Electronic Supporting Information for

Cadmium complexes bearing ^{Me2}N^E^O$^-$ (E = S, Se) organochalcogenoalkoxides and their zinc and mercury analogues

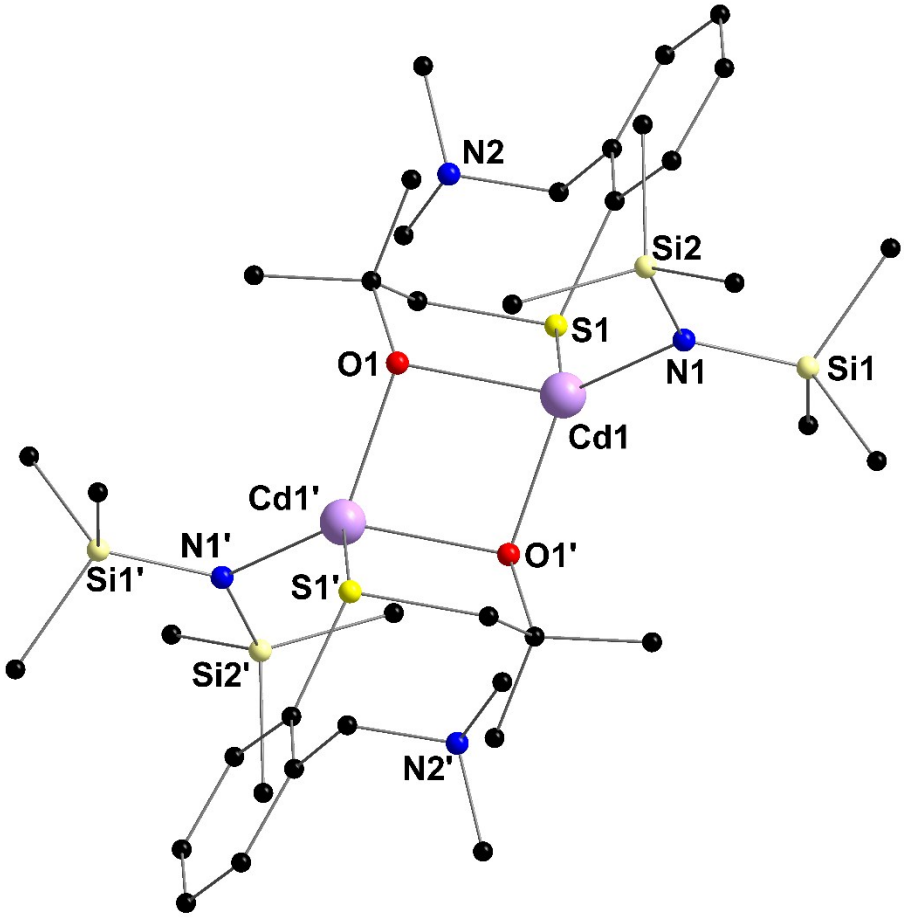
Alexandra Pop,[a] Clément Bellini,[b] Răzvan Șuteu,[a] Vincent Dorcet,[b] Thierry Roisnel,[b] Jean-François Carpentier,[b] Anca Silvestru*[a] and Yann Sarazin*[b]

[a] Supramolecular Organic and Organometallic Chemistry Centre, Chemistry Department, Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, RO-400028 Cluj-Napoca, Romania. E-mail: ancas@chem.ubbcluj.ro; Fax: (+40) 264-590818; Tel: (+40) 264-593833

[b] Université de Rennes 1, CNRS, Institut des Sciences Chimiques de Rennes, UMR 6226, Campus de Beaulieu, F-35042 Rennes Cedex, France. E-mail: yann.sarazin@univ-rennes1.fr; Fax: (+33) 2 23 23 69 39; Tel: (+33) 2 23 23 30 19

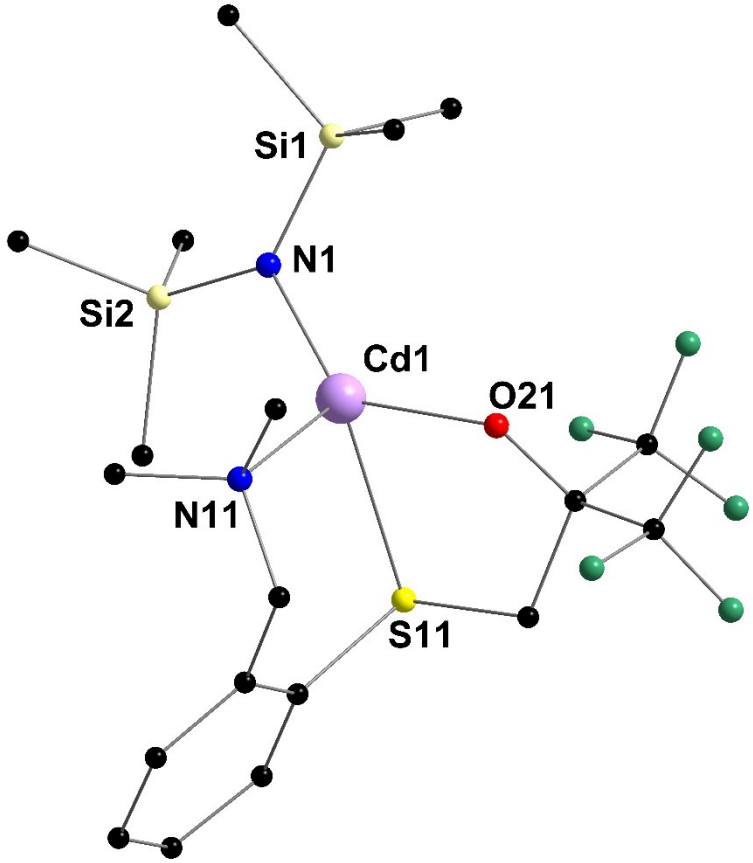
Contents

Figure S1. X-ray structure of [{$L^{S,(CH3)2}$}$CdN(SiMe_3)_2]_2$ ([**1**]$_2$)



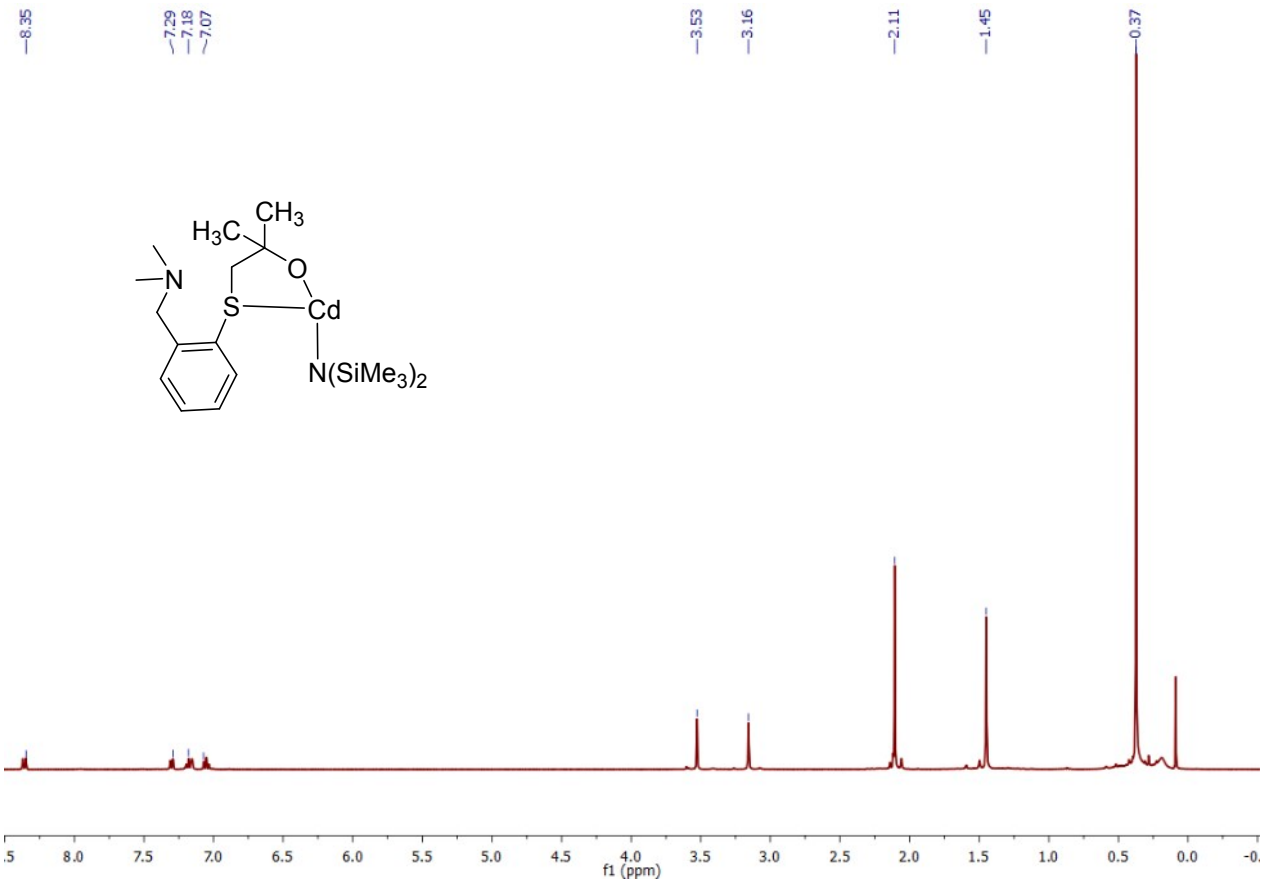
Rendering of the molecular solid-state structure of [{$L^{S,(CH3)2}$}$CdN(SiMe_3)_2]_2$ ([**1**]$_2$). H atoms omitted for clarity. Selected bond lengths (Å) and angles (°): Cd1-N1 = 2.099(2), C1-O1 = 22.1903(16), Cd1-O1' = 22.1975(17), Cd1-S1' = 22.7390(6); N(1)-Cd(1)-O(1) = 2128.96(7), N1-Cd1-O1' = 2136.79(8), O1-Cd1-O1' = 281.34(6), N1-Cd1-S1' = 2117.18(6), O1-Cd1-S1' = 2100.40(5), O1#1-Cd1-S1' = 278.18(5).

