl], 6.99 [s, 3H of aryl ring], 7.01 [s, 3H of aryl ring], 7.02 [d, J_{H-H} = 2, 3H of imidazole ring], 7.24 [d, J_{H-H} = 2, 3H of imidazole ring]. ¹H NMR (CDCl₃): 1.98 [s, 9 H, 3 Me of 3 mesityl], 2.14 [s, 9 H, 3 Me of 3 mesityl], 2.31 [s, 9 H, 3 Me

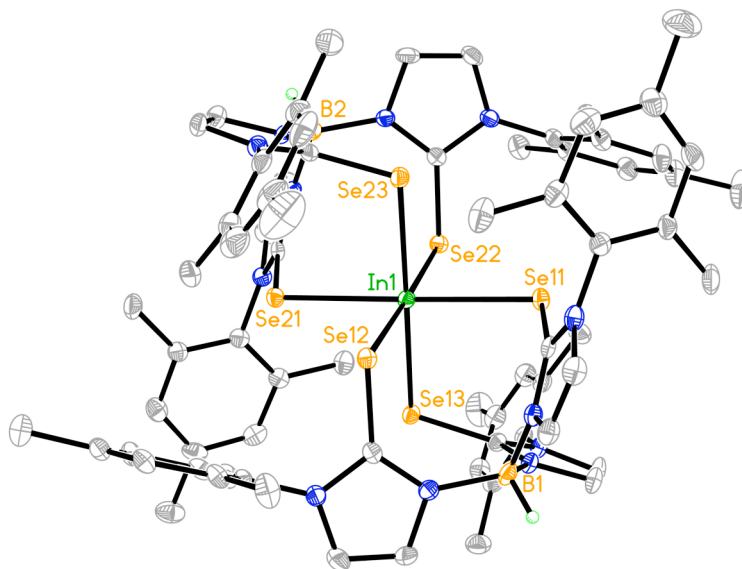
of 3 mesityl], 6.77 [d, $J_{\text{H-H}} = 2.1$ Hz, 3H of imidazole ring], 6.95 [s, 3H of aryl ring], 6.98 [s, 3H of aryl ring], 7.08 [d, $J_{\text{H-H}} = 2.1$ Hz, 3H of imidazole ring]. IR (KBr pellet, cm^{-1}): 3136 (w), 2919 (w), 2430 (w), 2365 (w), 2007 (s, ν_{CO}), 1890 (s, ν_{CO}), 1608 (w), 1559 (w), 1487 (w), 1439 (w), 1366 (m), 1323 (w), 1292 (w), 1192 (m), 1036 (w), 935 (w), 851 (w), 765 (w), 737 (w), 680 (w), 636 (w), 587 (w), 504 (w). Mass spectrum: $m/z = 934.0$ $\{\text{M}\}^+$.



Molecular structure of $[\text{Tm}^{\text{Mes}}]\text{Re}(\text{CO})_3$

Synthesis of {[Tse^{Mes}]₂In}[InCl₄]

