Supporting Information for: **Redox chemistry of bis(oxazolinyl)-cyclopentadienyl and -fluorenyl rhodium and iridium organometallic compounds**

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I. Cyclic Voltammograms.

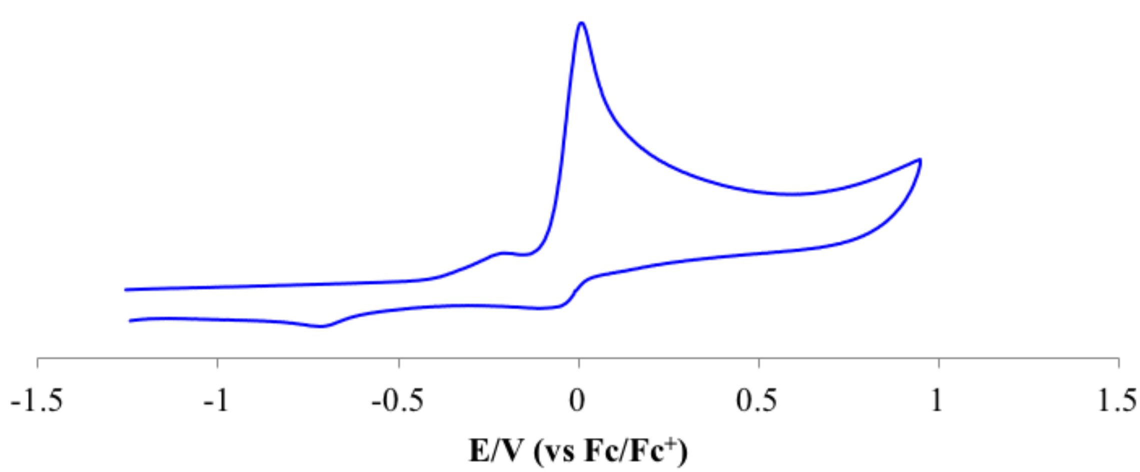

Figure S1. Cyclic voltammogram of {Bo^{M}Cp}Rh(η^4-C_8H_{12}). Conditions: 1 mM in CH_3CN, 0.1 M [$(nBu)_4N$][BF_4], 0.5 V·s^{-1}. E values are given in V vs Cp_2Fe/Cp_2Fe^{+}.

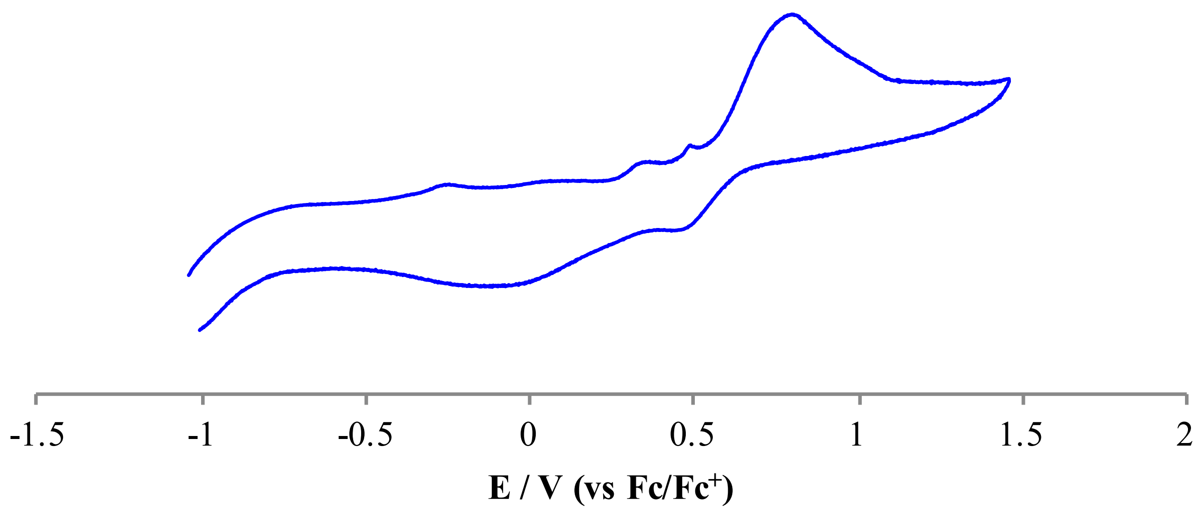

Figure S2. Cyclic voltammogram of {Bo^{M}Cp}$RhBr_2$. Conditions: 1 mM in CH_3CN, 0.1 M $[(nBu)_4N][BF_4]$, 0.1 V·s^{-1}. *E* values are given in V versus Cp_2Fe/Cp_2Fe^+.

