Electronic Supporting Information for

Mono- and bimetallic pentacoordinate silicon complexes of a chelating bis(catecholimine) ligand

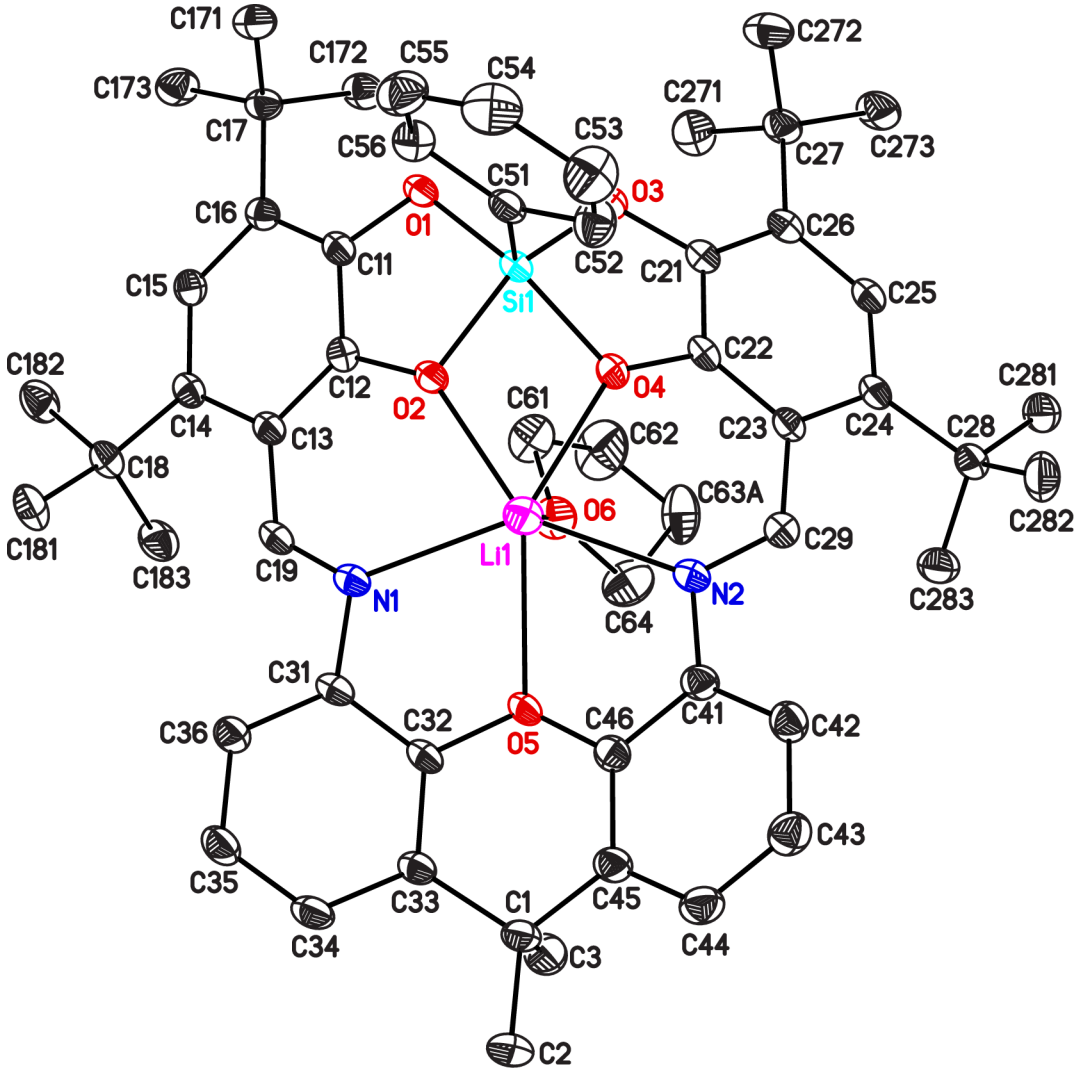
Thomas H. Do and Seth N. Brown*

251 Nieuwland Science Hall
Department of Chemistry and Biochemistry
University of Notre Dame
Notre Dame, Indiana 46556-5670 USA
E-mail: Seth.N.Brown.114@nd.edu

Contents:

I. X-ray Crystallography

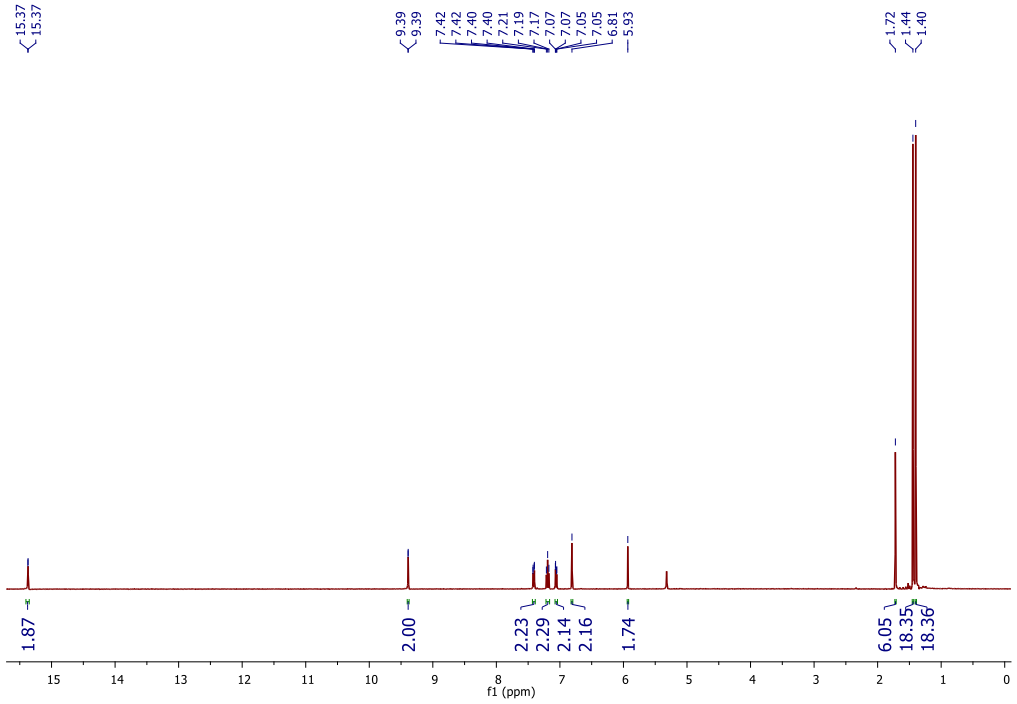
Figure S1. Thermal ellipsoid plot of (THF)Li(Xbic)SiPh•2 THF. Only the major conformation of the disordered THF ligand is shown. Hydrogen atoms and solvent have been omitted for clarity.



II. ^{1}H, $^{13}C\{^{1}H\}$, and $^{29}Si\{^{1}H\}$ NMR Spectra

Figure S2. NMR Spectra for $XbicH_4$.

^{1}H NMR (CD_2Cl_2):



$^{13}C\{^{1}H\}$ NMR ($CDCl_3$):

