Supproting Information for the Article Entitled "Synthesis, Structures, and Electronic Properties of Triple- and Double-Decker Ruthenocenes Incorporated by a Group 14 Metallole Dianion Ligand"

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1. Crystal data for **2a**, **2b**, **3b**

2. ^{1}H and ^{13}C NMR for **2a**

3. ^{1}H and ^{13}C NMR for **3b**

4. The Cartesian coordinates of the optimized geometry for **2a**

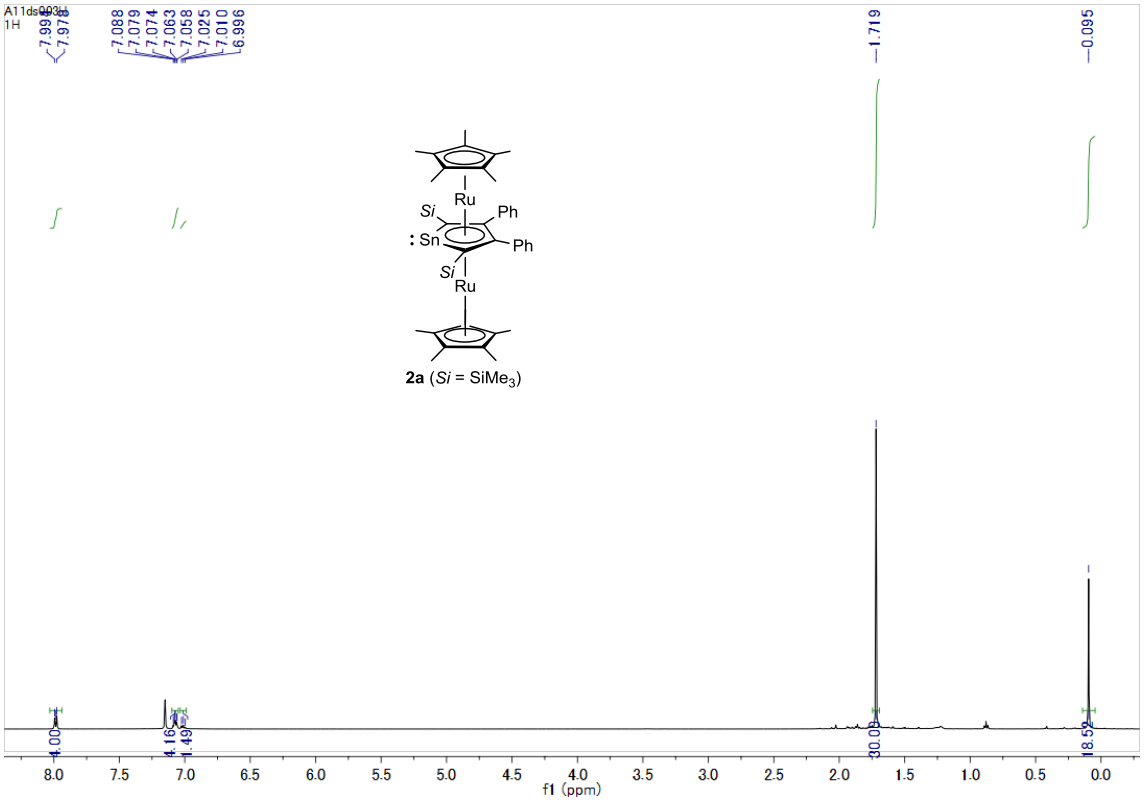
1. Crystal data for **2a**, **2b**, **3b**