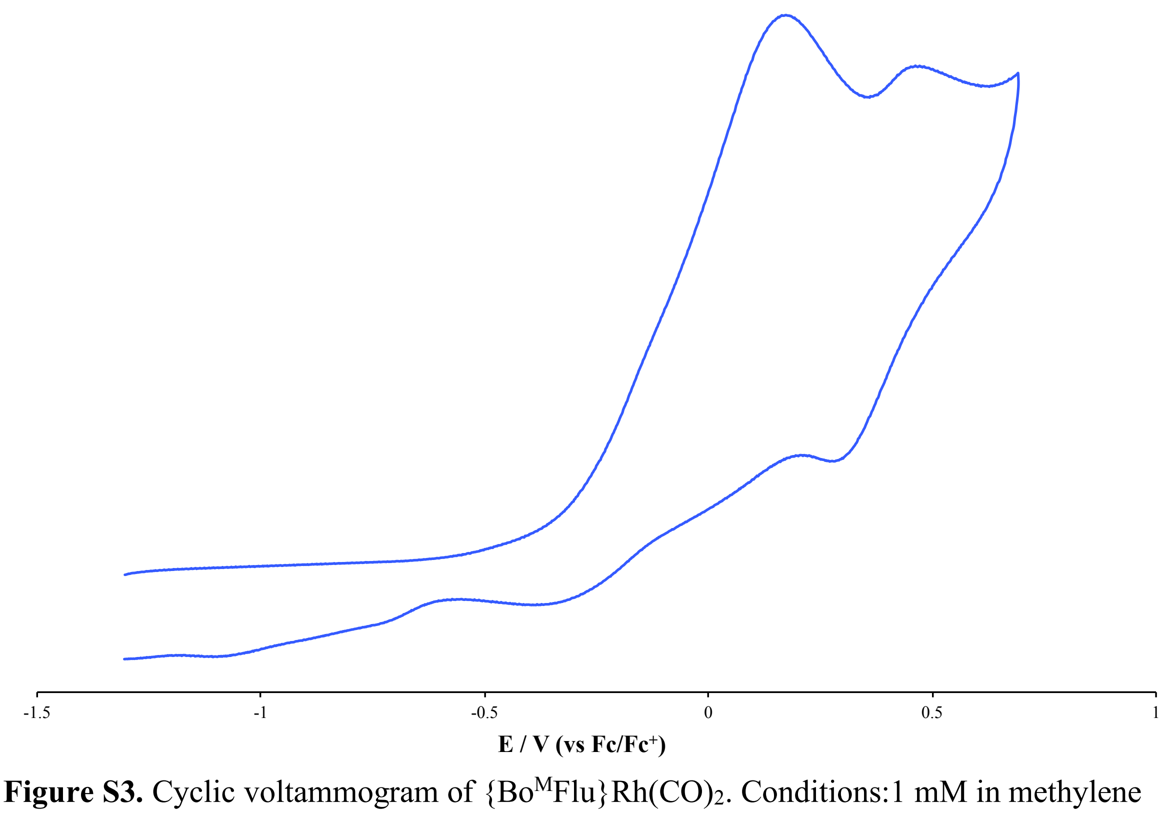

Figure S3. Cyclic voltammogram of {Bo^{M}Flu}$Rh(CO)_2$. Conditions:1 mM in methylene chloride, 0.1 M $[(nBu)_4N][BF_4]$, 0.1 V·s^{-1}. *E* values are given in V versus Cp_2Fe/Cp_2Fe^+.