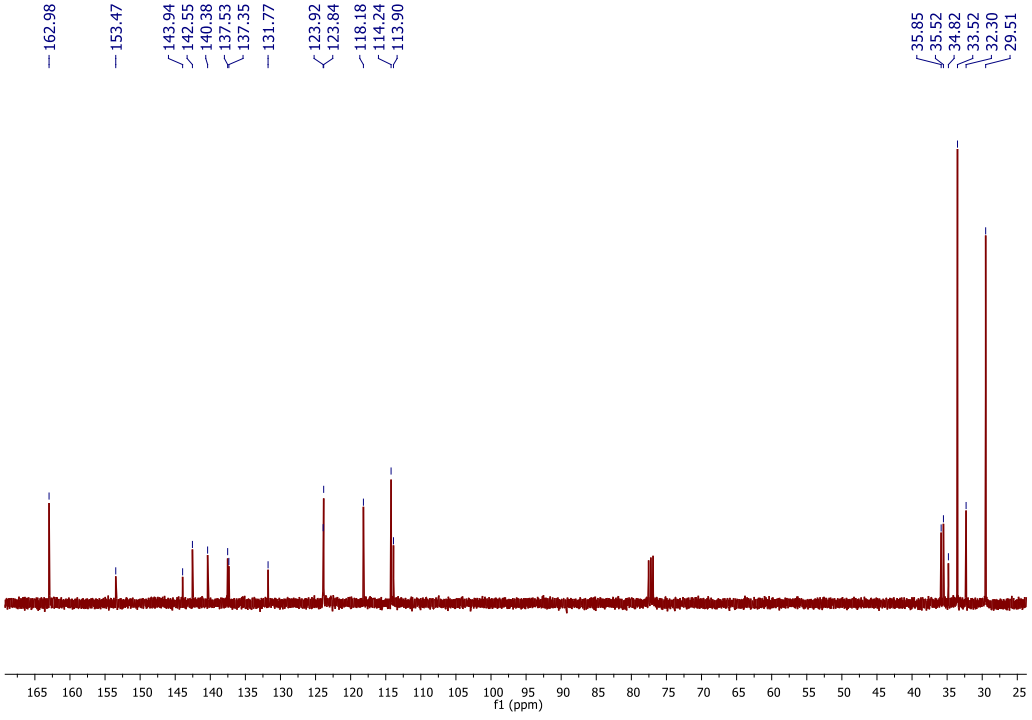
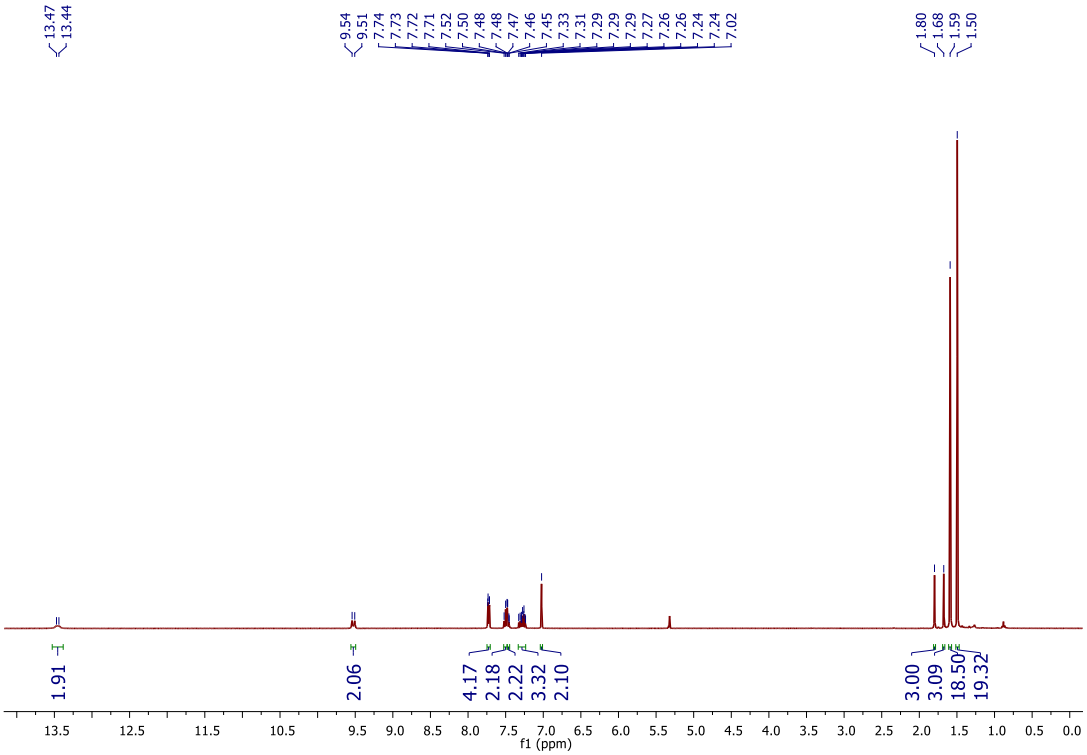
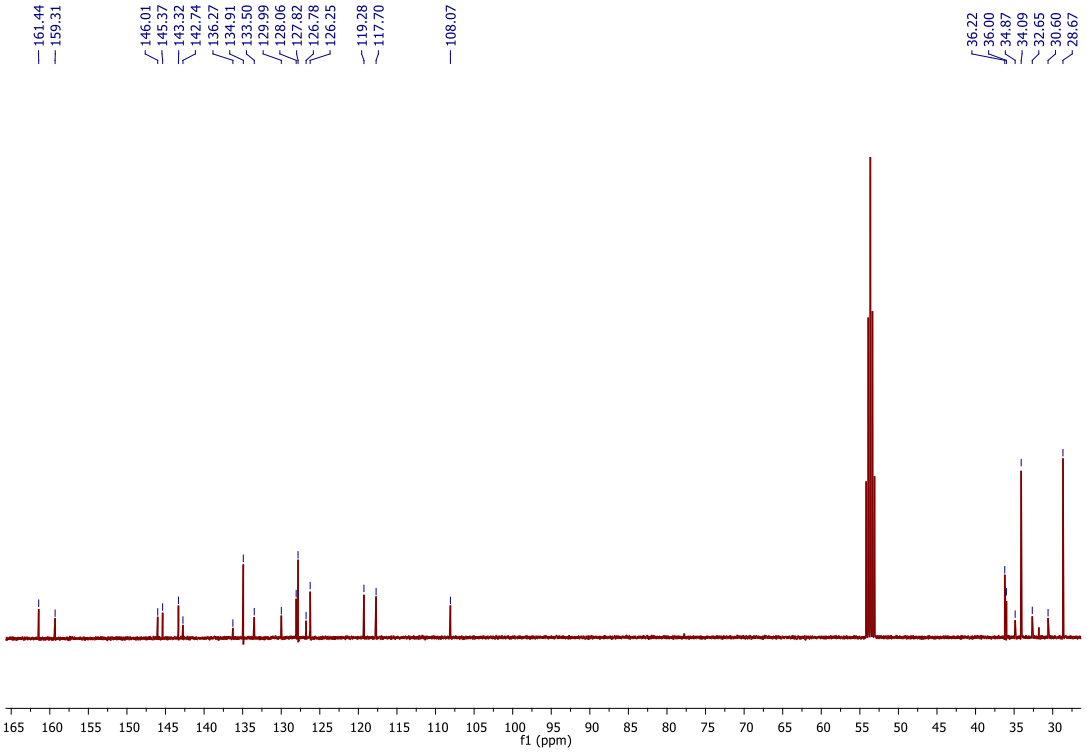


Figure S3. NMR Spectra for [(XbicH$_2$)SiPh][HCl$_2$] in CD_2Cl_2.

^{1}H NMR:



^{13}C{^{1}H} NMR:



$^{29}Si\{^{1}H\}$ NMR:

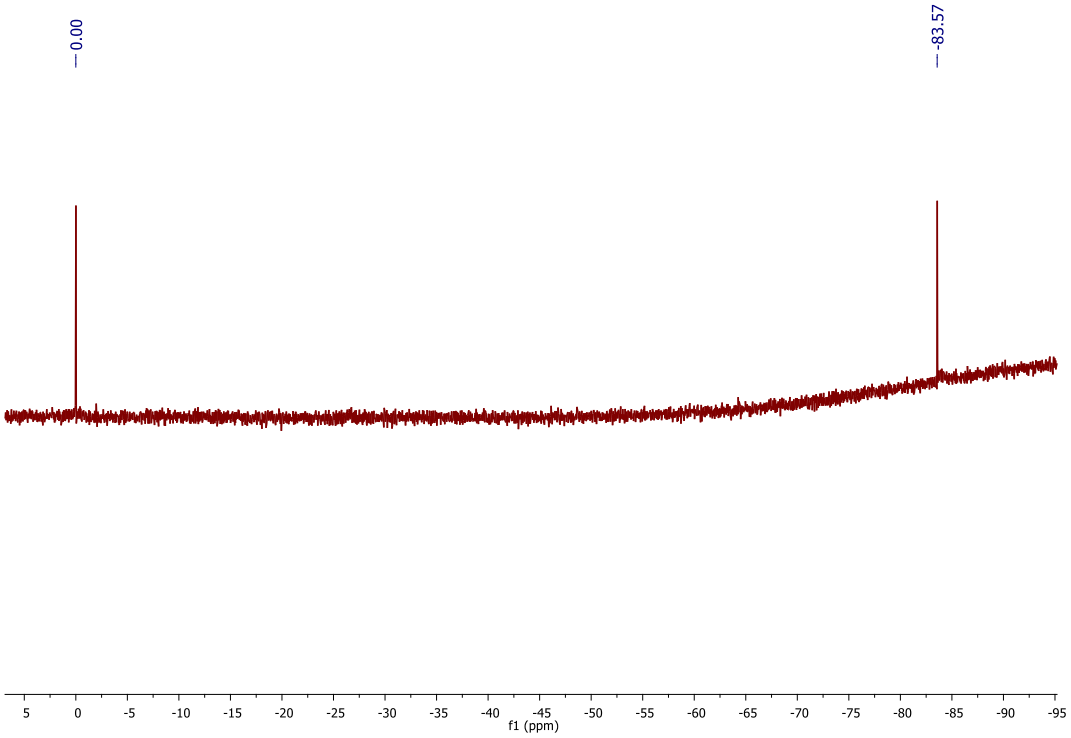
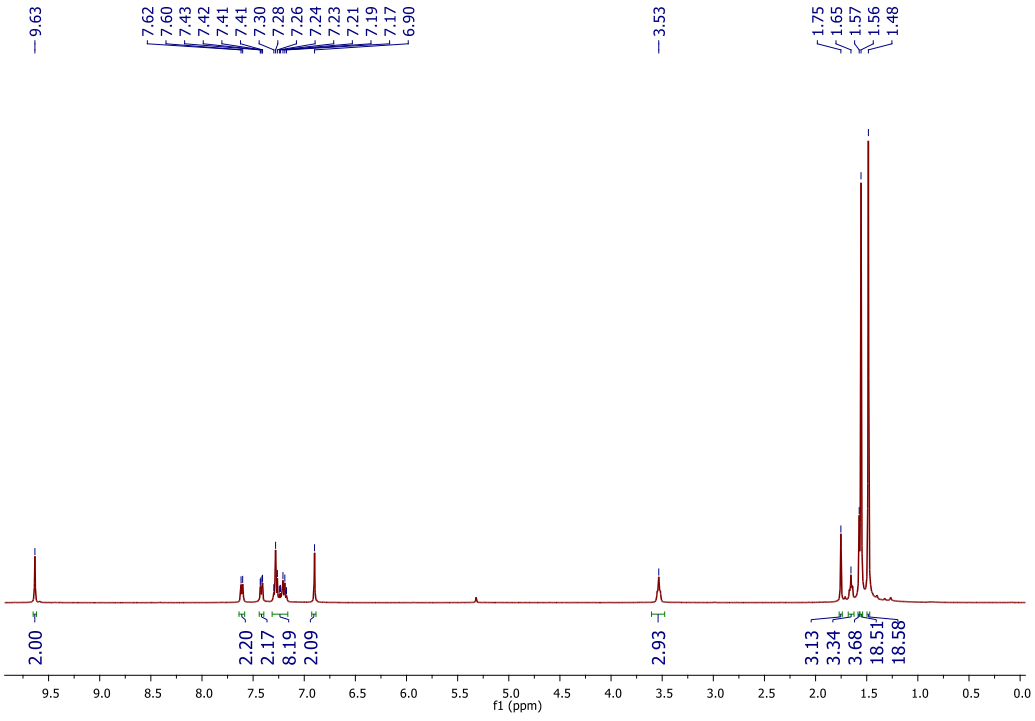
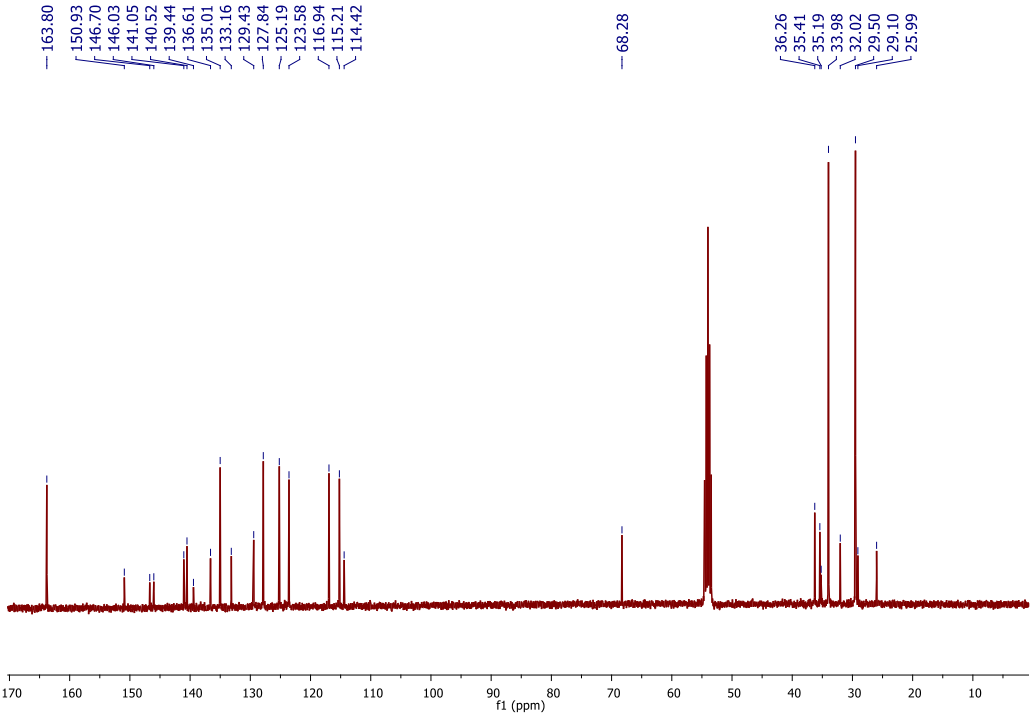


Figure S4. NMR Spectra for (THF)Li(Xbic)SiPh in CD_2Cl_2.