Figure S2. X-ray structure of [{$L^{S,(CF3)2}$}$CdN(SiMe_3)_2$] (**3**)



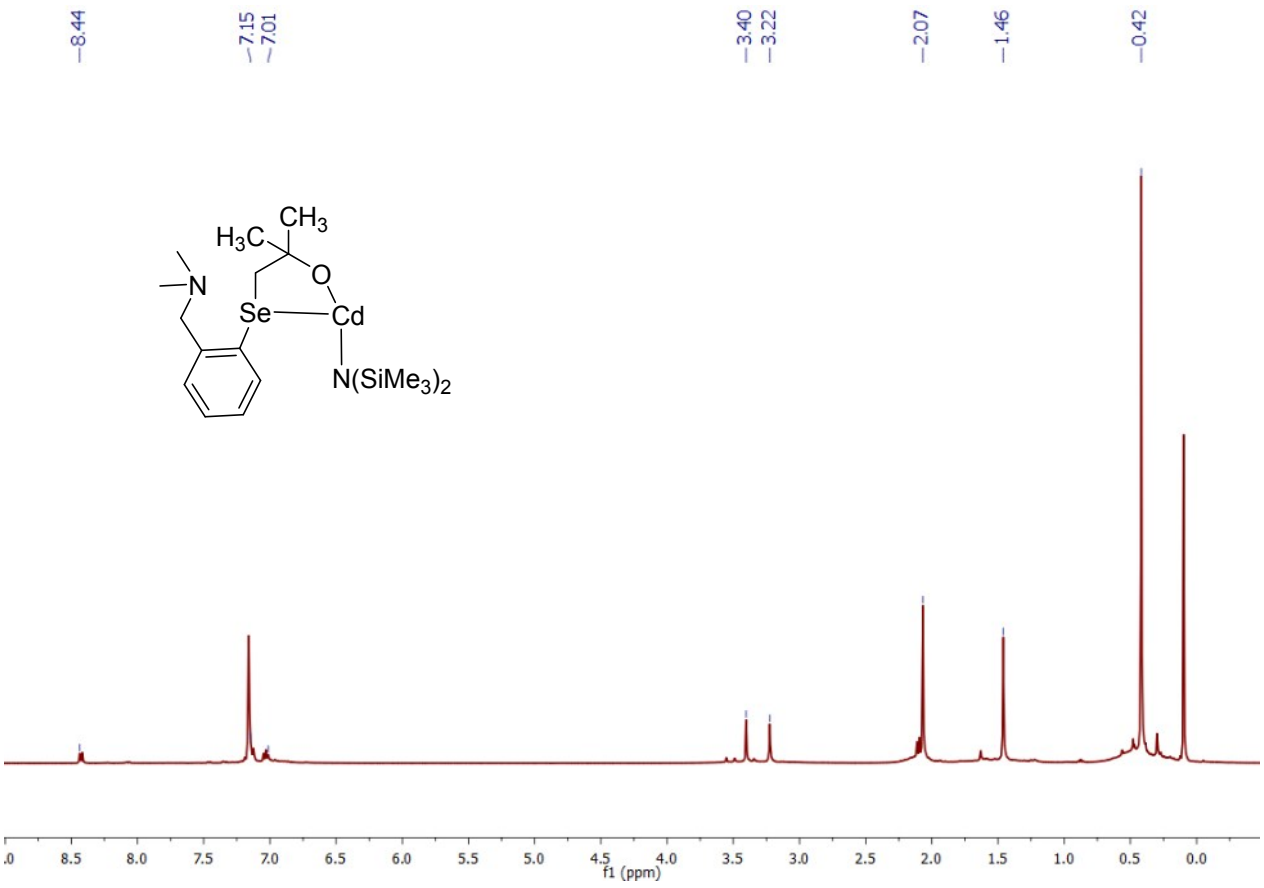
Rendering of the molecular solid-state structure of [{$L^{S,(CF3)2}$}$CdN(SiMe_3)_2$] (**3**). H atoms omitted for clarity. Selected bond lengths (Å) and angles (°): Cd1-N1 = 2.0849(15), Cd1-O21 = 2.1504(13), Cd1-N11 = 2.3384(15), Cd1-S11 = 2.6563(5); N1-Cd1-O21 = 136.04(6), N1-Cd1-N11 = 119.19(6), O21-Cd1-N11 = 89.33(5), N1-Cd1-S11 = 126.91(5), O21-Cd1-S11 = 79.22(4), N11-Cd1-S11 = 93.04(4).

Figure S3. ^{1}H NMR spectrum of complex **1**



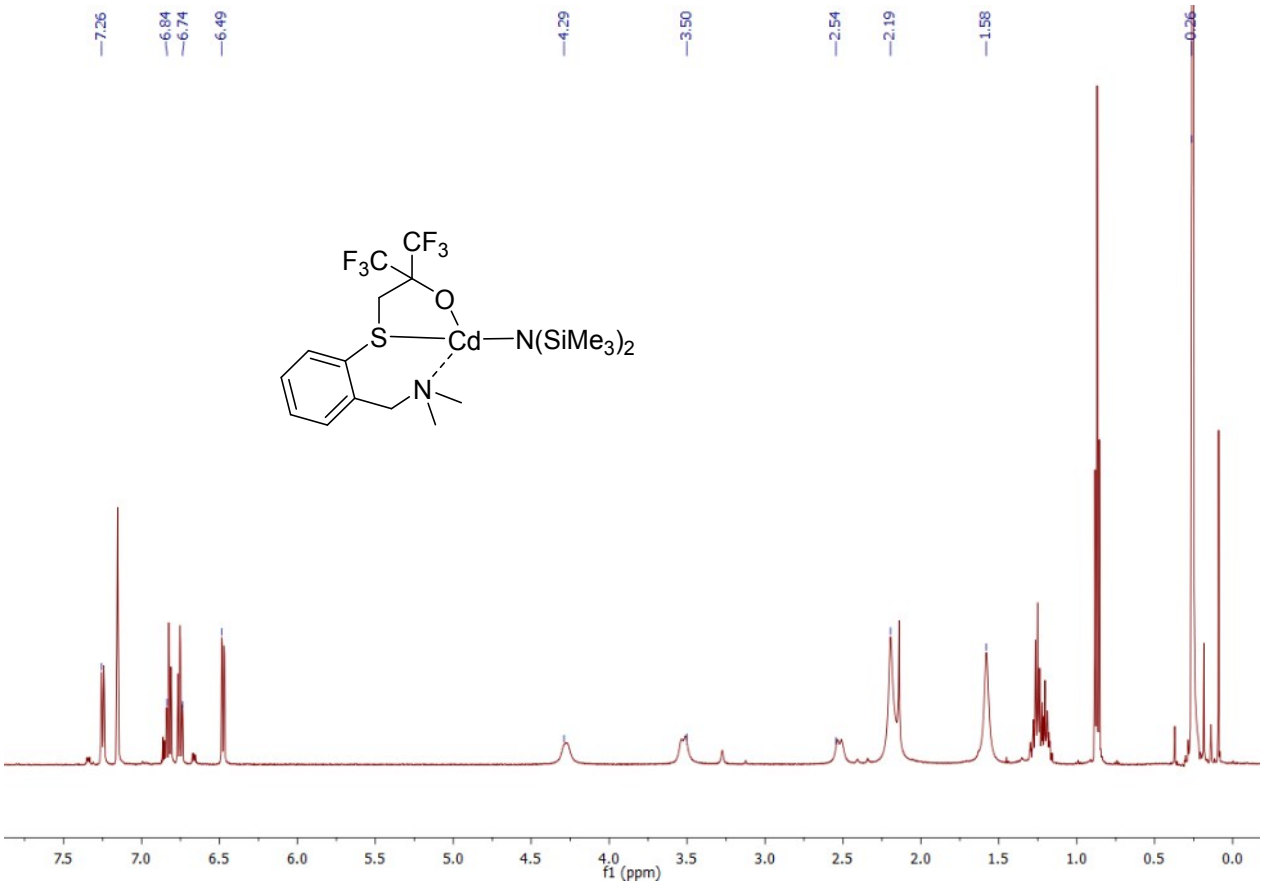
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 8.35 (dd, $^{4}J_{HH}$ = 1.1 Hz, $^{3}J_{HH}$ = 7.8 Hz, 1H, arom-H_6), 7.29 (dd, $^{4}J_{HH}$ = 1.3 Hz, $^{3}J_{HH}$ = 7.7 Hz, 1H, arom-H_3), 7.18 (dt, $^{4}J_{HH}$ = 1.6 Hz, $^{3}J_{HH}$ = 7.6 Hz, 1H, arom-H_5), 7.07 (dt, $^{4}J_{HH}$ = 1.1 Hz, $^{3}J_{HH}$ = 7.5 Hz, 1H, arom-H_5), 3.53 (s, 2H, ArCH_2N), 3.16 (s, 2H, SCH_2), 2.11 (s, 6H, N(CH_3)$_2$), 1.45 (s, 6H, C(CH_3)$_2$O), 0.37 (s, 18H, SiCH_3) ppm.