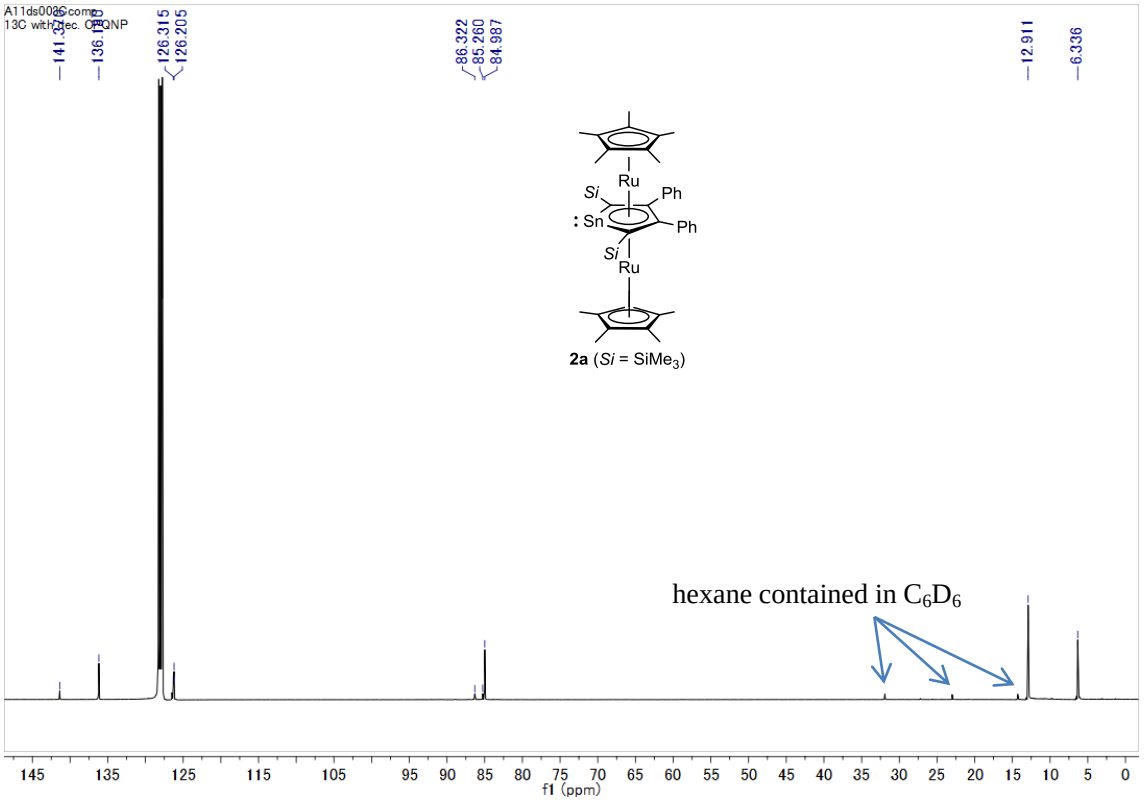
Crystal Data for **2a**: Formula, $C_{42}H_{58}Ru_2Si_2Sn$, FW=939.91, Crystal Dimension 0.10 × 0.04 × 0.04, Monoclinic, $P2_1/n$, a=11.505(2), b=19.578(4), c=17.558(4) Å, β=90.019(5)˚, V=3954.9(13) Å^3, Z=4, D_{calcd}=1.579 g cm^{-3}. R_1=0.056 ($I > 2\sigma(I)$, 6165 reflections), wR_2=0.109 (for all reflections) for 7767 reflections and 440 parameters. GOF=1.107.

Crystal Data for **2b**: Formula, $C_{48}H_{70}Ru_2Si_2Sn$, FW=1024.07, Crystal Dimension 0.06 × 0.06 × 0.04, Monoclinic, $P2_1/n$, a=10.7817(10), b=17.3180(16), c=24.015(2) Å, β=100.853(2)˚, V=4403.8(7) Å^3, Z=4, D_{calcd}=1.545 g cm^{-3}. R_1=0.046 ($I > 2\sigma(I)$, 7697 reflections), wR_2=0.108 (for all reflections) for 10514 reflections and 498 parameters. GOF=1.009.