^{1}H NMR:



$^{13}C\{^{1}H\}$ NMR:



$^{29}Si\{^{1}H\}$ NMR:

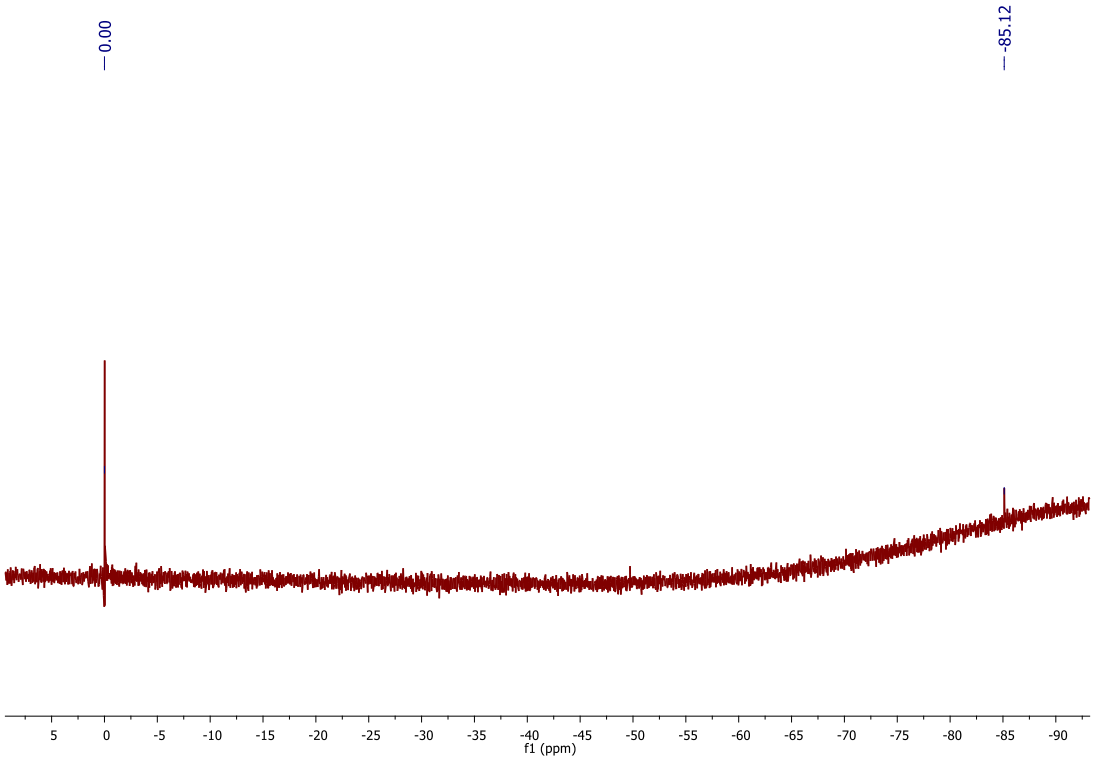
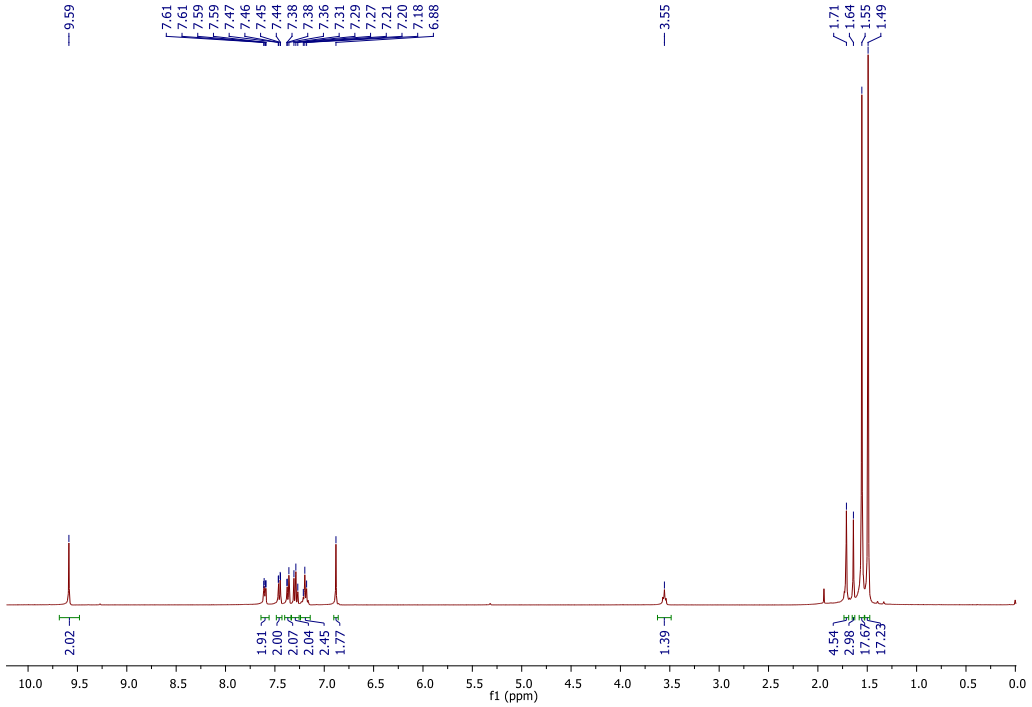
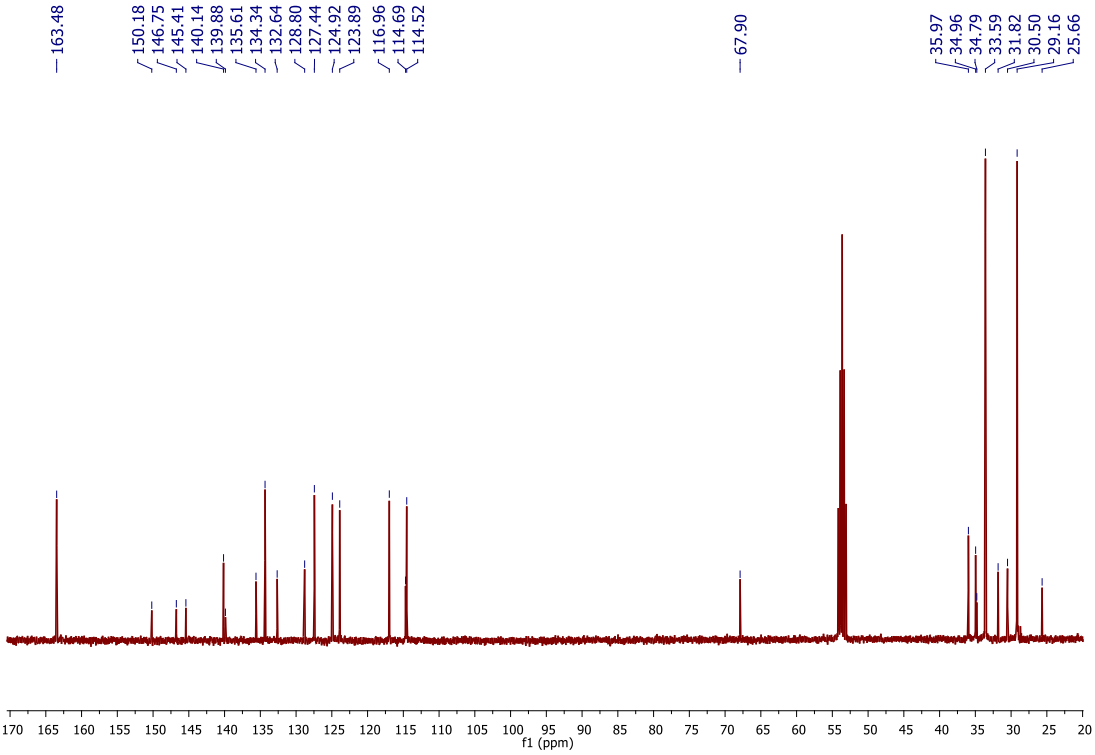


Figure S5. NMR Spectra for (THF)Na(Xbic)SiPh in CD_2Cl_2.