Figure S4. ^{1}H NMR spectrum of complex **2**



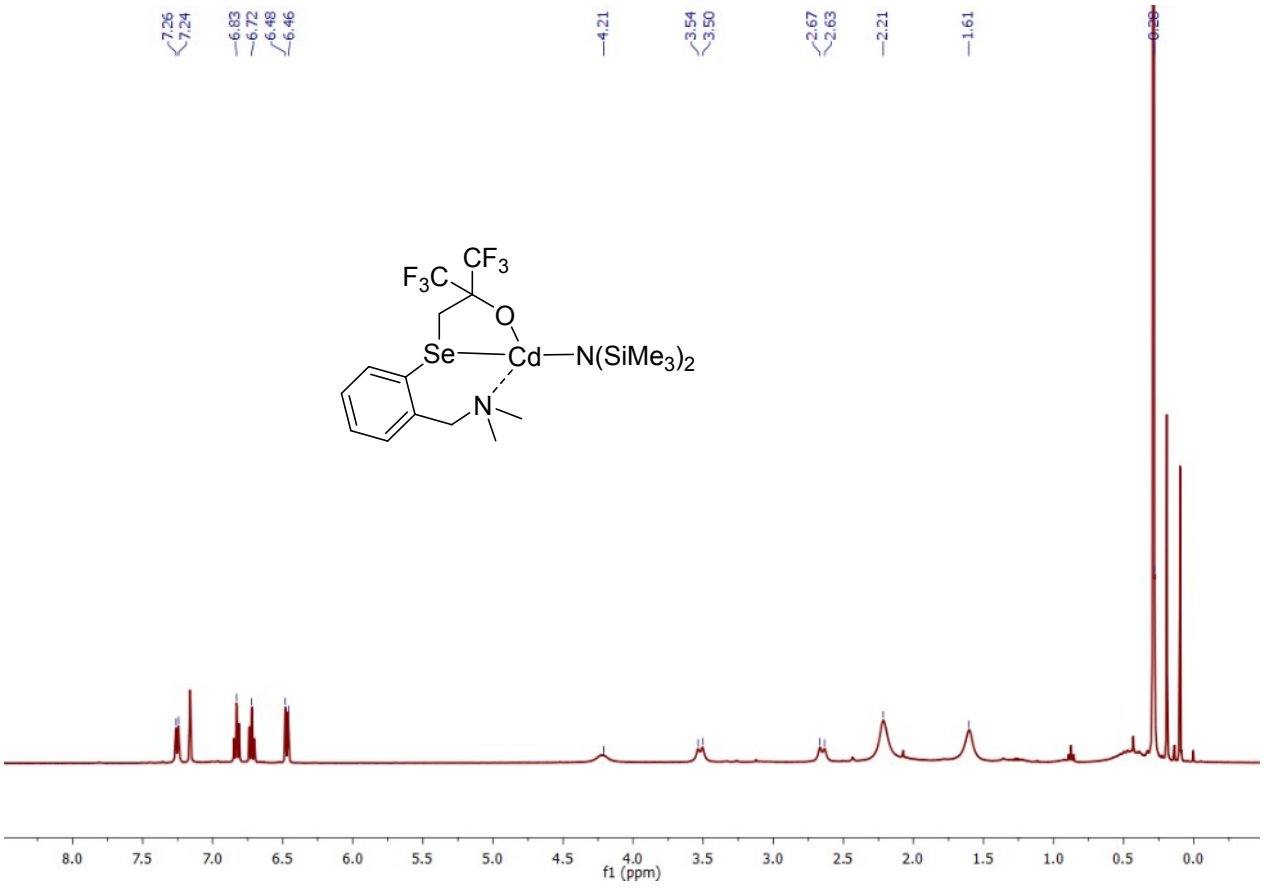
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 8.44 (dd, $^{4}J_{HH}$ = 1.0 Hz, $^{3}J_{HH}$ = 7.7 Hz, 1H, arom-H_6), 7.13-7.17 (overlapping m, 2H, arom-H_3 + arom-H_4), 7.03 (dt, $^{4}J_{HH}$ = 1.0 Hz, $^{3}J_{HH}$ = 7.4 Hz, 1H, arom-H_5), 3.40 (s, 2H, ArCH_2N), 3.22 (s, 2H, SeCH_2), 2.07 (s, 6H, NCH_3), 1.46 (s, 6H, C(CH_3)$_2$O), 0.42 (s, 18H, SiCH_3) ppm.

Figure S5. ^{1}H NMR spectrum of complex **3**



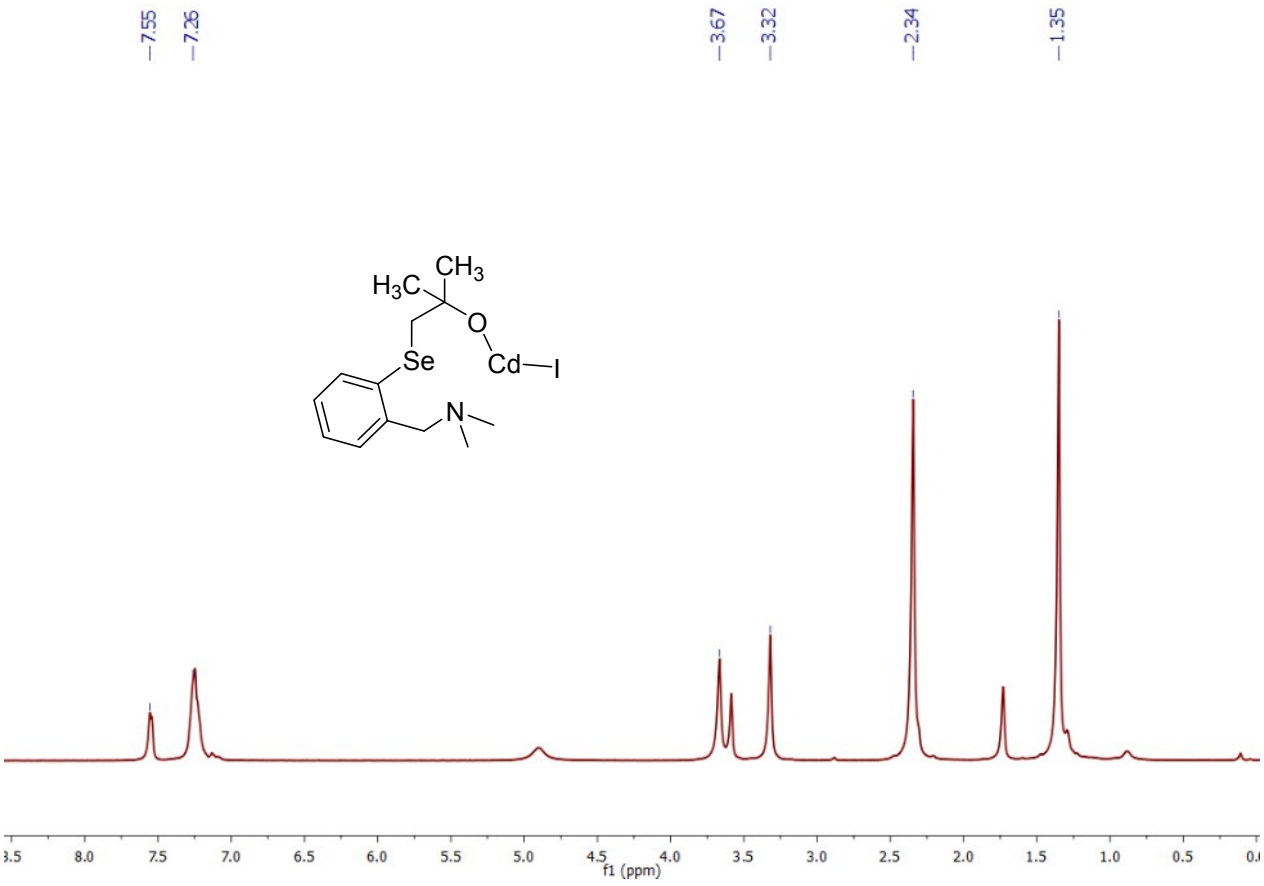
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 7.26 (d, $^{3}J_{HH}$ = 7.9 Hz, 1H, arom-H_6), 6.84 (dt, $^{4}J_{HH}$ = 1.4, $^{3}J_{HH}$ = 7.4 Hz, 1H, arom-H_5), 6.74 (dt, $^{4}J_{HH}$ = 1.5 Hz, $^{3}J_{HH}$ = 7.5 Hz, 1H, arom-H_4), 6.49 (dd, $^{4}J_{HH}$ = 1.6 Hz, $^{3}J_{HH}$ = 7.4 Hz, 1H, arom-H_3), 4.29 (br m, 1H, SCH_2), 3.50 (d, $^{2}J_{HH}$ = 13.2 Hz, 1H, ArCH*H*N), 2.54 (d, $^{2}J_{HH}$ = 13.2 Hz, 1H, ArC*H*HN), 2.19 (overlapping m, 4H, SCH_2 + NCH_3), 1.58 (s, 3H, NCH_3), 0.26 (s, 18H, SiCH_3) ppm.

Figure S6. ^{1}H NMR spectrum of complex **4**



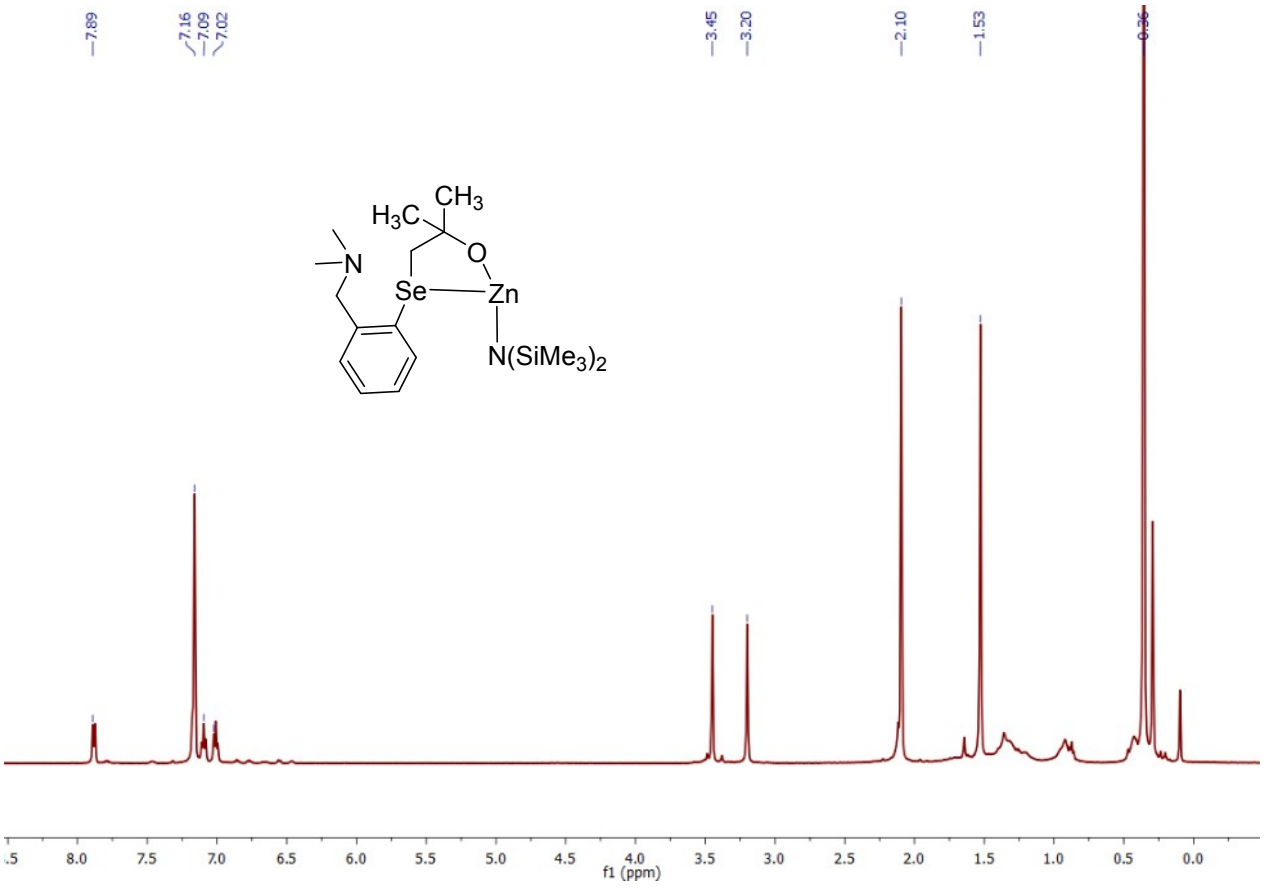
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 7.25 (d, $^{3}J_{HH}$ = 8.0 Hz, 1H, arom-H_6), 6.83 (dt, $^{4}J_{HH}$ = 1.4, $^{3}J_{HH}$ = 7.4 Hz, 1H, arom-H_5), 6.72 (dt, $^{4}J_{HH}$ = 1.6 Hz, $^{3}J_{HH}$ = 7.6 Hz, 1H, arom-H_4), 6.47 (dd, $^{4}J_{HH}$ = 1.3 Hz, $^{3}J_{HH}$ = 7.8 Hz, 1H, arom-H_3), 4.21 (br s, 1H, SeCH*H*), 3.52 (d, $^{2}J_{HH}$ = 13.0 Hz, 1H, ArCH*H*N), 2.65 (d, $^{2}J_{HH}$ = 13.0 Hz, 1H, ArC*H*HN), 2.21 (overlapping m, 4H, SeC*H*H + NCH_3), 1.61 (s, 3H, NCH_3), 0.25 (s, 18H, SiCH_3) ppm.