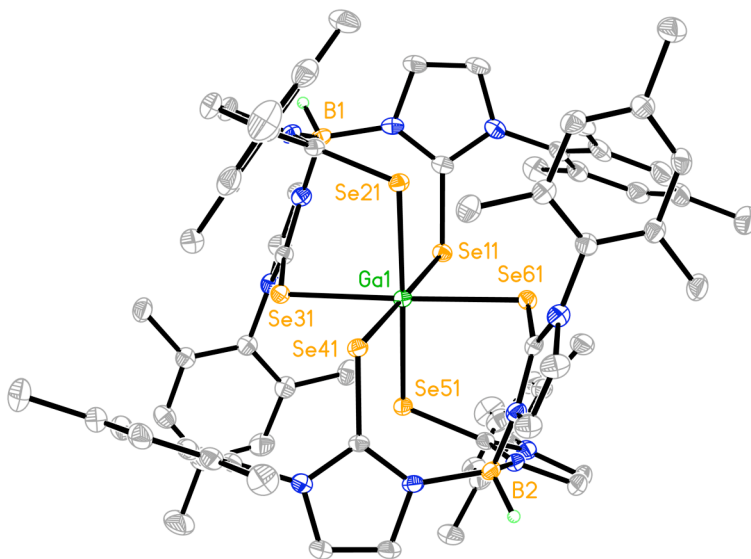
A mixture of [Tse^{Mes}]K (20 mg, 0.024 mmol) and InCl₃ (6 mg, 0.027 mmol) was treated with CDCl₃ (1 mL) and monitored by ¹H NMR spectroscopy, thereby demonstrating the immediate conversion to {[Tse^{Mes}]₂In}[InCl₄]. The mixture was filtered and the filtrate was allowed to evaporate slowly to deposit colorless crystals of {[Tse^{Mes}]₂In}[InCl₄] that were isolated and dried *in vacuo* (7 mg, 29 %). ¹H NMR (CDCl₃): 1.41 [s, 9 H, 3 Me of 3 mesityl], 1.93 [s, 9 H, 3 Me of 3 mesityl], 2.31 [s, 18 H, 6 Me of 6 mesityl], 6.68 [s, 6 H, 6 CH of 6 mesityl], 6.84 [d, 6 H, ³J_{H-H} = 2, 6 H of 6 imidazole], 6.96 [s, 6 H, 6 CH of 6 mesityl], 7.07 [d, 6 H, ³J_{H-H} = 2, 6 H of 6 imidazole]. Anal. Calcd. for C₇₂H₈₀B₂N₁₂Se₆In₂Cl₄: C, 43.7%; H, 4.1%; N, 8.5%. Found: C, 43.6%; H, 4.1%; 8.4%. Mass spectrum: *m/z* = 1724.2 {M + 1}⁺ (M = [Tse^{Mes}]₂In).



Molecular structure of {[Tse^{Mes}]₂In}⁺ (anion not shown)

Synthesis of $\{[\text{Tse}^{\text{Mes}}]_2\text{Ga}\}[\text{GaCl}_4]$

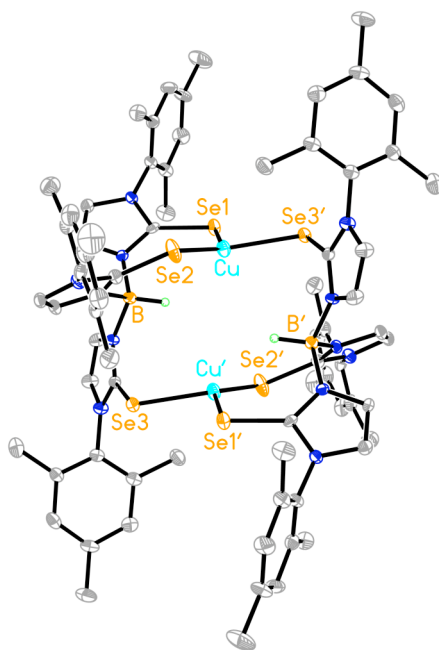
A mixture of $[\text{Tse}^{\text{Mes}}]\text{K}$ (20 mg, 0.024 mmol) and GaCl_3 (4 mg, 0.023 mmol) were combined in a J. Young NMR tube, dissolved in CD_3CN (1 mL), and shaken vigorously. The solution was filtered and allowed to evaporate slowly in a N_2 atmosphere. After 1 day, large yellow crystals had formed that were isolated and dried *in vacuo* (9 mg, 40 %). ^1H NMR (CDCl_3): 1.44 [s, 9 H, 3 Me of 3 mesityl], 1.89 [s, 18 H, 6 Me of 6 mesityl], 2.31 [s, 18 H, 6 Me of 6 mesityl], 6.71 [s, 6 H, 6 CH of 6 mesityl], 6.81 [d, 6 H, $^3J_{\text{H-H}} = 2$, 6 H of 6 imidazole], 6.95 [s, 6 H, 6 CH of 6 mesityl], 7.08 [d, 6H, $^3J_{\text{H-H}} = 2$, 6 H of 6 imidazole]. Anal. Calcd. for $\text{C}_{72}\text{H}_{80}\text{B}_2\text{N}_{12}\text{Se}_6\text{Ga}_2\text{Cl}_4$: C, 45.7%; H, 4.3%; N, 8.9%. Found: C, 45.9%; H, 4.0%; 9.1%. Mass spectrum: $m/z = 1678.1 \{M + 1\}^+$ ($M = [\text{Tse}^{\text{Mes}}]_2\text{Ga}$).