^{1}H NMR:



^{13}C{^{1}H} NMR:



$^{29}Si\{^{1}H\}$ NMR:

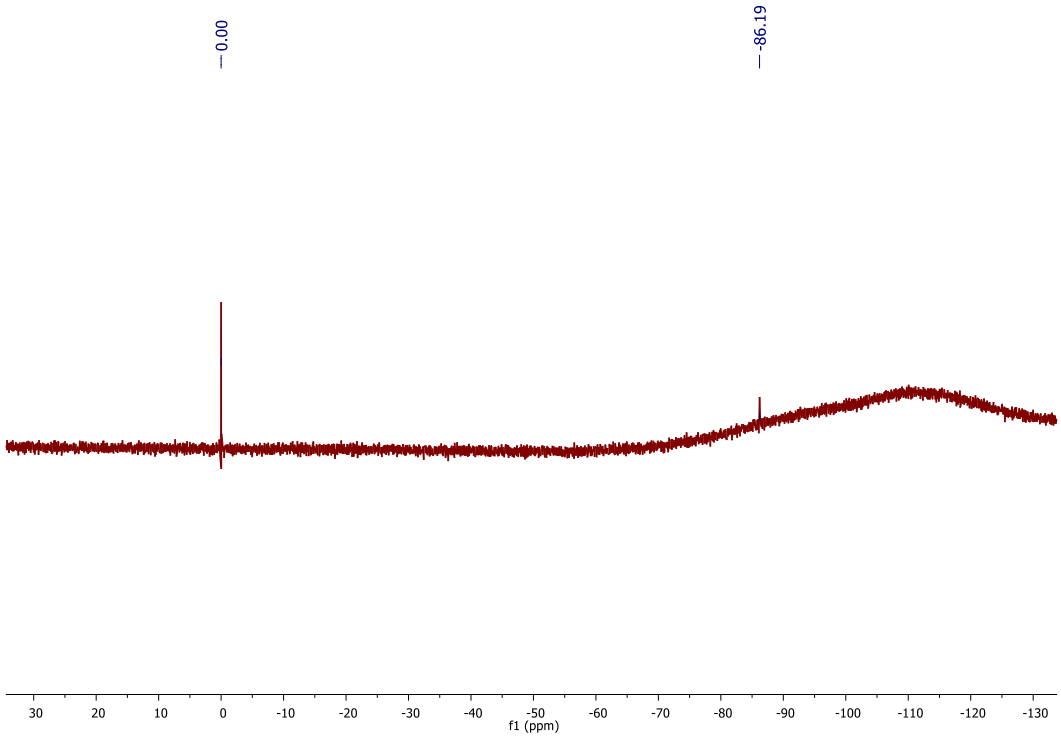
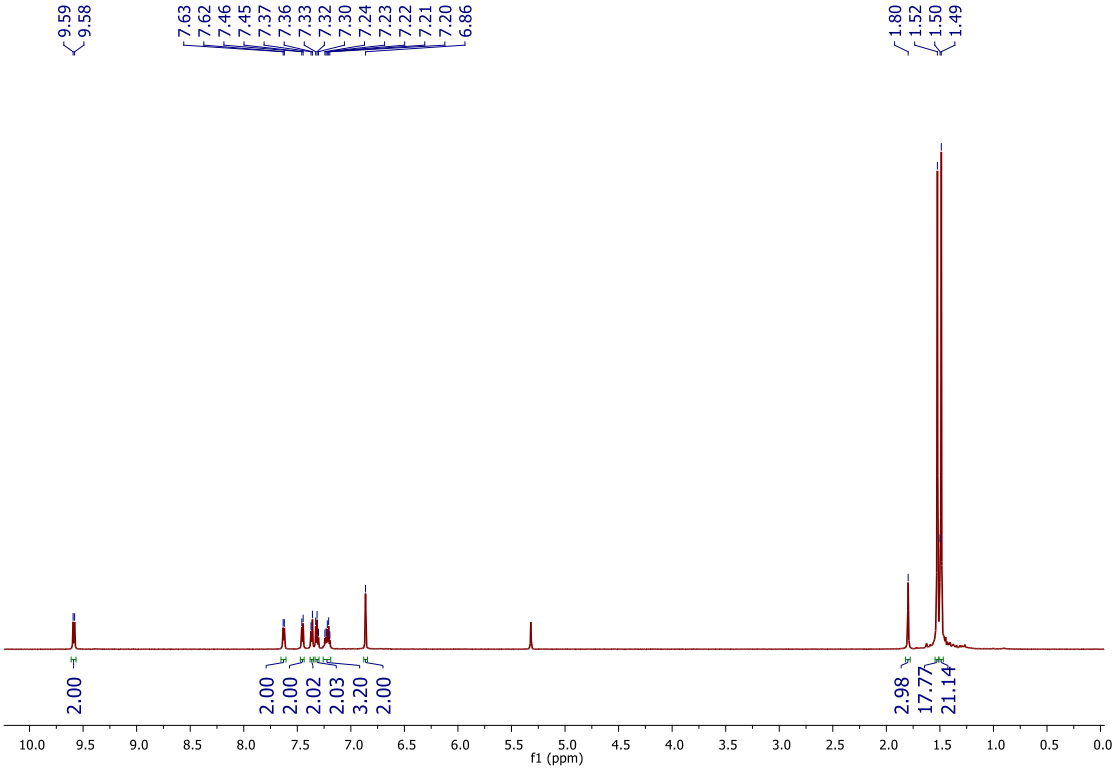
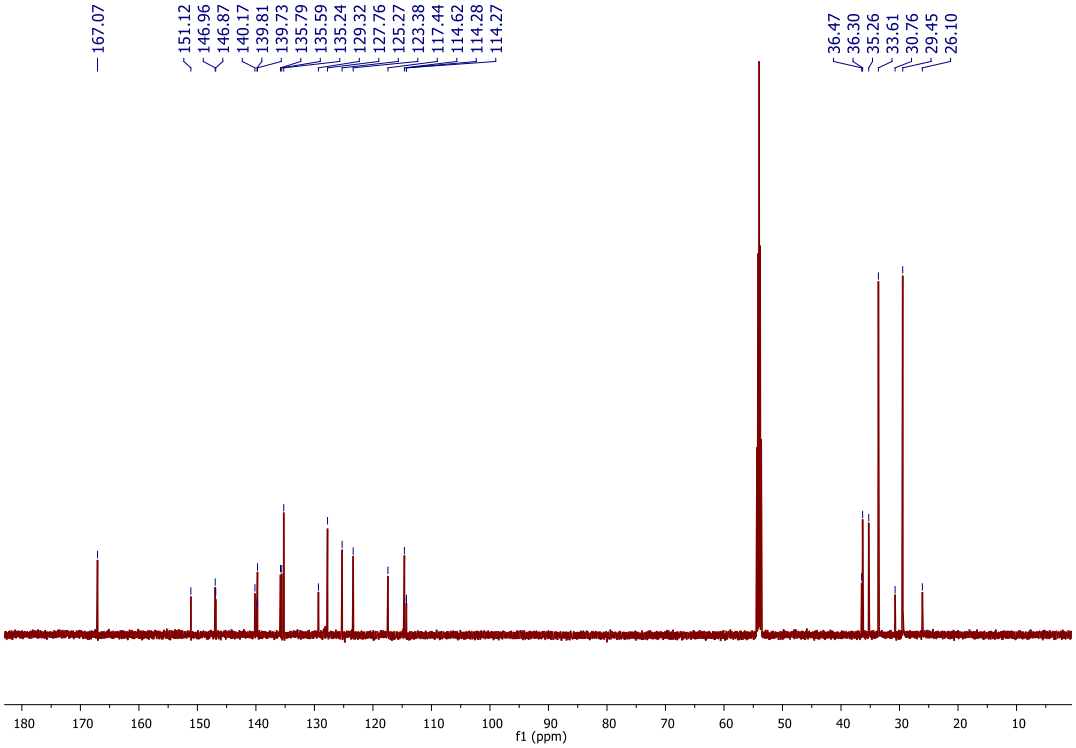


Figure S6. NMR Spectra for Ag(Xbic)SiPh in CD_2Cl_2.

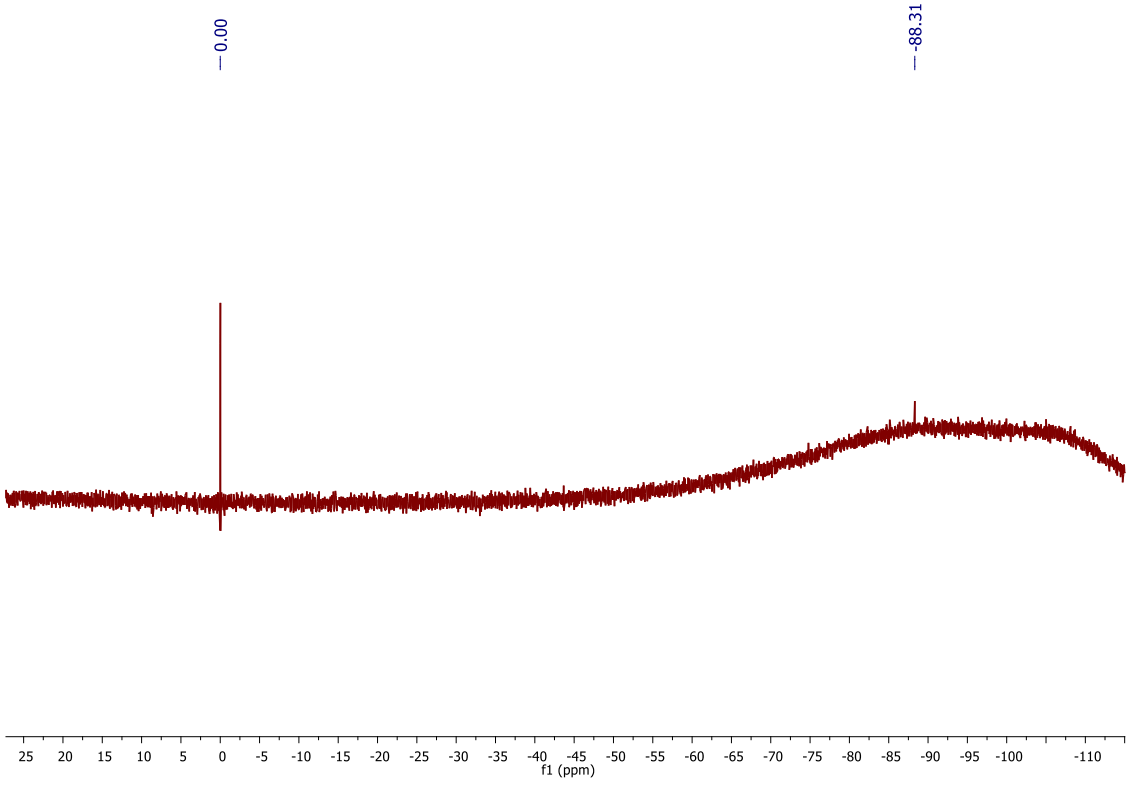
^{1}H NMR:



$^{13}C\{^{1}H\}$ NMR:



$^{29}Si\{^{1}H\}$ NMR:



III. UV-Visible Spectra

Figure S7. UV-visible spectrum of $XbicH_4$ (1.4×10^{-5} M in CH_2Cl_2).