Figure S7. ^{1}H NMR spectrum of complex **5**



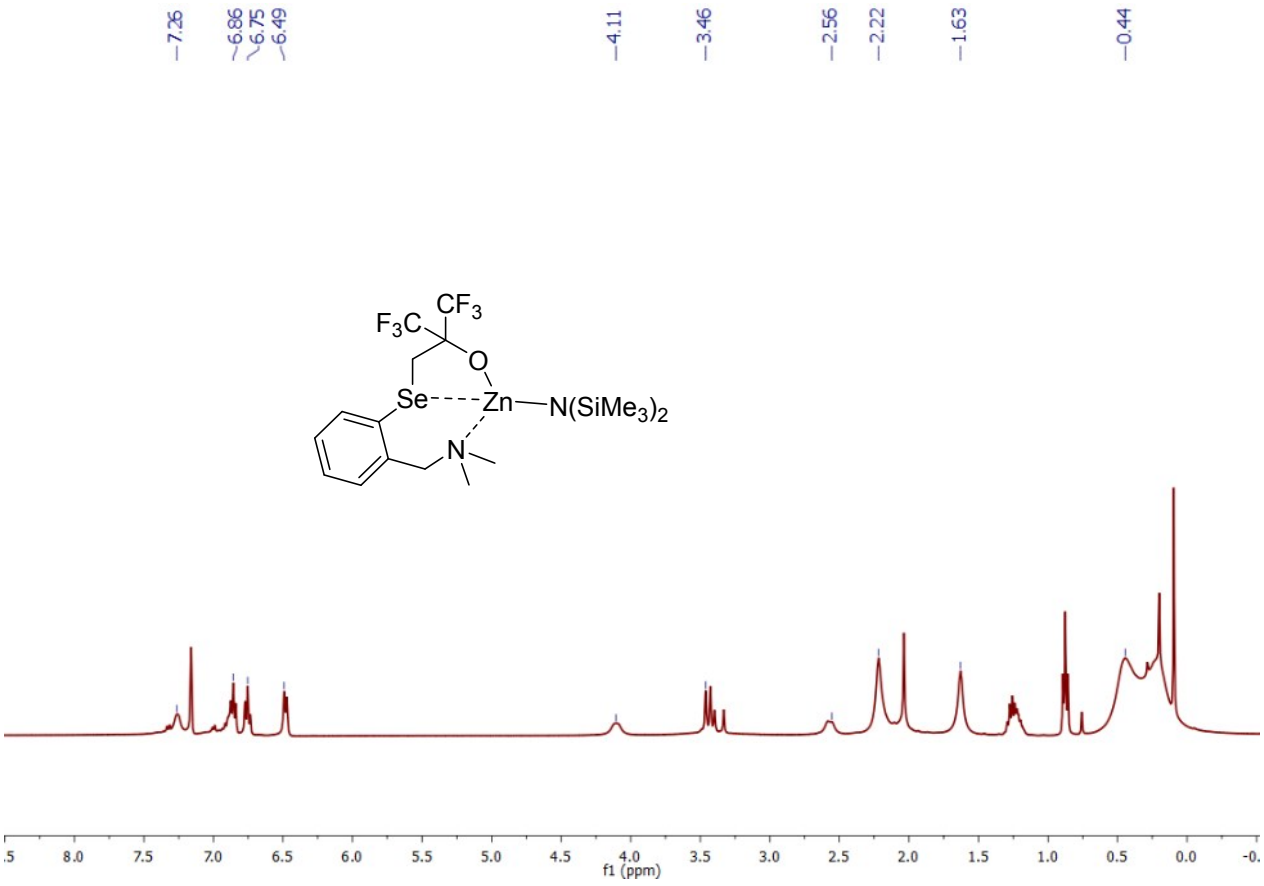
^{1}H NMR (THF-d_8, 500.1 MHz, 298 K): δ = 7.56 (d, $^{3}J_{HH}$ = 8.3 Hz, 1H, arom-H_6), 7.22-7.27 (m, 3H, arom-H_3 + arom-H_4 + arom-H_5), 3.67 (s, 2H, ArCH_2N), 3.32 (s, 2H, SeCH_2), 2.34 (s, 6H, NCH_3), 1.35 (s, 6H, C(CH_3)$_2$O) ppm.

Figure S8. ^{1}H NMR spectrum of complex **6**



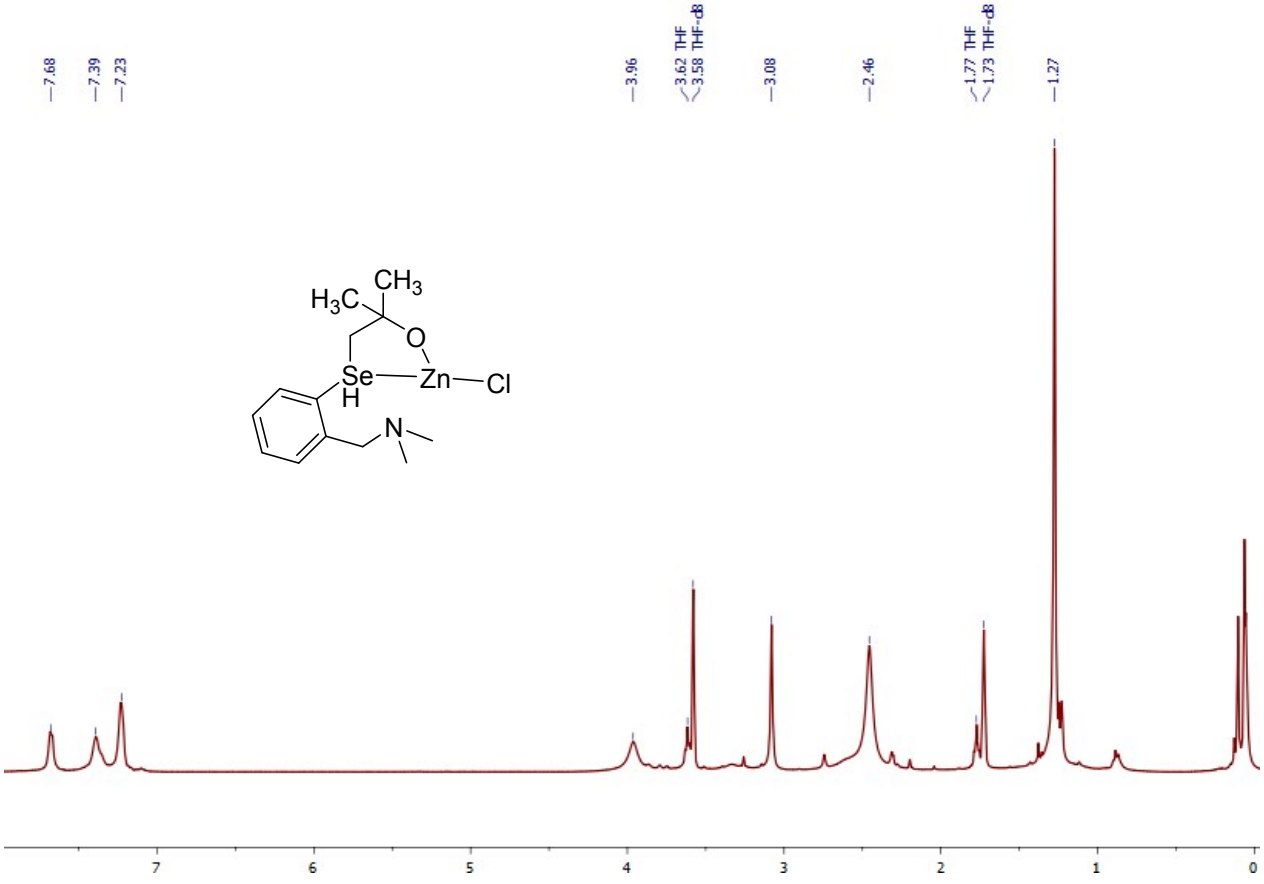
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 7.89 (d, 1H, $^{3}J_{HH}$ = 8.7 Hz, arom-H_6), 7.16 (m, 1H, arom-H_3), 7.09 (t, 1H, $^{3}J_{HH}$ = 7.7 Hz, arom-H_4), 7.02 (t, 1H, $^{3}J_{HH}$ = 7.3 Hz, arom-H_5), 3.45 (s, 2H, ArCH_2N), 3.20 (s, 2H, SeCH_2), 2.10 (s, 6H, N(CH_3)$_2$), 1.53 (s, 6H, C(CH_3)$_2$O), 0.36 (s, 18H, SiCH_3) ppm.