Molecular structure of $\{[\text{Tse}^{\text{Mes}}]_2\text{Ga}\}^+$ (anion not shown)

Synthesis of $[\text{Tse}^{\text{Mes}}]_2\text{Cu}_2$

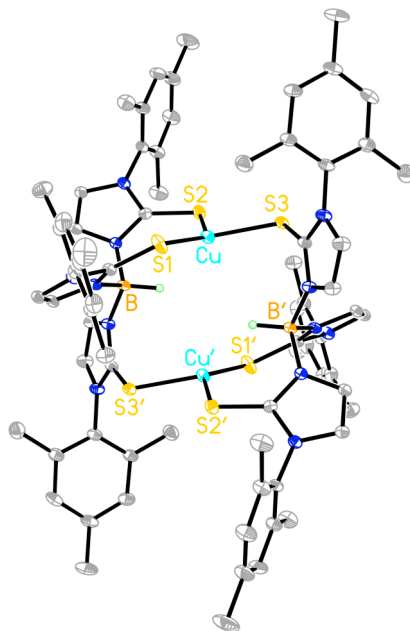
A solution of $[\text{Tse}^{\text{Mes}}]\text{K}$ (30 mg, 0.036 mmol) in MeCN (0.7 mL) was treated with CuCl (4 mg, 0.041 mmol). The solution was shaken vigorously and then filtered. The solution was allowed to evaporate slowly over a period of 2 days giving small colorless crystals of $[\text{Tse}^{\text{Mes}}]_2\text{Cu}_2$ that were isolated and dried *in vacuo* (3 mg, 10 % yield). ^1H NMR (CD_3CN): 1.85 (s, 36H of mesityl *o*- CH_3), 2.36 (s, 18H of mesityl *p*- CH_3), 7.02 (s, 12H of mesityl), 7.10 (br doublet, 6H of imidazole), 7.19 (br, 6H of imidazole). Anal. calcd. for $\text{C}_{36}\text{H}_{40}\text{BCuN}_6\text{Se}_3\text{Cu}$: C, 49.6%; H, 4.6%; N, 9.7%. Found: C, 49.6%; H, 4.5%; N, 9.4%.



Molecular structure of $\{[\text{Tse}^{\text{Mes}}]\text{Cu}\}_2$

Synthesis of $\{[\text{Tm}^{\text{Mes}}]\text{Cu}\}_2$

A solution of $[\text{Cu}(\text{MeCN})_4][\text{BF}_4]$ (0.019 g, 0.06 mmol) in CH_3CN (2 mL) was added to a solution of $\text{Tm}^{\text{Mes}}\text{Li}$ (0.04 g, 0.06 mmol) in CH_3CN (2 mL) resulting in the formation of a green precipitate and a colorless solution. The mixture was filtered and colorless crystals were obtained after several days. Anal. calcd. for $\text{C}_{36}\text{H}_{40}\text{N}_6\text{S}_3\text{BCu}$: C, 59.5%; H, 5.5%; N, 11.6%. Found: C, 58.6%; H, 6.1%; N, 12.9%.



Molecular structure of $\{[\text{Tse}^{\text{Mes}}]\text{Cu}\}_2$

Table 1. Crystal, intensity collection and refinement data.