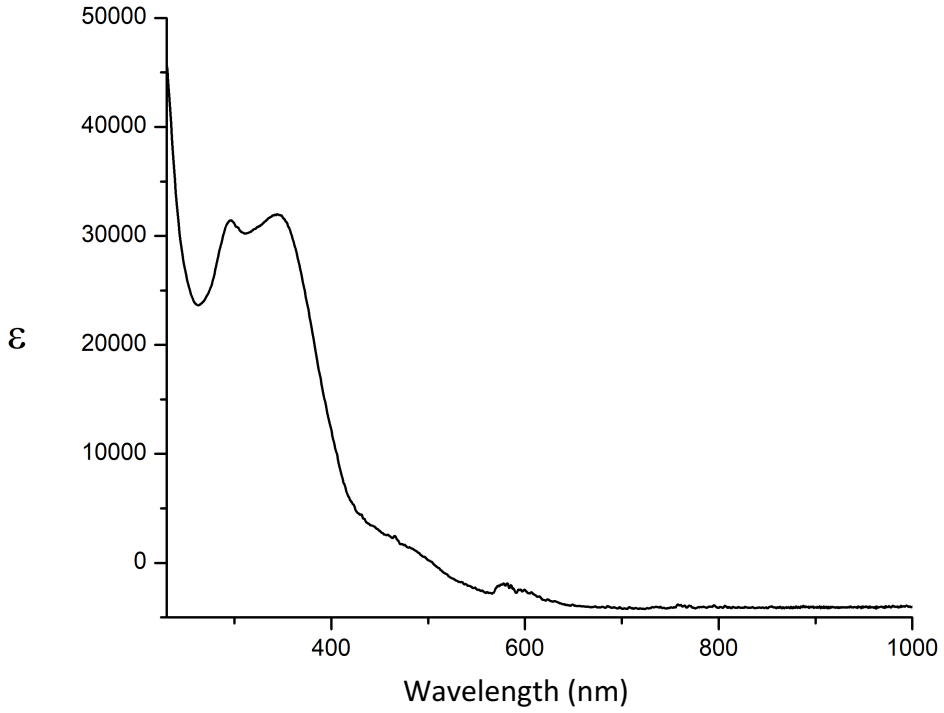


Figure S8. UV-visible spectrum of $[(XbicH_2)SiPh][HCl_2]$ (1.0×10^{-5} M in CH_2Cl_2).

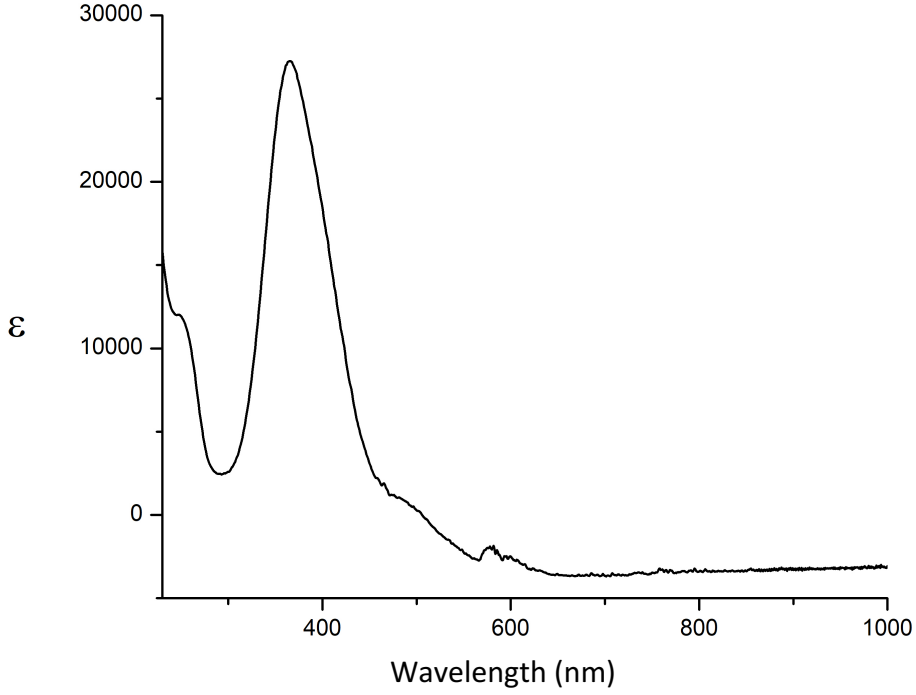


Figure S9. UV-visible spectrum of (THF)Li(Xbic)SiPh (1.0×10^{-5} M in CH_2Cl_2).

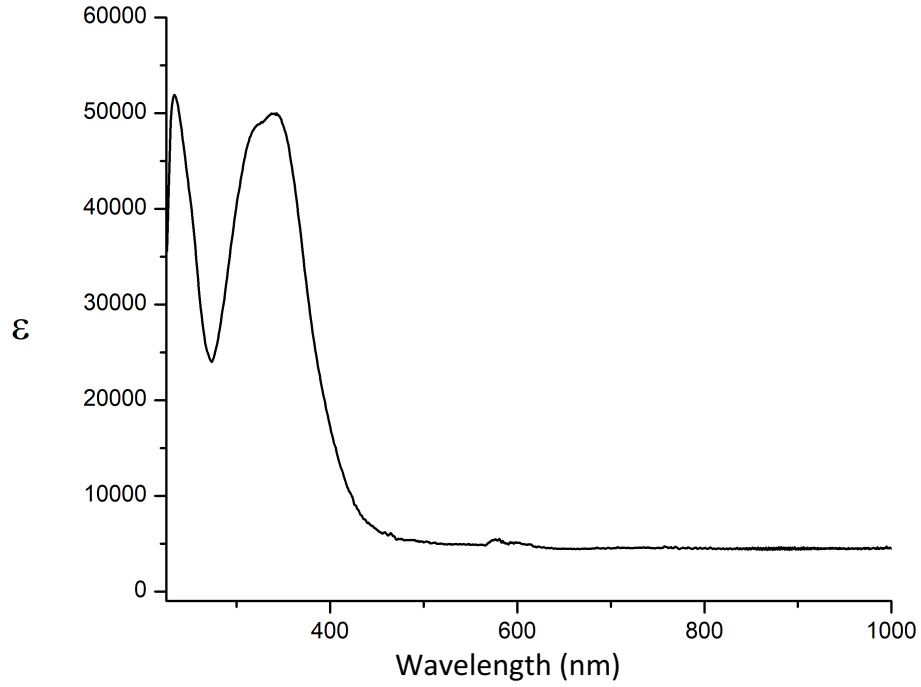


Figure S10. UV-visible spectrum of (THF)Na(Xbic)SiPh (1.0×10^{-5} M in CH_2Cl_2).

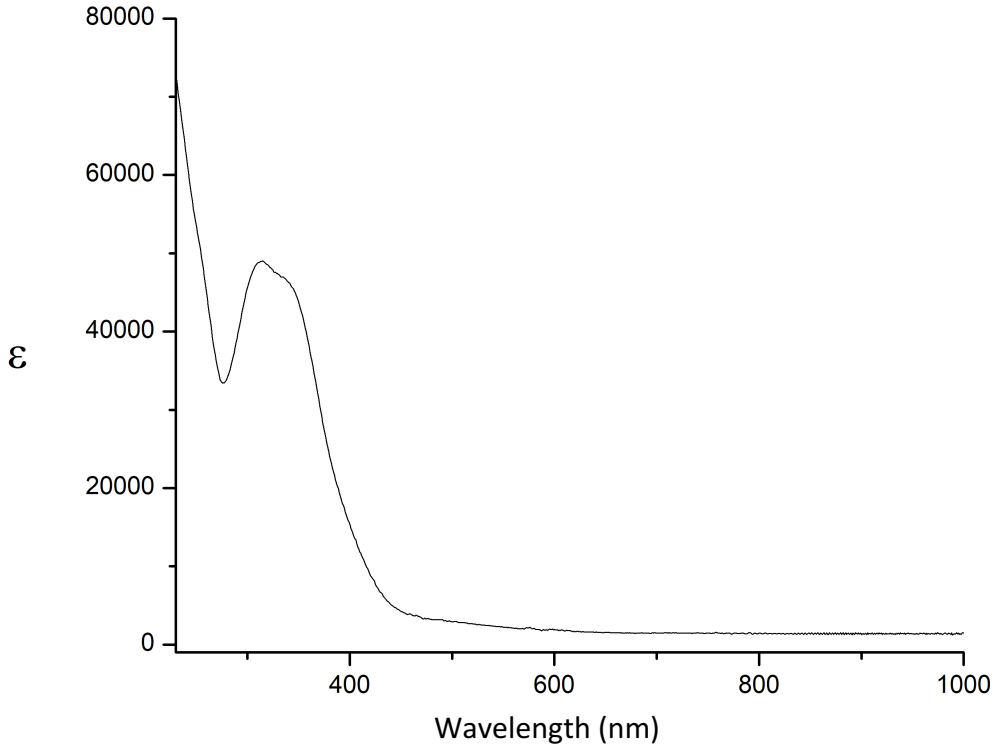
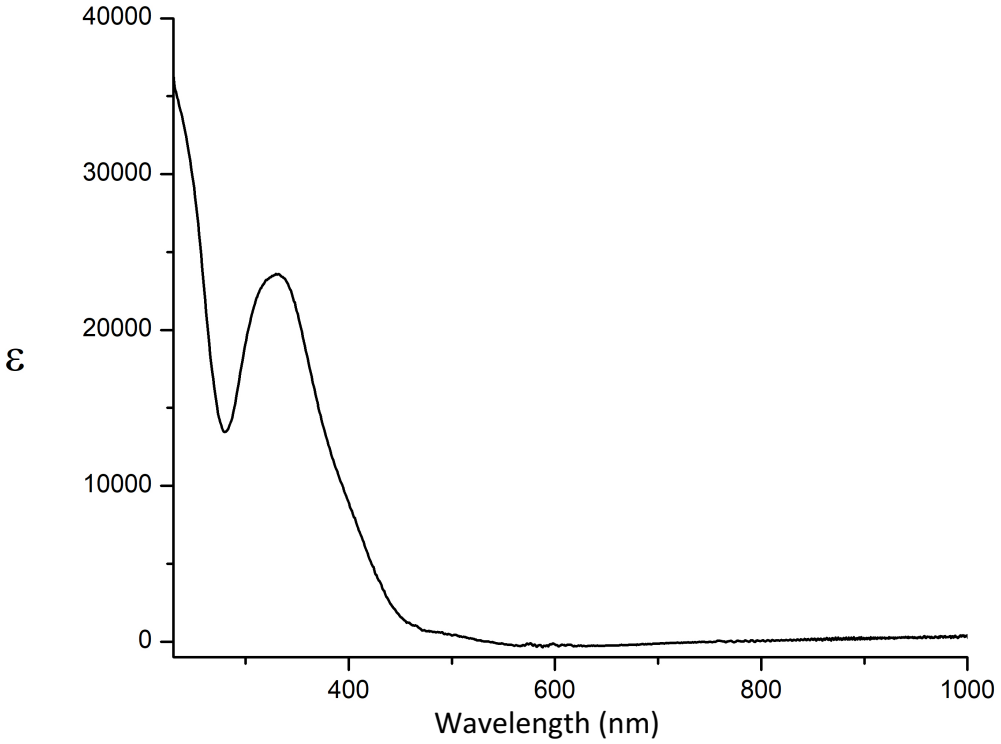


Figure S11. UV-visible spectrum of Ag(Xbic)SiPh (1.2×10^{-5} M in CH_2Cl_2).