Figure S9. ^{1}H NMR spectrum of complex **7**



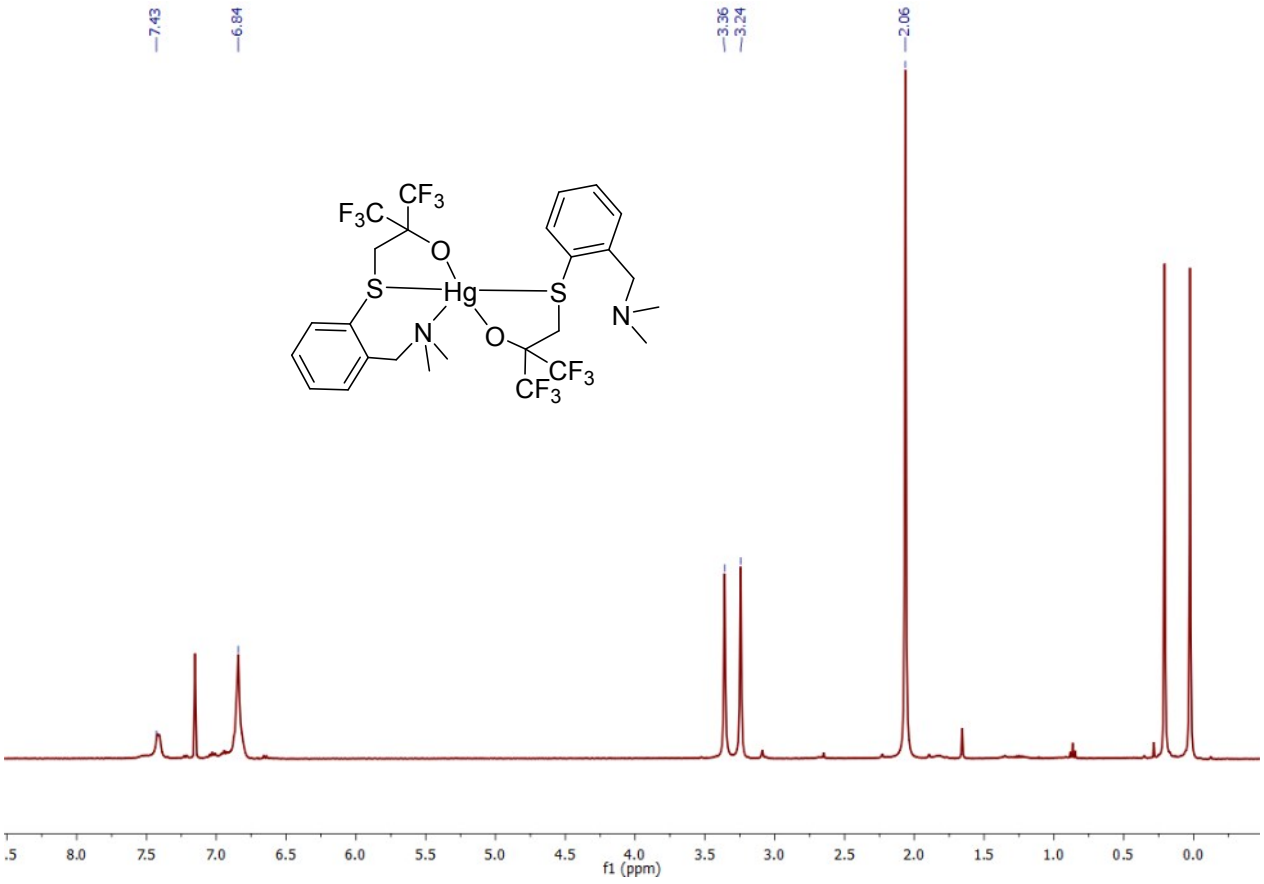
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 7.26 (br m, 1H, arom-H_6), 6.86 (t, $^{3}J_{HH}$ = 7.60 Hz, 1H, arom-H_5), 6.75 (t, $^{3}J_{HH}$ = 7.7 Hz, 1H, arom-H_4), 6.49 (d, $^{3}J_{HH}$ = 7.4 Hz, 1H, arom-H_3), 4.11 (br m, 1H, SeCHH), 3.46 (d, $^{2}J_{HH}$ = 13.5 Hz, 2H, ArCH_2N), 2.56 (br m, 1H SeCHH), 2.22 (s, 3H, NCH_3), 1.63 (s, 3H, NCH_3), 0.44 (br, 18H, SiCH_3) ppm.

Figure S10. ^{1}H NMR spectrum of complex **8**



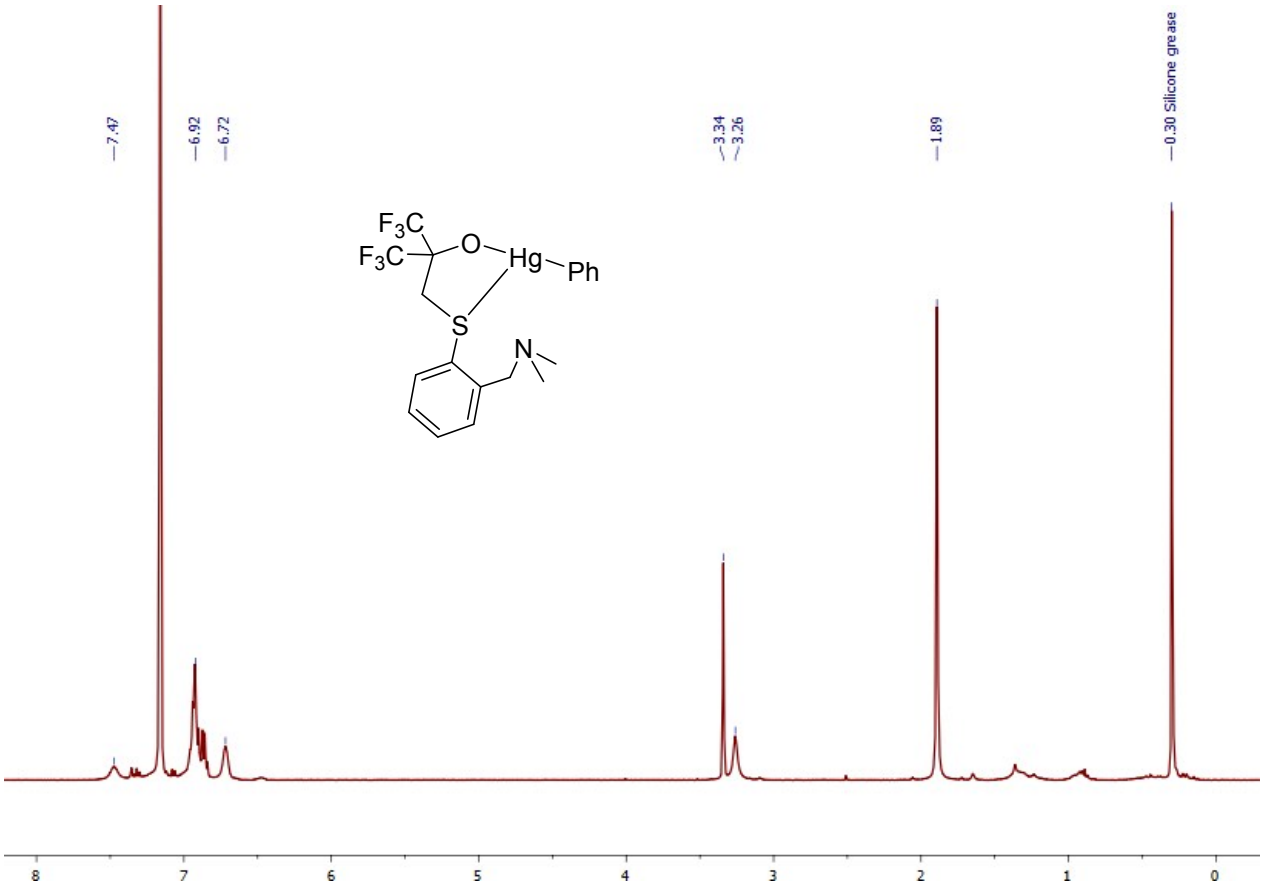
^{1}H NMR (THF-d_8, 400.1 MHz, 298 K): δ = 7.68 (br, 1H, arom-H_6), 7.39 (br, 1H, arom-H_3), 7.23 (overlapping m, 2H, arom-H_4 + arom-H_5), 3.96 (s, 2H, ArCH_2N), 3.08 (s, 2H, SeCH_2), 2.46 (br s, 6H, NCH_3), 1.27 (s, 6H, C(CH_3)$_2$O) ppm.

Figure S11. ^{1}H NMR spectrum of complex **9**



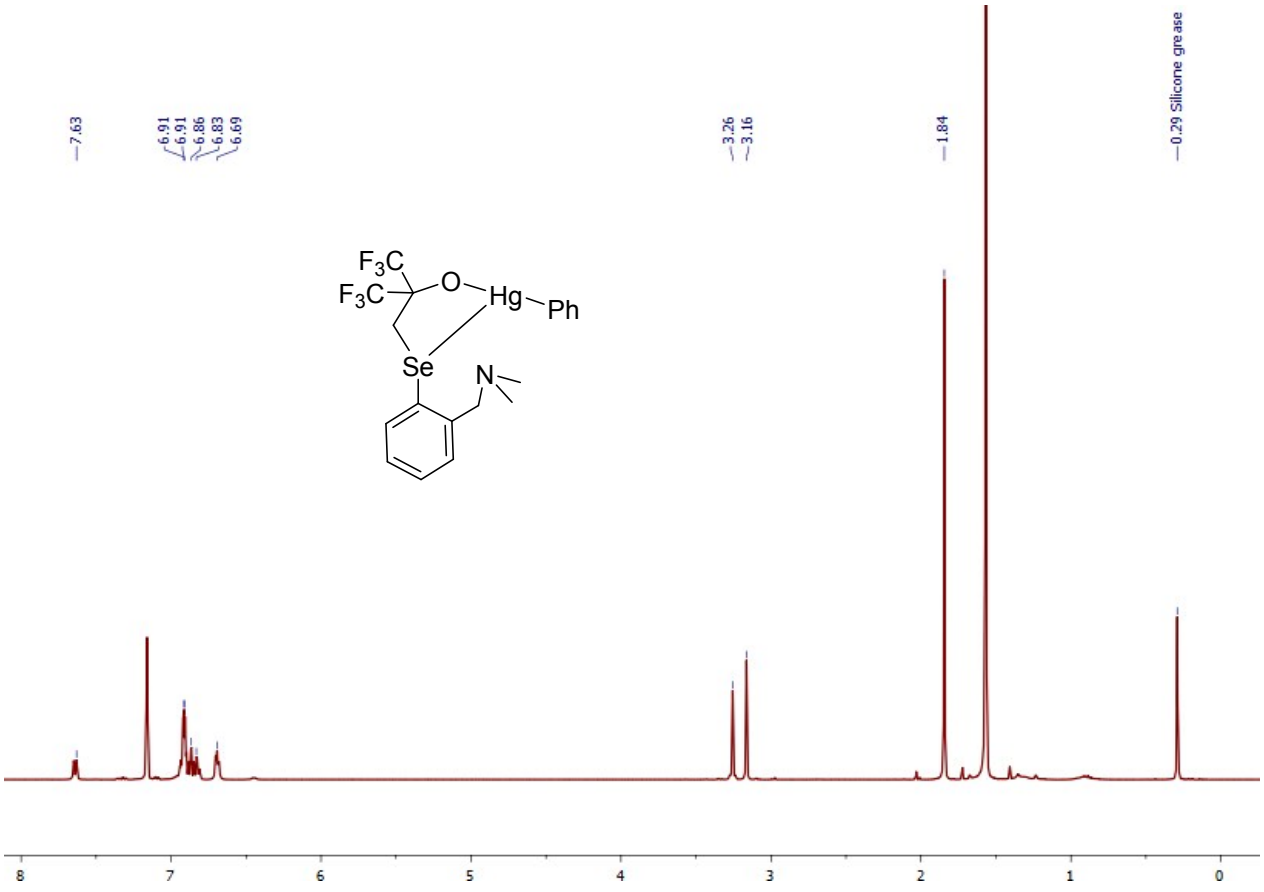
^{1}H NMR (benzene-d_6, 500.1 MHz, 298 K): δ = 7.43 (br., s, 2H, arom-H_6), 6.84 (overlapping m, 6H, arom-H_3 + arom-H_5 + arom-H_4), 3.36 (br s, 4H, SCH_2), 3.24 (br s, 4H, ArCH_2N), 2.06 (br s, 12H, NCH_3) ppm.