	[Tse ^{Mes}]ZnI·3MeCN	[Tse ^{Mes}]CdI·3MeCN
lattice	Rhombohedral	Rhombohedral
formula	C ₄₂ H ₄₉ BI ₉ Se ₃ Zn	C ₄₂ H ₄₉ BCdI ₉ Se ₃
formula weight	1119.86	1166.89
space group	R-3c	R-3c
<i>a</i> /Å	14.618(1)	14.6142(7)
<i>b</i> /Å	14.619(1)	14.6142(7)
<i>c</i> /Å	77.980(1)	78.868(5)
α /°	90.00	90.00
β /°	90.00	90.00
γ /°	120.00	120.00
<i>V</i> /Å ³	14431(3)	14588(1)
<i>Z</i>	12	12
temperature (K)	243	243
radiation (λ , Å)	0.71073	0.71073
ρ (calcd.), g cm ⁻³	1.546	1.594
μ (Mo K α), mm ⁻¹	3.461	3.368
θ max, deg.	28.27	28.28
no. of data	3921	3951
no. of parameters	149	203
<i>R</i> ₁	0.0406	0.0586
<i>wR</i> ₂	0.1294	0.1266
GOF	1.022	1.006

	[Tse ^{Mes}]HgI·3MeOH	[Tse ^{Mes}]CoI·3MeCN
lattice	Rhombohedral	Rhombohedral
formula	C ₃₉ H ₅₂ BHgIN ₆ O ₃ Se ₃	C ₄₂ H ₄₉ BCoIN ₉ Se ₃
formula weight	1228.05	1113.42
space group	R-3	R-3
<i>a</i> /Å	14.823(1)	14.7744(8)
<i>b</i> /Å	14.823(1)	14.7744(8)
<i>c</i> /Å	37.136(5)	38.319(2)
α /°	90.00	90.00
β /°	90.00	90.00
γ /°	120.00	120.00
<i>V</i> /Å ³	7066.1(12)	7243.7(7)
<i>Z</i>	6	6
temperature (K)	243	243
radiation (λ , Å)	0.71073	0.71073
ρ (calcd.), g cm ⁻³	1.732	1.531
μ (Mo K α), mm ⁻¹	6.280	3.294
θ max, deg.	28.24	28.23
no. of data	3695	3783
no. of parameters	168	179
<i>R</i> ₁	0.0512	0.0307
<i>wR</i> ₂	0.1315	0.0793
GOF	1.003	1.016

	[Tse ^{Mes}]ZnSPh	[Tse ^{Mes}] ₂ Zn•5MeCN
lattice	Triclinic	Monoclinic
formula	C ₄₂ H ₄₅ BN ₆ SSe ₃ Zn	C ₈₂ H ₉₅ B ₂ N ₁₇ Se ₆ Zn
formula weight	978.96	1879.50
space group	<i>P</i> -1	<i>C</i> 2/ <i>c</i>
<i>a</i> /Å	9.3041(8)	20.640(3)
<i>b</i> /Å	21.886(2)	18.829(3)
<i>c</i> /Å	22.382(2)	24.172(4)
α /°	73.753(2)	90
β /°	85.956(2)	92.623(2)
γ /°	89.978(2)	90
<i>V</i> /Å ³	4363.7(7)	9384(2)
<i>Z</i>	4	4
temperature (K)	243	243
radiation (λ , Å)	0.71073	0.71073
ρ (calcd.), g cm ⁻³	1.490	1.330
μ (Mo K α), mm ⁻¹	3.149	2.673
θ max, deg.	26.02	28.35
no. of data	17021	10934
no. of parameters	973	423
<i>R</i> ₁	0.0791	0.0521
<i>wR</i> ₂ ^a	0.1839	0.0840
GOF	1.109	1.007