IV. Infrared spectra

Figure S12. Infrared spectrum of $XbicH_4$.

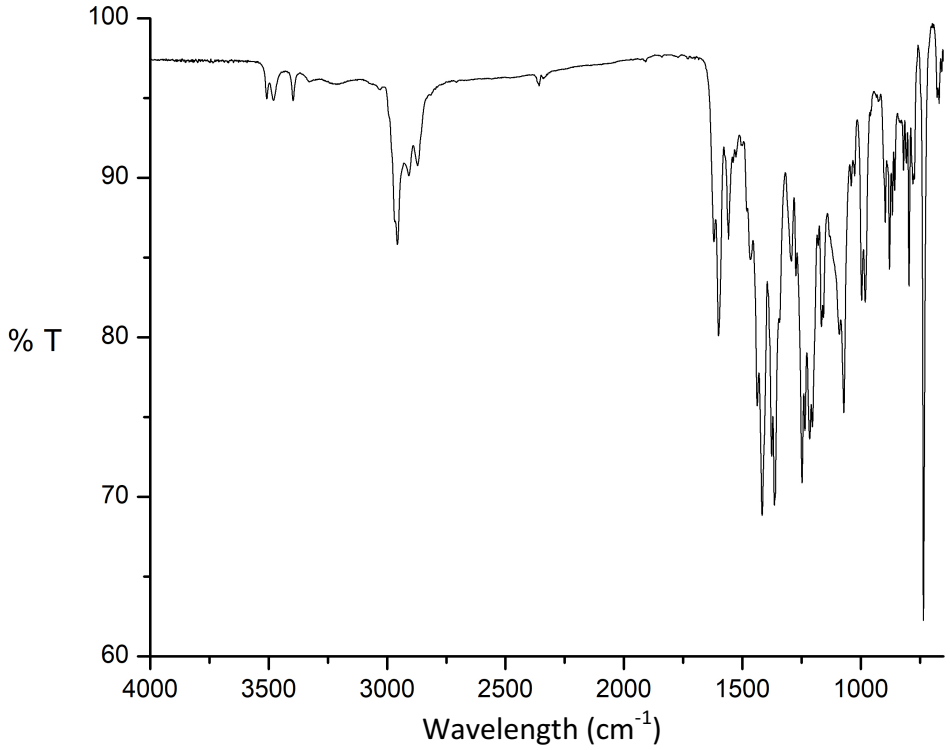


Figure S13. Infrared spectrum of [(XbicH_2)SiPh][HCl_2].

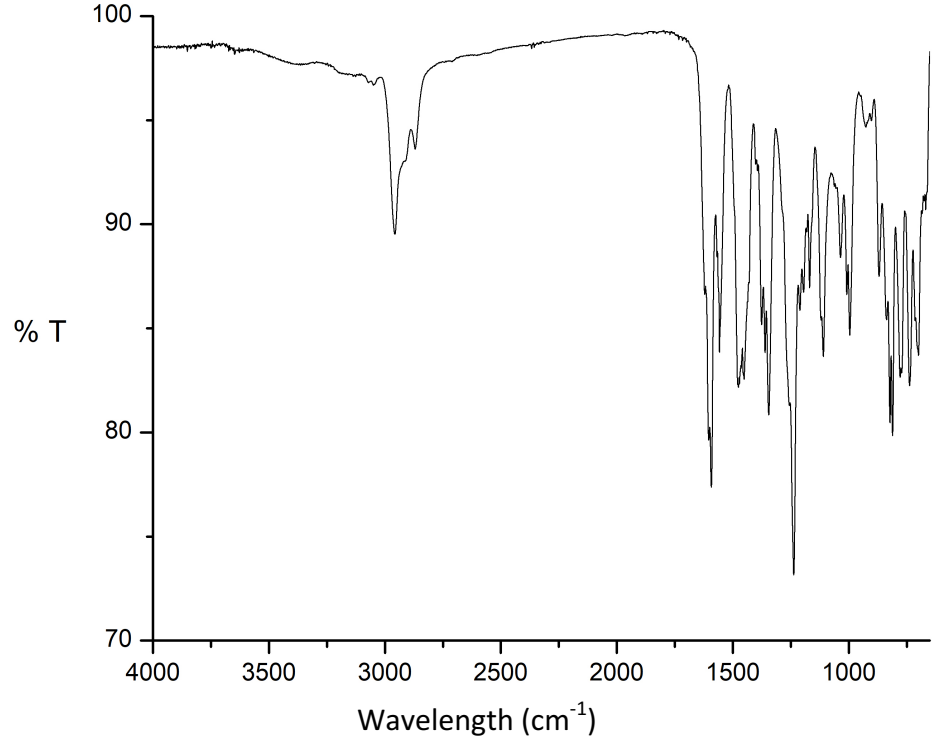


Figure S14. Infrared spectrum of (THF)Li(Xbic)SiPh.

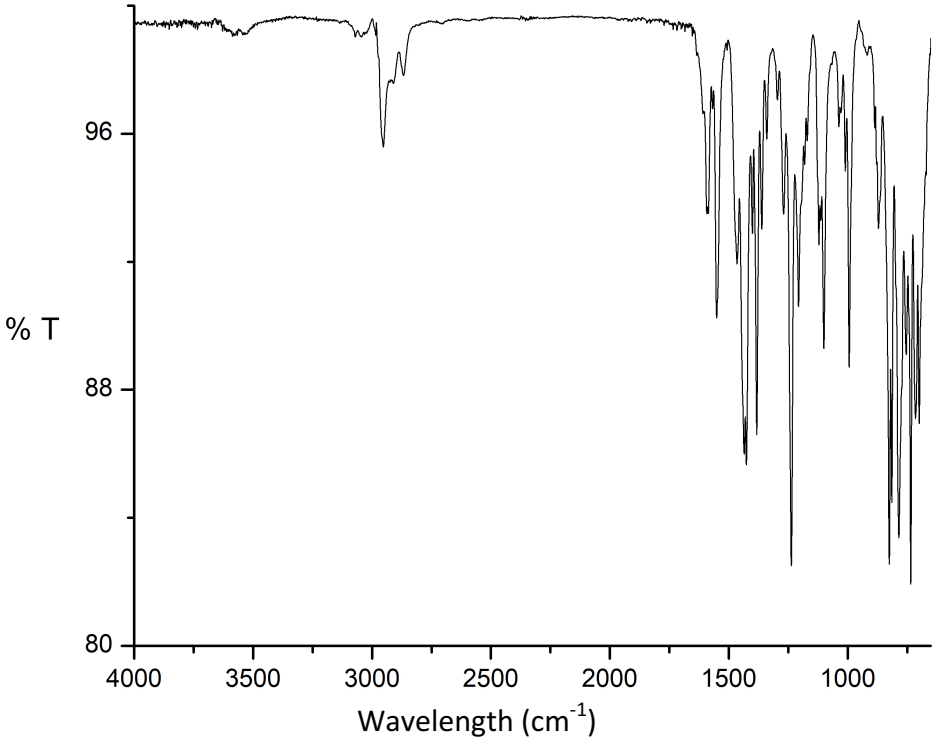


Figure S15. Infrared spectrum of (THF)Na(Xbic)SiPh.

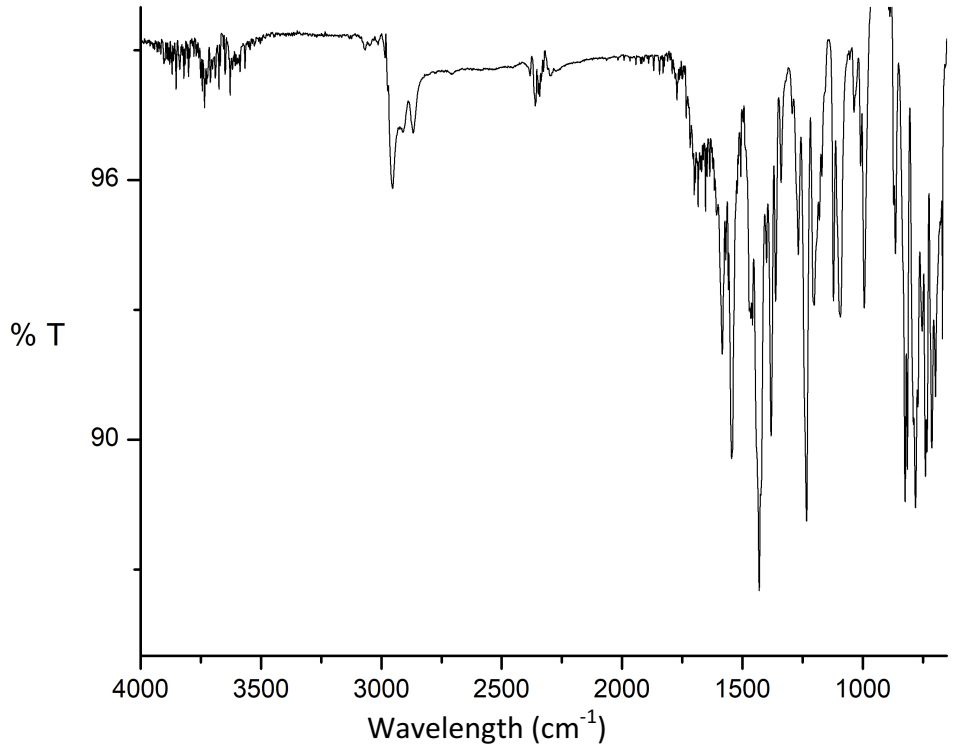
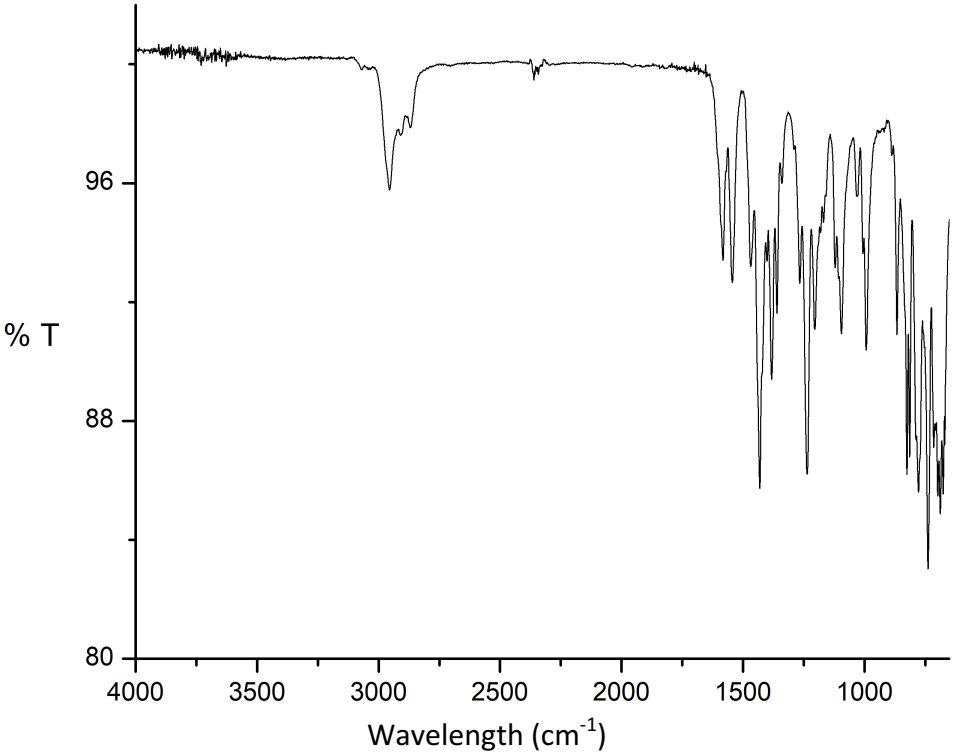