Figure S12. ^{1}H NMR spectrum of complex **10**



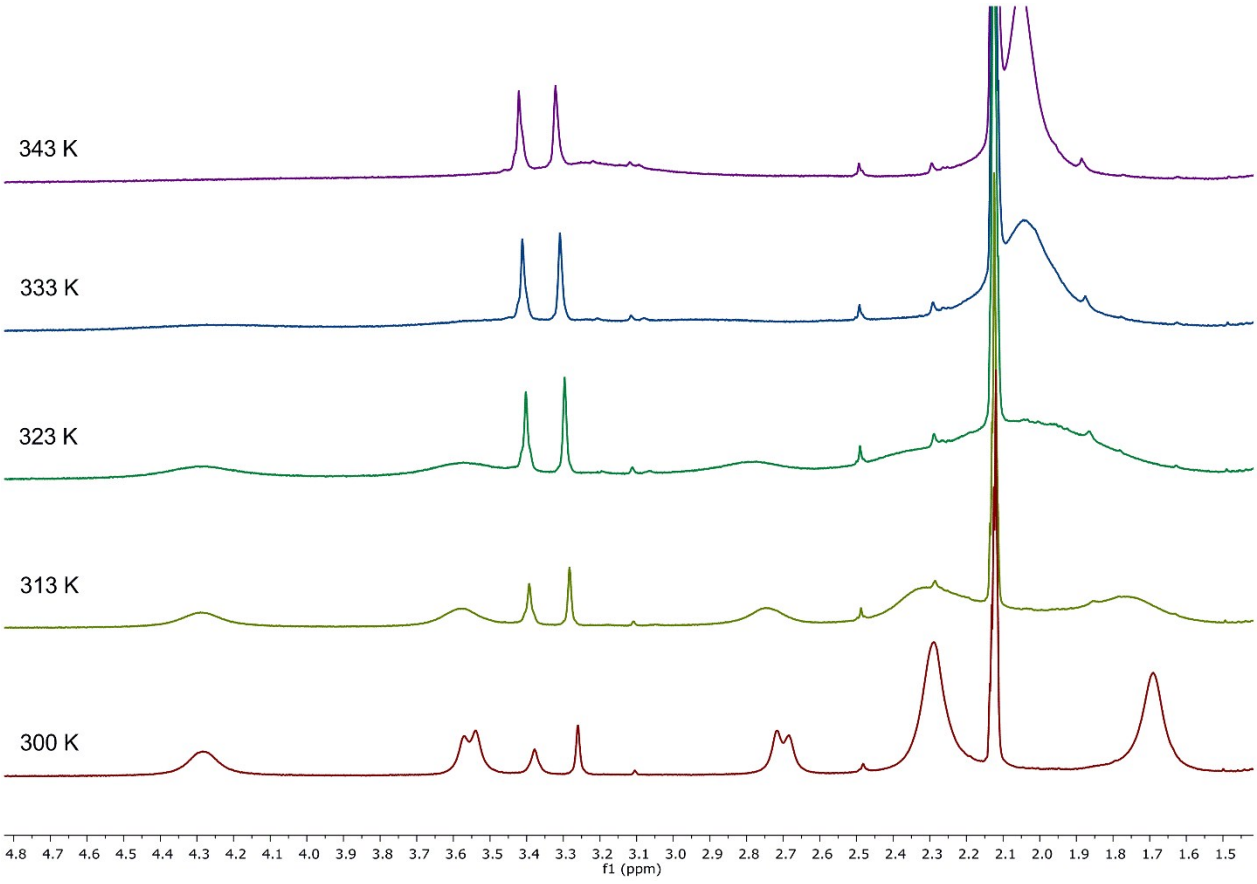
^{1}H NMR (benzene-d_6, 400.1 MHz, 298 K): δ = 7.47 (br, 1H, arom-H_6), 6.92 (overlapping m, 4H, *o*-C_6H_5 + *m*-C_6H_5), 6.85 (overlapping m, 2H, arom-H_4 + arom-H_5), 6.72 (overlapping m, 2H, arom-H_3 + *p*-C_6H_5), 3.34 (s, 2H, ArCH_2N), 3.26 (s, 2H, SCH_2), 1.89 (s, 6H, NCH_3) ppm.

Figure S13. ^{1}H NMR spectrum of complex **11**



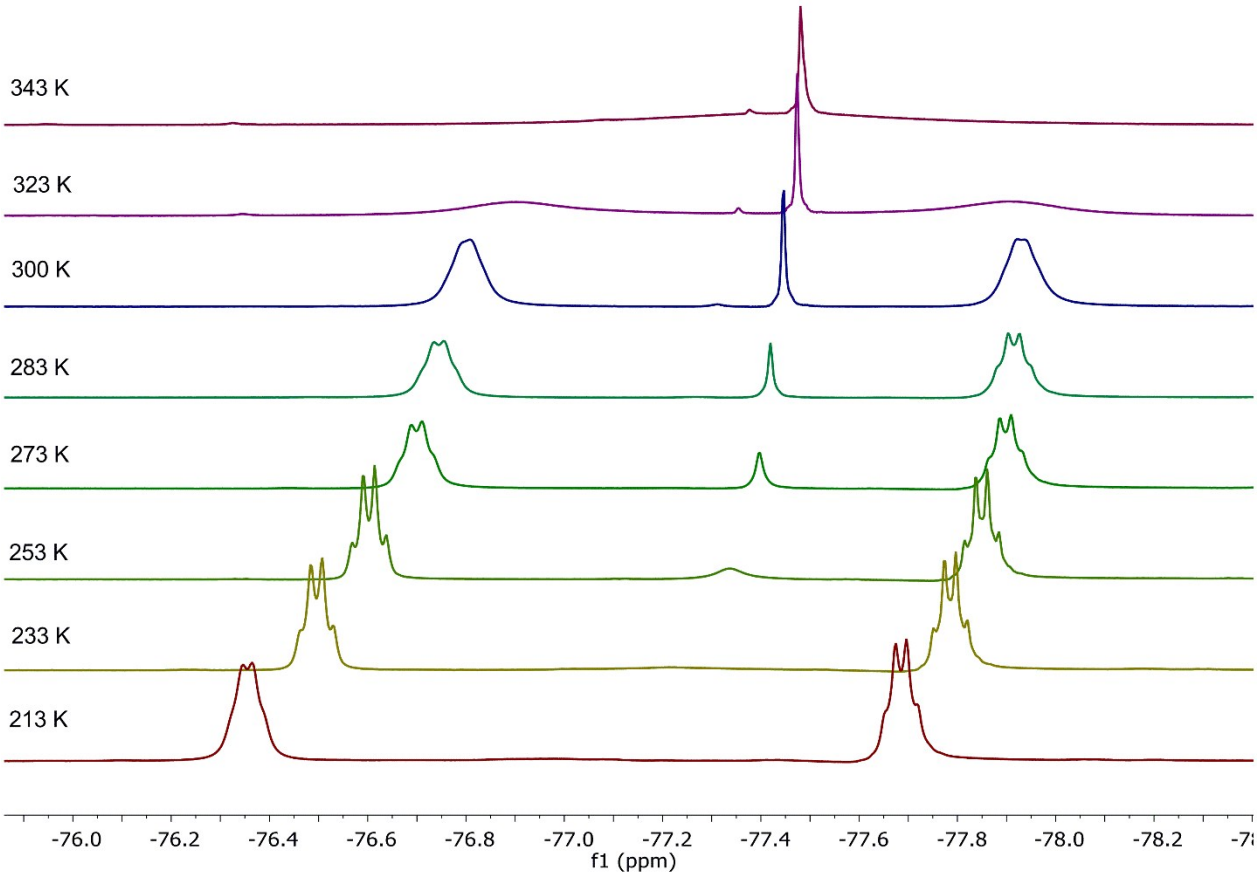
^{1}H NMR (benzene-d_6, 400.1 MHz, 298 K): δ = 7.63 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, arom-CH_6), 6.91 (overlapping m, 4H, *o*-C$_6H_5$ + *m*-C$_6H_5$), 6.86 (overlapping m, 2H, arom-H_4 + arom-H_5), 6.83 (d, $^{3}J_{HH}$ = 7.1 Hz, 1H, arom-H_3), 6.69 (m, 1H, *p*-C$_6H_5$), 3.26 (s, 2H, ArCH_2N), 3.16 (s, 2H, SeCH_2), 1.84 (s, 6H, NCH_3) ppm. Peak at 1.55 ppm = residual rinsing acetone.