	$\{[\text{Tse}^{\text{Mes}}]_2\text{Ga}][\text{GaCl}_4] \cdot 2\text{MeCN}\}$	$\{[\text{Tse}^{\text{Mes}}]_2\text{In}][\text{InCl}_4] \cdot 2\text{MeCN}\}$
lattice	Monoclinic	Monoclinic
formula	$\text{C}_{76}\text{H}_{86}\text{B}_2\text{Cl}_4\text{Ga}_2\text{N}_{14}\text{Se}_6$	$\text{C}_{76}\text{H}_{86}\text{B}_2\text{Cl}_4\text{In}_2\text{N}_{14}\text{Se}_6$
formula weight	1972.21	2062.41
space group	$P2_1/c$	$P2_1/c$
$a/\text{\AA}$	16.366(1)	16.464(1)
$b/\text{\AA}$	22.280(2)	22.369(1)
$c/\text{\AA}$	24.541(2)	24.862(2)
$\alpha/^\circ$	90	90
$\beta/^\circ$	109.217(1)	108.965(1)
$\gamma/^\circ$	90	90
$V/\text{\AA}^3$	8450(1)	8658.9(9)
Z	4	4
temperature (K)	243	243
radiation (λ , \AA)	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.550	1.582
μ (Mo $K\alpha$), mm^{-1}	3.398	3.227
θ max, deg.	28.33	28.32
no. of data	19616	19970
no. of parameters	976	976
R_1	0.0556	0.0425
wR_2	0.1222	0.0528
GOF	1.006	1.016

	$\{[\text{Tse}^{\text{Mes}}]\text{Cu}\}_2 \cdot 6\text{MeCN}$	$\{[\text{Tm}^{\text{Mes}}]\text{Cu}\}_2 \cdot 6\text{MeCN}$
lattice	Triclinic	Triclinic
formula	$\text{C}_{84}\text{H}_{98}\text{B}_2\text{Cu}_2\text{N}_{18}\text{Se}_6$	$\text{C}_{84}\text{H}_{98}\text{B}_2\text{Cu}_2\text{N}_{18}\text{S}_6$
formula weight	1982.26	1700.86
space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> /Å	13.111(3)	12.835(2)
<i>b</i> /Å	13.614(3)	13.514(2)
<i>c</i> /Å	15.098(3)	15.052(2)
α /°	69.291(4)	70.472(4)
β /°	81.177(3)	83.347(3)
γ /°	63.195(4)	64.730(3)
<i>V</i> /Å ³	2249.9(9)	2224.1(6)
<i>Z</i>	1	1
temperature (K)	243	243
radiation (λ , Å)	0.71073	0.71073
ρ (calcd.), g cm ⁻³	1.463	1.270
μ (Mo K α), mm ⁻¹	2.952	0.672
θ max, deg.	23.26	25.00
no. of data	5974	7417
no. of parameters	512	506
R_1	0.0508	0.0683
wR_2^a	0.1098	0.1740
GOF	1.245	1.083

	[Tse ^{Mes}]Re(CO) ₃ ·5C ₆ H ₆	[Tm ^{Mes}]Re(CO) ₃ ·4C ₆ H ₆
lattice	Monoclinic	Monoclinic
formula	C ₆₉ H ₇₀ BN ₆ O ₃ ReSe ₃	C ₆₃ H ₆₄ BN ₆ O ₃ ReS ₃
formula weight	1465.20	1246.39
space group	<i>P2₁/c</i>	<i>P2₁/n</i>
<i>a</i> /Å	10.3336(7)	10.1948(9)
<i>b</i> /Å	21.623(2)	21.590(2)
<i>c</i> /Å	30.390(2)	27.969(2)
α /°	90	90
β /°	92.894(2)	96.845(2)
γ /°	90	90
<i>V</i> /Å ³	6781.7(9)	6112.2(9)
<i>Z</i>	4	4
temperature (K)	243	243
radiation (λ , Å)	0.71073	0.71073
ρ (calcd.), g cm ⁻³	1.435	1.354
μ (Mo K α), mm ⁻¹	3.450	2.139
θ max, deg.	28.30	28.32
no. of data	15488	14302
no. of parameters	753	687
<i>R</i> ₁	0.0500	0.0705
<i>wR</i> ₂	0.1164	0.1183
GOF	1.027	1.009