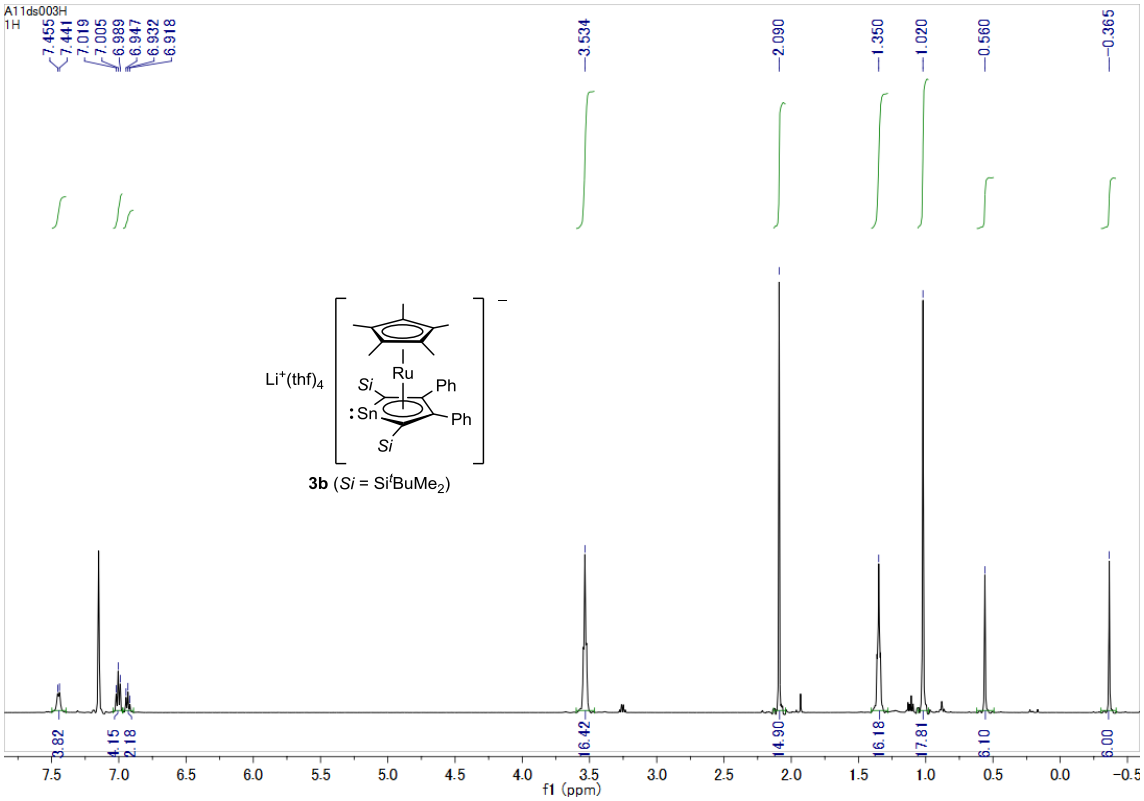
Crystal Data for **3b**: Formula, $C_{54}H_{87}LiO_4RuSi_2Sn$, FW=1083.14, Crystal Dimension 0.12 × 0.06 × 0.04, Triclinic, P-1, a=12.7833(15), b=14.3558(17), c=15.1393(18) Å, α=97.677(3)˚, β=96.928(2)˚, γ=93.321(3)˚, V=2725.5(6) Å^3, Z=2, D_{calcd}=1.320 g cm^{-3}. R_1=0.050 ($I > 2\sigma(I)$, 8672 reflections), wR_2=0.109 (for all reflections) for 11187 reflections and 573 parameters. GOF=1.015.