Figure S16. Infrared spectrum of Ag(Xbic)SiPh.



V. Electrochemistry

Figure S17. Cyclic voltammogram of $XbicH_4$ in CH_2Cl_2 (0.1 M Bu_4NPF_6, 60 mV s^{-1}).

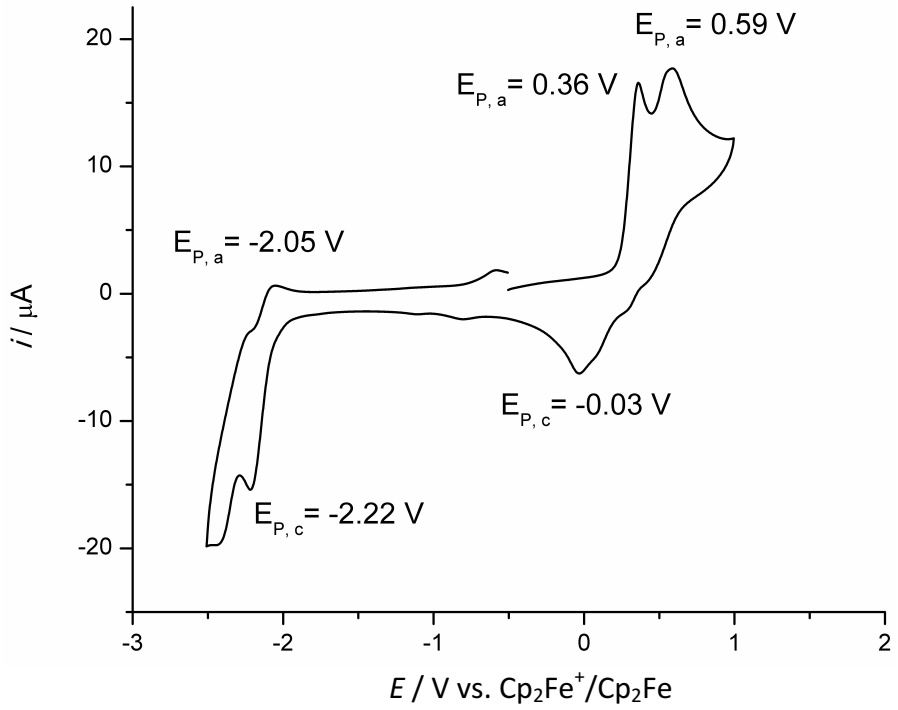


Figure S18. Cyclic voltammogram of $[(XbicH_2)SiPh][HCl_2]$ in CH_2Cl_2 (0.1 M Bu_4NPF_6, 60 mV s^{-1}).

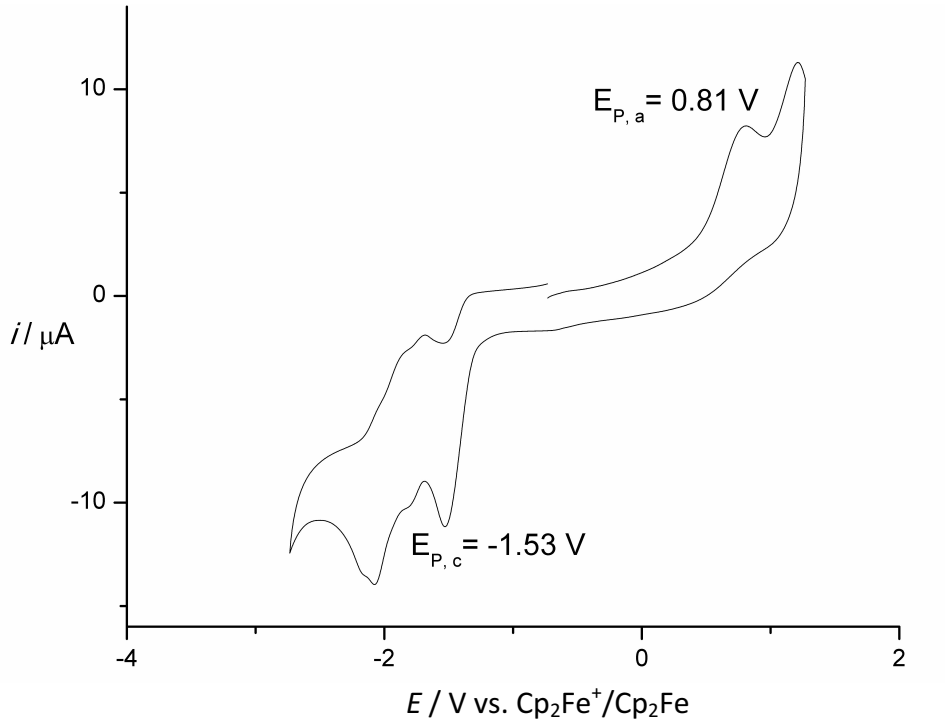


Figure S19. Cyclic voltammogram of (THF)Li(Xbic)SiPh in CH_2Cl_2 (0.1 M Bu_4NPF_6, 60 mV s^{-1}).

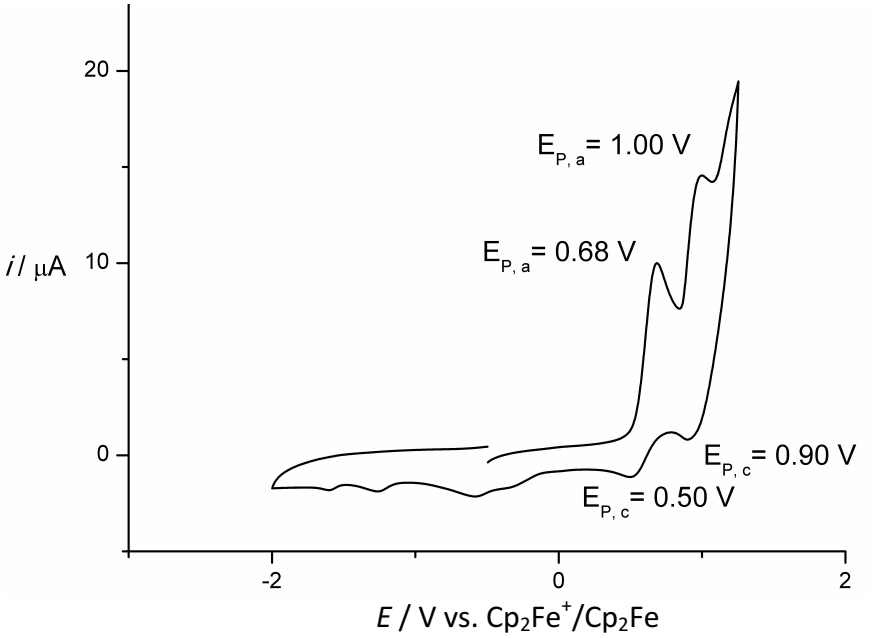


Figure S20. Cyclic voltammogram of (THF)Na(Xbic)SiPh in CH_2Cl_2 (0.1 M Bu_4NPF_6, 60 mV s^{-1}).