Figure S14. ^{1}H VT NMR for complex **4**



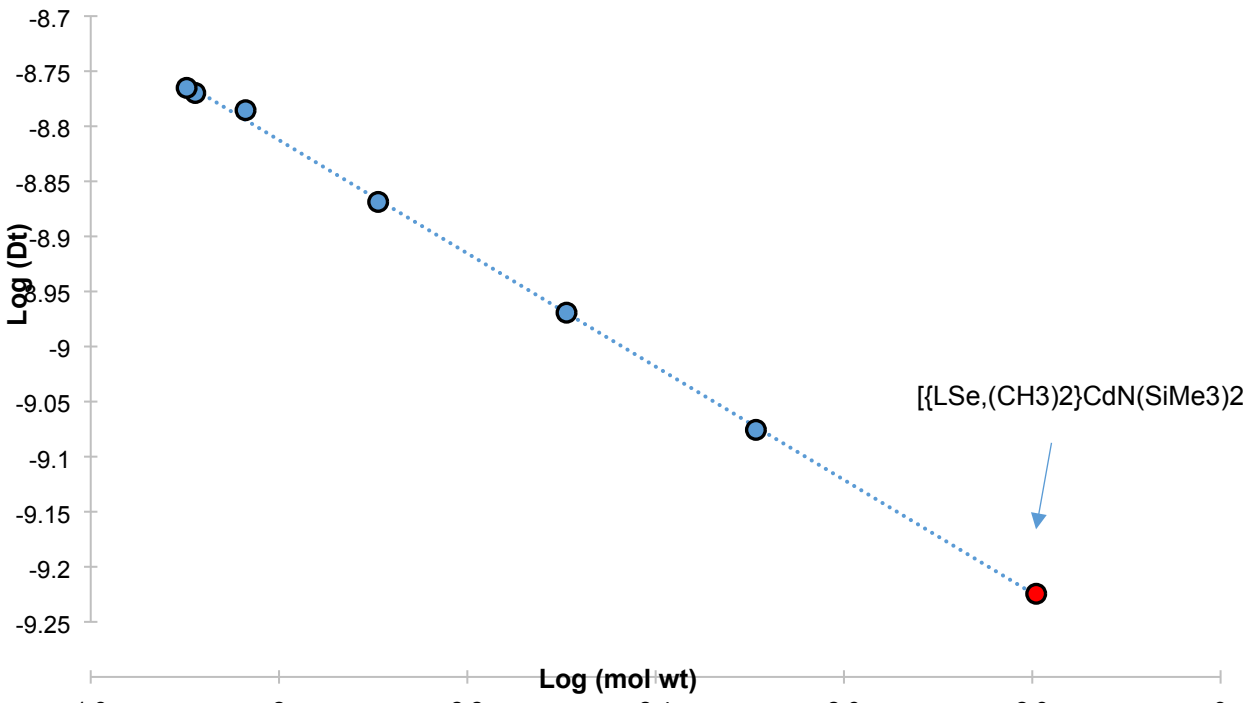
^{1}H VT NMR (toluene-d_8, 400.1 MHz) for [{$L^{Se,(CF3)2}$}CdN($SiMe_3$)$_2$] (**4**).

Figure S15. ^{19}F VT NMR for complex **4**



^{19}F VT NMR (toluene-d_8, 376.2 MHz) for [{$L^{Se,(CF3)2}$}$CdN(SiMe_3)_2$] (**4**).

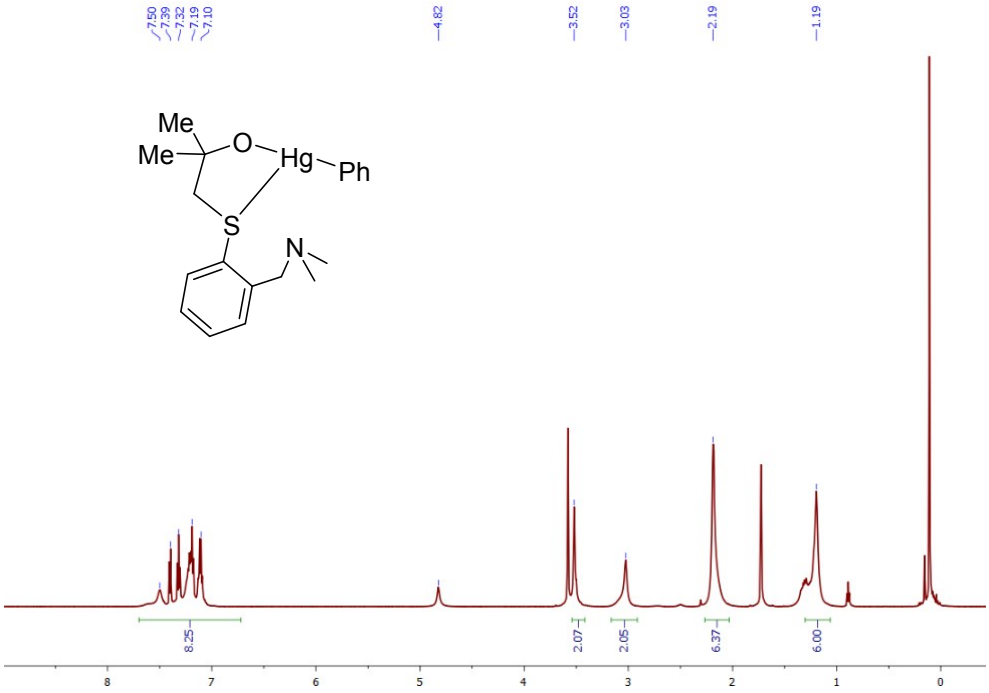
Figure S16. Diffusion – molecular weight analysis for complex **2**



Diffusion-molecular weight analysis for $[\{L^{Se,(CH3)2}\}CdN(SiMe_3)_2]_2$ in benzene-d_6 at 293 K. Calibrants: benzene, pyridine, toluene, naphthalene, pyrene, tetrakis(trimethylsilyl)silane (resp. 78.1, 79.1, 92.1, 128.1, 202.1 and 320.8 $g \cdot mol^{-1}$).

Figure S17. Synthesis and ^{1}H NMR spectrum of [{L$^{S,(CH3)2}$}HgPh] (**12**).

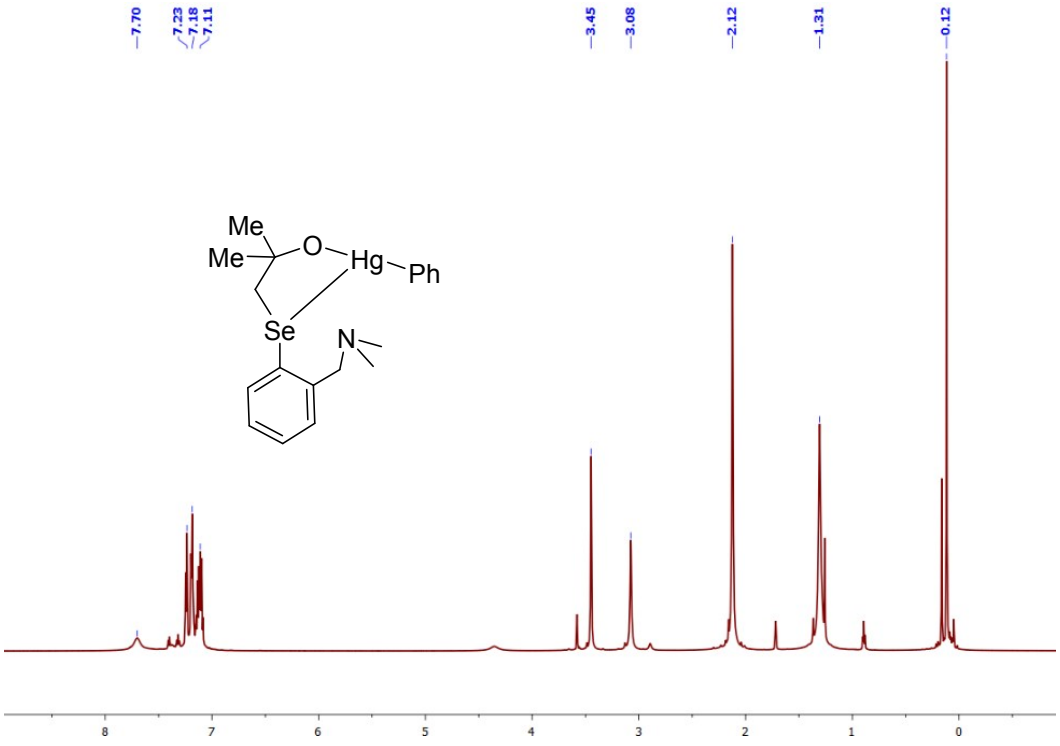
[PhHgN(SiMe$_3$)$_2$] (0.46 g, 1.04 mmol) was dissolved in THF (10 mL), and a solution of {L$^{S,(CH3)2}$}H (0.25 g, 1.04 mmol) in THF (15 mL) was added dropwise at room temperature. The reaction mixture was stirred overnight at room temperature, and the solvent was removed under vacuum. Compound **12** was obtained as an oily material upon washing with *n*-hexane (3×5 mL). Yield 0.29 g (55%). ^{1}H NMR (THF-d_8, 400.1 MHz, 298 K): δ = 7.50 (br, 1H, arom-C$_6$*H*), 7.39 (d, $^{3}J_{HH}$ = 7.7 Hz, 1H, arom-C$_3$*H*), 7.32 (m, 2H, arom-C$_4$*H* + arom-C$_5$*H*), 7.19 (m, 2H, *o*-C$_6$*H*$_5$), 7.10 (overlapping m, 3H, *m*-C$_6$*H*$_5$ + *p*-C$_6$*H*$_5$), 3.52 (s, 2H, ArC*H*$_2$N), 3.03 (s, 2H, SC*H*$_2$), 2.19 (s, 6H, NC*H*$_3$), 1.19 (s, 6H, C(C*H*$_3$)$_2$O) ppm. ^{13}C{^{1}H} NMR (THF-d_8, 100.6 MHz, 298 K): δ = 140.13 (arom-*C*$_1$), 138.69 (arom-*C*$_2$), 138.18 (arom-*C*$_3$), 132.71 (*i*-*C*$_6$H$_5$), 131.06 (arom-*C*$_6$), 129.23 (arom-*C*$_5$), 129.02 (arom-*C*$_4$), 128.86 (*p*-*C*$_6$H$_5$), 128.41 (*o*-*C*$_6$H$_5$), 126.68 (*m*-*C*$_6$H$_5$), 70.88 (*C*(CH$_3$)$_2$O), 63.22 (Ar*C*H$_2$N), 51.17 (S*C*H$_2$), 45.46 (N*C*H$_3$), 29.71 (C(*C*H$_3$)$_2$O) ppm. ^{199}Hg{^{1}H} NMR (THF-d_8, 71.6 MHz, 298 K) : δ = –801 ppm.