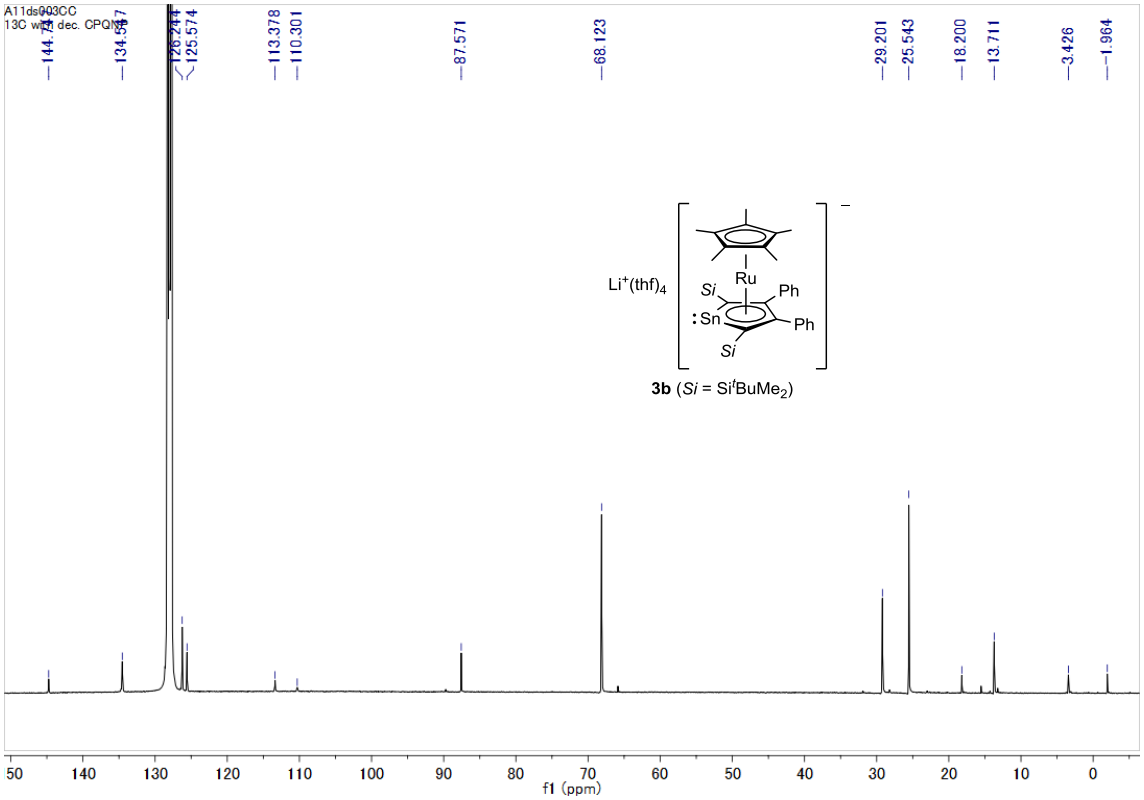
2. ^{1}H and ^{13}C NMR for **2a**





3. ^{1}H and ^{13}C NMR for **3b**





4. The Cartesian coordinates of the optimized geometry for **2a**

H	2.844373	-0.839781	-3.743942
H	4.425905	-1.557157	-3.389021
H	-1.090473	2.872354	-3.300398
H	-0.175592	4.381316	-3.181219
H	-3.334601	0.097925	-3.430697
H	0.672982	2.843409	-3.392297
H	2.854204	1.414141	-3.496861
H	-0.283027	-3.342112	-3.153818
H	-4.931784	-0.577361	-3.058710
C	3.415270	-1.388355	-2.989389
H	2.937273	-2.364932	-2.869409
C	-0.176809	3.321636	-2.892662
H	-3.505305	-1.618883	-3.070494
H	4.507040	1.892655	-3.082000
C	-3.863036	-0.622716	-2.799780
H	-1.363392	-4.552613	-2.456631
C	3.492169	1.762883	-2.679128
C	-1.023991	-3.512417	-2.362202
H	-3.272254	2.463817	-2.288266
H	-4.978051	2.033980	-2.144741
H	-1.872055	-2.856131	-2.570867
Sn	-0.147012	-0.095924	-2.299271
H	3.128363	2.746878	-2.377053
H	1.954943	-4.051221	-1.627634
H	0.957243	-5.352064	-0.976059
C	-4.057131	2.206989	-1.570970
C	3.475279	-0.642608	-1.691952
C	1.312167	-4.329451	-0.786927
C	3.503300	0.790038	-1.541070
H	-4.234916	3.081442	-0.941368
C	-3.672147	-0.331531	-1.342929
H	-1.781734	5.004204	-1.042820
H	-2.443183	3.621979	-0.163940
H	3.811841	-3.327247	-0.903806