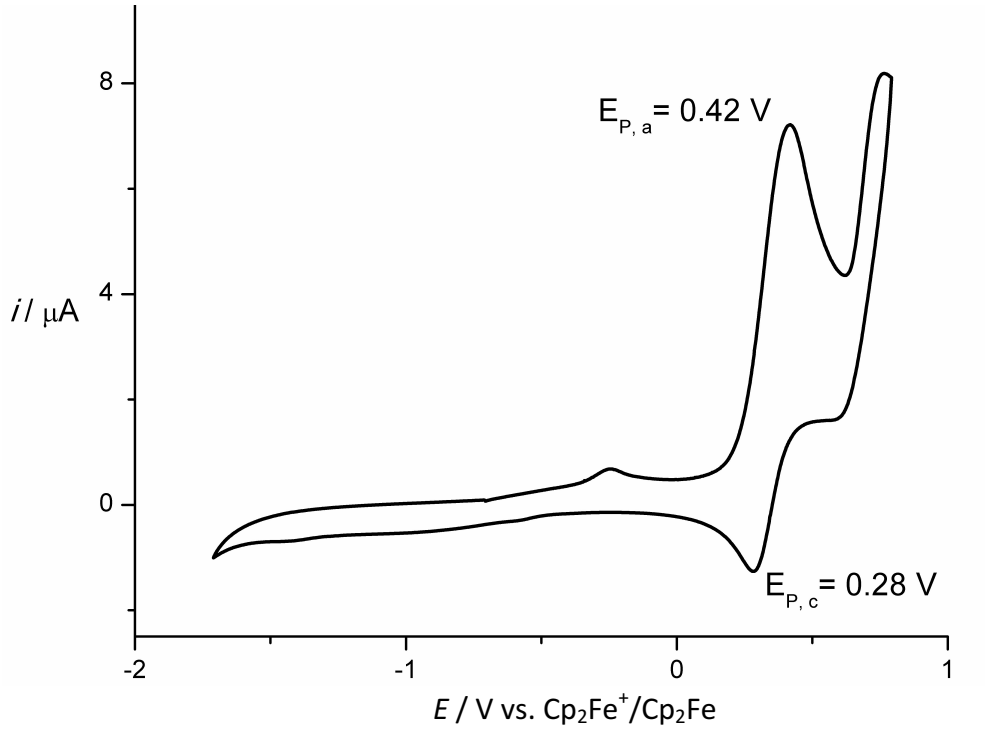
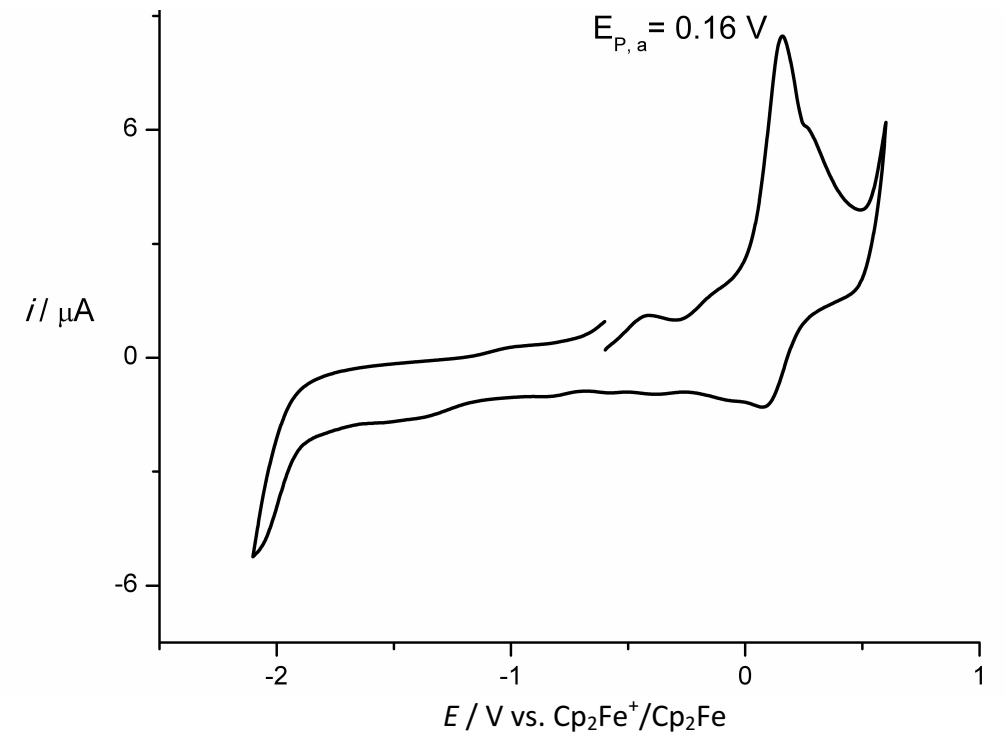


Figure S21. Cyclic voltammogram of Ag(Xbic)SiPh in CH_2Cl_2 (0.1 M Bu_4NPF_6, 60 mV s^{-1}).



VI. Energies and Cartesian coordinates of calculated structures

A. $[(XbicH_2)SiPh]^+$ E = –2046.44470102 a.u.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	-2.582043	-0.102236	-0.008478
2	8	-3.459487	-1.209590	-1.016507
3	8	-1.123615	-1.276097	-0.212077
4	8	-3.729009	1.160542	-0.466121
5	8	-1.265138	1.093594	-0.372691
6	8	2.756773	0.111144	-0.294422
7	7	1.385144	-2.287648	-0.370027
8	1	0.777696	-1.496943	-0.133299
9	7	1.168022	2.378274	-0.479486
10	1	0.669371	1.507159	-0.279561
11	6	-2.793060	-2.321073	-1.385735
12	6	-1.454892	-2.323269	-0.945528
13	6	-0.565236	-3.356255	-1.330979
14	6	-1.089529	-4.436053	-2.112569
15	1	-0.427844	-5.246405	-2.404164
16	6	-2.411484	-4.436698	-2.493372
17	1	-2.803834	-5.258331	-3.083215
18	6	-3.279017	-3.367447	-2.144744
19	1	-4.312908	-3.361411	-2.474385
20	6	0.803734	-3.290850	-1.012544
21	1	1.459001	-4.096631	-1.332758
22	6	-3.155263	2.303047	-0.860663
23	6	-1.750758	2.261149	-0.791795
24	6	-0.954337	3.368408	-1.155385
25	6	-1.624588	4.538590	-1.638100
26	1	-1.036478	5.405016	-1.925505
27	6	-2.999670	4.564984	-1.712504
28	1	-3.502299	5.456891	-2.071778
29	6	-3.783059	3.448978	-1.323323
30	1	-4.865899	3.482683	-1.386575
31	6	0.444689	3.367291	-0.985754
32	1	0.994050	4.260578	-1.267202
33	6	2.750548	-2.260855	0.007327
34	6	3.459260	-1.043608	0.026298
35	6	4.820502	-1.034280	0.339085
36	6	5.452145	-2.236279	0.671870
37	1	6.508972	-2.218687	0.923512
38	6	4.751879	-3.438416	0.688953
39	1	5.248012	-4.361056	0.970699
40	6	3.400999	-3.448216	0.359498
41	1	2.834530	-4.372185	0.411423
42	6	2.537530	2.487514	-0.123531
43	6	3.085354	3.740843	0.177747
44	1	2.447132	4.616943	0.204170
45	6	4.431609	3.865328	0.497568
46	1	4.842935	4.840251	0.736439
47	6	5.235900	2.730662	0.532113
48	1	6.289993	2.817460	0.780613
49	6	4.710154	1.464657	0.263223

50	6	3.352619	1.339323	-0.046915
51	6	-2.872213	-0.285403	1.822562
52	6	-2.041073	-1.069802	2.645657
53	1	-1.192920	-1.592166	2.213805
54	6	-2.288109	-1.194127	4.012443
55	1	-1.632851	-1.804407	4.628374
56	6	-3.379013	-0.539976	4.587756
57	1	-3.574994	-0.639634	5.651912
58	6	-4.218555	0.239575	3.790754
59	1	-5.071561	0.747534	4.232220
60	6	-3.966031	0.368055	2.424948
61	1	-4.627954	0.976344	1.816940
62	6	5.603767	0.250728	0.264692
63	1	6.219484	0.249938	-0.647685
64	1	6.309782	0.308072	1.101537

B. (THF)Li(Xbic)SiPh E = –2285.54193953 a.u.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	2.711394	-0.070369	0.275427
2	3	-0.409318	0.037574	-0.166746
3	8	3.784781	1.139726	-0.452421
4	8	1.368443	1.067279	-0.036605
5	8	3.487261	-1.318775	-0.662882
6	8	1.261151	-1.188261	0.386750
7	8	-2.861933	0.182320	0.107498
8	8	-0.522627	-0.240532	-2.192888
9	7	-1.166744	2.307141	-0.064024
10	7	-1.399948	-2.074745	0.404324
11	6	3.149831	2.270335	-0.815290
12	6	1.763142	2.231180	-0.574589
13	6	0.911216	3.288526	-0.906421
14	6	1.510014	4.430845	-1.500885
15	1	0.880200	5.277313	-1.763262
16	6	2.875871	4.478299	-1.736090
17	1	3.312672	5.364106	-2.188160
18	6	3.714855	3.396610	-1.398349
19	1	4.782788	3.431336	-1.589952
20	6	-0.510096	3.273606	-0.625412
21	1	-1.033112	4.193917	-0.918231
22	6	2.747188	-2.443909	-0.818131
23	6	1.459248	-2.338826	-0.255162
24	6	0.498957	-3.343906	-0.437318
25	6	0.911440	-4.522527	-1.113814
26	1	0.194139	-5.329328	-1.244949
27	6	2.196629	-4.644494	-1.618063
28	1	2.491362	-5.554779	-2.131884
29	6	3.129415	-3.592928	-1.490338
30	1	4.126476	-3.668941	-1.912865
31	6	-0.875334	-3.182932	-0.017015
32	1	-1.498970	-4.082141	-0.120724
33	6	-2.508728	2.538797	0.288613

34	6	-3.387533	1.438716	0.381612
35	6	-4.732094	1.598661	0.725100
36	6	-5.204303	2.875451	1.039846
37	1	-6.246129	2.998335	1.324939
38	6	-4.348103	3.973151	1.005701
39	1	-4.710903	4.958855	1.282264
40	6	-3.016860	3.803667	0.637336
41	1	-2.343217	4.653628	0.663997
42	6	-2.737804	-2.089916	0.828564
43	6	-3.351950	-3.188955	1.453994
44	1	-2.759030	-4.073704	1.662858
45	6	-4.684658	-3.136631	1.854180
46	1	-5.134624	-3.992615	2.348725
47	6	-5.432714	-1.982827	1.631615
48	1	-6.476370	-1.937590	1.932477
49	6	-4.850379	-0.863854	1.029003
50	6	-3.503275	-0.916080	0.667404
51	6	3.256869	-0.048940	2.068802
52	6	2.525862	-0.711544	3.073227
53	1	1.620990	-1.249723	2.807207
54	6	2.941642	-0.689034	4.405281
55	1	2.357449	-1.205377	5.163324
56	6	4.105829	-0.007329	4.763687
57	1	4.432375	0.008822	5.800824
58	6	4.848467	0.653636	3.783888
59	1	5.756805	1.186166	4.055502
60	6	4.425384	0.635417	2.454202
61	1	5.008191	1.156885	1.701080
62	6	0.589232	-0.049519	-3.105310
63	1	1.418865	-0.677384	-2.764116
64	1	0.899990	0.998186	-3.064933
65	6	0.084149	-0.476972	-4.490065
66	1	-0.306693	0.385909	-5.041884
67	1	0.874166	-0.933128	-5.093438
68	6	-1.055547	-1.447795	-4.144218
69	1	-0.655513	-2.436413	-3.891061
70	1	-1.785438	-1.565584	-4.951040
71	6	-1.650517	-0.788126	-2.902394
72	1	-2.342022	0.023155	-3.170872
73	1	-2.163691	-1.478305	-2.230262
74	6	-5.634568	0.388872	0.725128
75	1	-6.120660	0.289555	-0.259433
76	1	-6.446080	0.518143	1.450512