^{1}H NMR of [{L$^{S,(CH3)2}$}HgPh] (**12**) (THF-d_8, 400.1 MHz, 298 K)

Figure S18. Synthesis and ^{1}H NMR spectrum of [{L$^{Se,(CH3)2}$}HgPh] (**13**).

Following the protocol given for **12**, [PhHgN(SiMe$_3$)$_2$] (0.25 g, 0.57 mmol) was reacted with {L$^{Se,(CH3)2}$}H (0.16 g, 0.57 mmol) to give **13** which was isolated as an oily material (0.15 g, 48%). ^{1}H NMR (THF-d_8, 400.1 MHz, 298 K): δ = 7.70 (br, 1H, arom-C$_6$*H*), 7.23 (br, 1H, arom-C$_3$*H*), 7.18 (overlapping m, 4H, arom-C$_4$*H* + arom-C$_5$*H* + *o*-C$_6$*H*$_5$), 7.11 (overlapping m, 3H, *m*-C$_6$*H*$_5$ + *p*-C$_6$*H*$_5$), 3.45 (s, 2H, ArC*H*$_2$N), 3.08 (s, 2H, SeC*H*$_2$), 2.12 (s, 6H, NC*H*$_3$), 1.31 (s, 6H, C(C*H*$_3$)$_2$O) ppm. ^{13}C{^{1}H} NMR (THF-d_8, 100.6 MHz, 298 K): δ = 141.32 (arom-*C*$_1$), 138.70 (arom-*C*$_2$), 138.17 (arom-*C*$_3$), 136.03 (*i*-*C*$_6$H$_5$), 133.85 (arom-*C*$_6$), 130.67 (arom-*C*$_5$), 129.27 (arom-*C*$_4$), 129.02 (*p*-*C*$_6$H$_5$), 128.81 (*o*-*C*$_6$H$_5$), 126.80 (*m*-*C*$_6$H$_5$), 70.71 (*C*(CH$_3$)$_2$O), 65.50 (Ar*C*H$_2$N), 45.19 (Se*C*H$_2$), 44.95 (N*C*H$_3$), 30.25 (C(*C*H$_3$)$_2$O) ppm. ^{77}Se{^{1}H} NMR (THF-d_8, 76.3 MHz, 298 K) : δ = +202 ppm. ^{199}Hg{^{1}H} NMR (THF-d_8, 71.6 MHz, 298 K): δ = –798 ppm. Anal. Calcd. for C$_{19}$H$_{25}$HgNOSe (562.97 g mol^{-1}): C 40.5; H 4.5; N 2.5. Found: C 40.1, H 4.7, N 2.7 %.



^{1}H NMR of [{L$^{Se,(CH3)2}$}HgPh] (**13**) (THF-d_8, 400.1 MHz, 298 K)

Table S1. Crystallographic data for compounds **1-3**

	1	**2**	**3**
Empirical formula	$C_{19}H_{38}CdN_2OSSi_2$	$C_{38}H_{76}Cd_2N_4O_2Se_2Si_4$	$C_{19}H_{32}CdF_6N_2OSSi_2$
Formula weight (g/mol)	511.15	1116.13	619.11
Temperature	150(2) K	150(2) K	150(2) K
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
a [Å]	9.1973(4)	9.2472(9)	a = 9.9892(3)
b [Å]	12.6308(4)	12.5669(10)	b = 10.8280(3)
c [Å]	13.1425(5)	13.1946(14)	c = 13.9517(4)
α [°]	71.180(2)	71.041(4)	α = 92.8170(10)
β [°]	70.430(2)	70.219(4)	β = 90.0630(10)
γ [°]	69.4360(10)	69.424(4)	γ = 97.4510(10)
Volume	1310.05(9) $Å^3$	1313.4(2) $Å^3$	1494.47(7) $Å^3$
Z	2	1	2
Density (calculated)	1.296 g/cm^3	1.411 g/cm^3	1.376 g/cm^3
Absorption coefficient	1.015 mm^{-1}	2.318 mm^{-1}	0.930 mm^{-1}
F(000)	380	568	628
Crystal size	0.6 × 0.27 × 0.19	0.3 × 0.15 × 0.1	0.56 × 0.48 × 0.37
θ range for data collection	3.3 to 27.48 °	3.29 to 27.48 °	2.92 to 27.45 °
Index ranges	–11 < h < 11	–12 < h < 12	–10 < h < 12
	–12 < k < 16	–15 < k < 16	–14 < k < 13
	–15 < l < 17	–17 < l < 17	–18 < l < 18
Reflections	18315 / 5938	16970 / 5927	20065 / 6712
collected/unique	[R(int) = 0.0356]	[R(int) = 0.0631]	[R(int) = 0.0254]
Completeness to θ max.	99%	98.5%	98.3%
Absorption correction	multi-scan		
Refinement method	Full-matrix least-squares on F^2		
Data / restrains / parameters	5938 / 0 / 245	5927 / 0 / 245	6712 / 0 / 297
Goodness-of-fit on F^2 -S	1.034	1.018	1.043
Final R indices	R1 = 0.033	R1 = 0.037	R1 = 0.0259
[I>2sigma(I)]	wR2 = 0.0651	wR2 = 0.0796	wR2 = 0.0667
R indices (all data)	R1 = 0.0403	R1 = 0.0498	R1 = 0.0305
	wR2 = 0.0679	wR2 = 0.0863	wR2 = 0.0688
Largest diff. peak and hole	0.878 and –0.467e/$Å^3$	0.483 and –0.391 e/$Å^3$	0.924 and –0.324 e/$Å^3$

Table S2. Crystallographic data for compounds **4**, **6** and **7**

	4	**6**	**7**
Empirical formula	$C_{19}H_{32}CdF_6N_2OSeSi_2$	$C_{19}H_{38}N_2OSeSi_2Zn$	$C_{19}H_{32}F_6N_2OSeSi_2Zn$
Formula weight (g/mol)	666.01	511.02	618.97
Temperature	150(2) K	150(2) K	150(2) K
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
a [Å]	9.9777(6)	9.1925(6)	a = 9.8542(5)
b [Å]	10.8108(7)	12.6472(8)	b = 10.5091(5)
c [Å]	13.9716(9)	12.9189(10)	c = 14.1922(7)
α [°]	92.875(3)	96.460(4)	α = 93.228(2)
β [°]	90.825(3)	109.961(3)	β = 90.915(2)
γ [°]	98.109(2)	111.277(3)	γ = 97.033(2)
Volume	1489.78(16) $Å^3$	1266.67(15) $Å^3$	1455.97(12) $Å^3$
Z	2	2	2
Density (calculated)	1.485 g/cm^3	1.34 g/cm^3	1.412 g/cm^3
Absorption coefficient	2.085 mm^{-1}	2.511 mm^{-1}	2.227 mm^{-1}
F(000)	664	532	628
Crystal size (mm)	0.57 × 0.29 × 0.24	0.6 × 0.59 × 0.5	0.35 × 0.26 × 0.17
Theta range for data collection	2.92 to 27.55°	3.33 to 27.48°	3.006 to 27.524 °
Index ranges	–11 < h < 12 –14 < k < 13 –18 < l < 15	–11 < h < 11 –16 < k < 16 –14 < l < 16	–12 < h < 12 –13 < k < 13 –18 < l < 18
Reflections collected/unique	13325 / 6730 [R(int) = 0.0368]	13325 / 5722 [R(int) = 0.0281]	24953 / 6586 [R(int) = 0.0245]
Completeness to theta max.	97.9%	98.5%	97.9%
Absorption correction	multi-scan		
Refinement method	Full-matrix least-squares on F^2		
Data / restrains / parameters	6730 / 0 / 297	5722 / 0 / 245	6586 / 0 / 297
Goodness-of-fit on F^2 -S	0.932	1.039	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0369 wR2 = 0.0764	R1 = 0.0336 wR2 = 0.0838	R1 = 0.0194 wR2 = 0.0601
R indices (all data)	R1 = 0.0558 wR2 = 0.0812	R1 = 0.0465 wR2 = 0.0897	R1 = 0.0214 wR2 = 0.0608
Largest diff. peak and hole	0.582 and –0.49 $e/Å^3$	1.418 and –0.551 $e/Å^3$	0.420 and –0.215$e/Å^3$

Table S3. Crystallographic data for compounds **9-10**

	9	**10**
Empirical formula	$C_{26}H_{28}F_{12}HgN_2O_2S_2$	$C19H_{19}F_6HgNOS$
Formula weight (g/mol)	893.21	624.00
Temperature	150(2) K	294(2) K
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a [Å]	10.0125(3)	5.5944(19)
b [Å]	10.4618(3)	85.854(6)
c [Å]	15.7074(3)	17.803(6)
α [°]	91.4789(9)	74.157(6)
β [°]	96.5048(9)	85.854(6)
γ [°]	109.0432(10)	78.605(5)
Volume	1541.82(7) Å^3	1266.67(15) Å^3
Z	2	2
Density (calculated)	1.924 g/cm^3	1.986 g/cm^3
Absorption coefficient	5.228 mm^{-1}	7.536 mm^{-1}
F(000)	868	596
Crystal size (mm)	0.37 × 0.32 × 0.11	0.23 × 0.19 × 0.17
Theta range for data collection	3.18 to 27.48 °	1.189 to 24.999 °
Index ranges	–12 < h < 12	–6 < h < 6
	–13 < k < 13	–13 < k < 13
	–20 < l < 16	–21 < l < 21
Reflections collected/unique	23655 / 7026	10061 / 3670
	[R(int) = 0.0348]	[R(int) = 0.0911]
Completeness to theta max.	99.4%	99.7%
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restrains / parameters	7026 / 0 / 410	3670 / 0 / 264
Goodness-of-fit on F^2 -S	0.881	0.924
Final R indices [I>2sigma(I)]	R1 = 0.0215	R1 = 0.0528
	wR2 = 0.0549	wR2 = 0.0699
R indices (all data)	R1 = 0.0241	R1 = 0.0907
	wR2 = 0.0564	wR2 = 0.0800
Largest diff. peak and hole	1.103 and –0.773e/Å^3	0.830 and –1.245 e/Å^3