Si	-0.080504	3.193304	-1.000954
H	-3.427664	-3.237321	-1.199249
C	-3.742386	0.981094	-0.764026
Si	-0.232121	-3.235415	-0.656708
H	1.139666	5.290604	-0.597699
C	-1.540326	4.208791	-0.325521
H	2.312546	4.039224	-1.011156
H	1.916465	-4.358994	0.123247
C	-0.042171	1.359229	-0.526064
H	-5.083580	-2.837393	-0.740316
C	3.735412	-1.223151	-0.403318
C	1.400031	4.234722	-0.445998
C	-0.013024	-1.376505	-0.391574
H	5.256438	-2.679491	-0.126860
Ru	1.814818	-0.021032	-0.404760
C	4.157102	-2.633885	-0.137198
C	-4.030935	-2.741640	-0.436386
C	-3.707897	-1.288436	-0.273200
Ru	-1.842179	-0.022472	-0.149698
H	4.059746	3.219483	-0.288237
C	3.771473	1.085523	-0.157423
H	-1.881135	-4.845176	0.348162
H	-1.268706	4.687353	0.621254
C	-1.243509	-4.040903	0.734476
H	3.818286	-3.004210	0.835061
H	1.616574	4.096701	0.618020
C	-3.780126	0.837590	0.662470
C	3.891489	-0.159444	0.535930
H	-3.912385	-3.295202	0.496488
C	4.140316	2.410093	0.438488
C	0.073606	0.808618	0.803681
H	-0.568314	-4.474257	1.479832
C	0.077390	-0.692845	0.883210
H	-3.842533	2.905759	1.304315
C	-3.740656	-0.568043	0.961732
H	5.185033	2.384542	0.778510

H	-1.873715	-3.314549	1.252768
H	3.518789	2.672619	1.300211
C	-4.113266	1.906950	1.657517
H	1.865444	-2.572759	1.571597
H	-5.195733	1.915488	1.851368
H	-1.649867	2.628005	1.804566
H	5.377191	-0.721868	1.972800
C	4.345933	-0.341073	1.952571
C	0.230642	1.641491	2.036949
C	0.203346	-1.381720	2.202734
C	1.193263	-2.353350	2.394755
H	-3.613472	1.748846	2.618038
C	-0.756353	2.558529	2.410559
C	-3.963343	-1.178999	2.310788
H	-5.018673	-1.463356	2.431645
H	3.723554	-1.057189	2.500328
H	4.340937	0.603440	2.503743
H	-3.358758	-2.077756	2.463723
H	2.132352	0.816450	2.571125
C	1.371142	1.538103	2.842092
H	-3.723411	-0.480146	3.117011
H	2.099295	-3.774232	3.732026
H	-1.410557	-0.328759	3.147095
C	1.324772	-3.020217	3.610921
C	-0.646396	-1.087606	3.275331
C	-0.604823	3.362475	3.539421
H	-1.386605	4.070828	3.804042
C	1.526511	2.335474	3.974051
C	0.540342	3.256282	4.327030
C	-0.515832	-1.747527	4.495809
C	0.468490	-2.719271	4.669965
H	2.421002	2.233451	4.584204
H	0.661433	3.880442	5.208832
H	-1.187319	-1.499180	5.314292
H	0.569379	-3.234970	5.621620

Method: B3PW91//[431]<Sn>/Lanl2dz+f<Ru>/6-31G(d) <others>

Total energy (optimization) = -8422.779570 au