II. Solution IR Spectra.

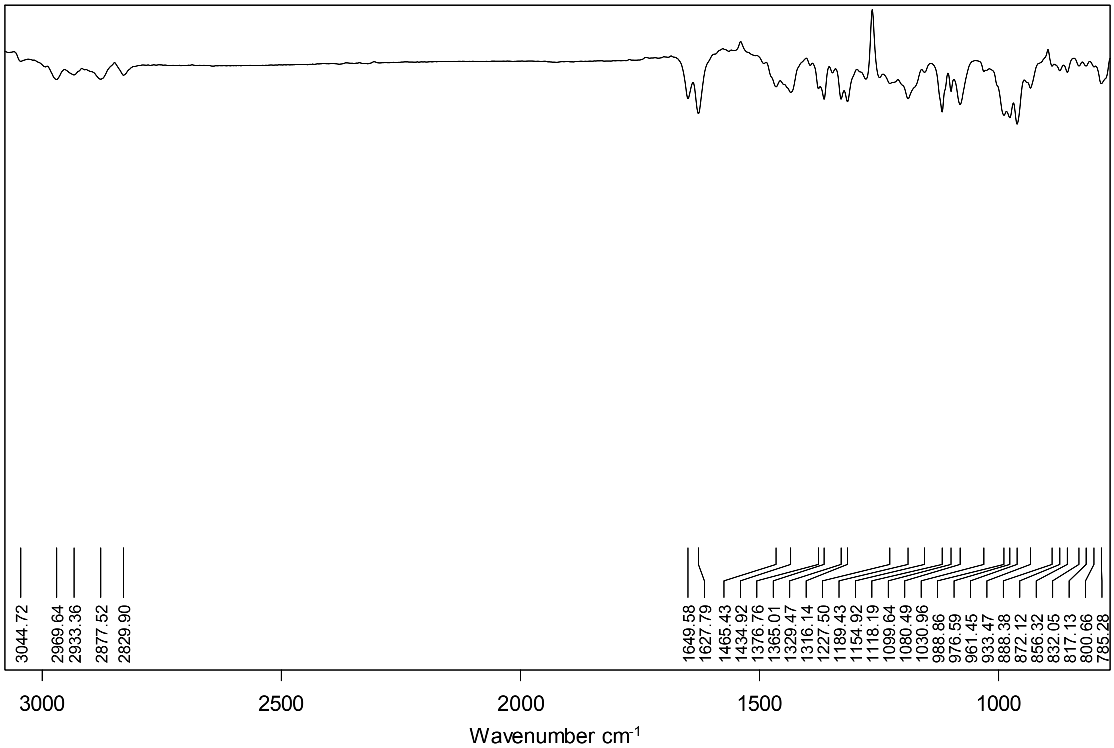

Figure S4. Solution ATR infrared spectra of {Bo^{M}Flu}Rh(η^4-C_8H_{12}) as 0.1 M solution in CH_2Cl_2.

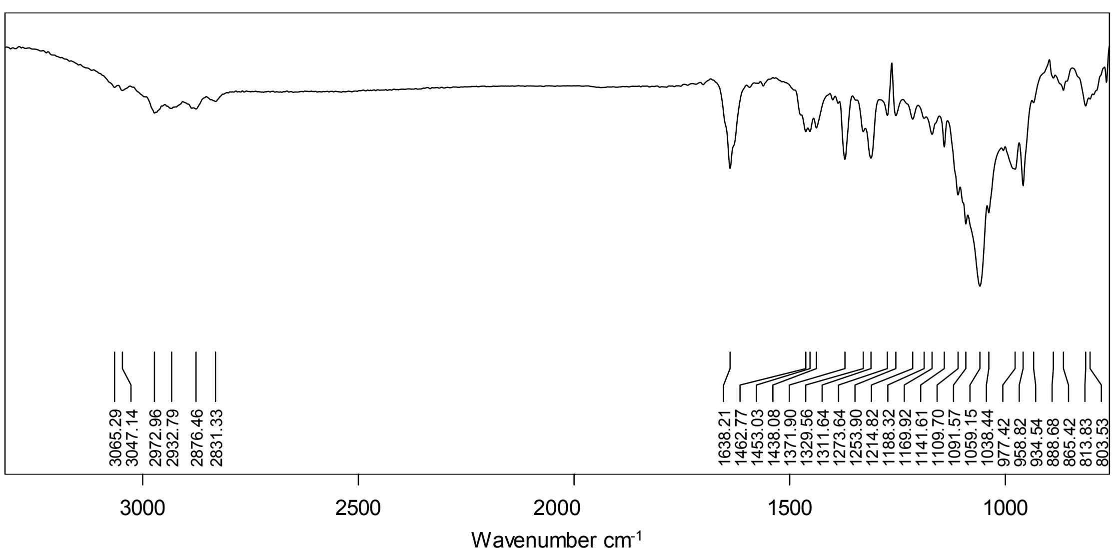

Figure S5. Solution ATR infrared spectra of the filtered reaction {Bo^{M}Flu}Rh(η^4-C_8H_{12}) + 1 eq. $AgBF_4$ as a 0.1 M solution in CH_2Cl_2.

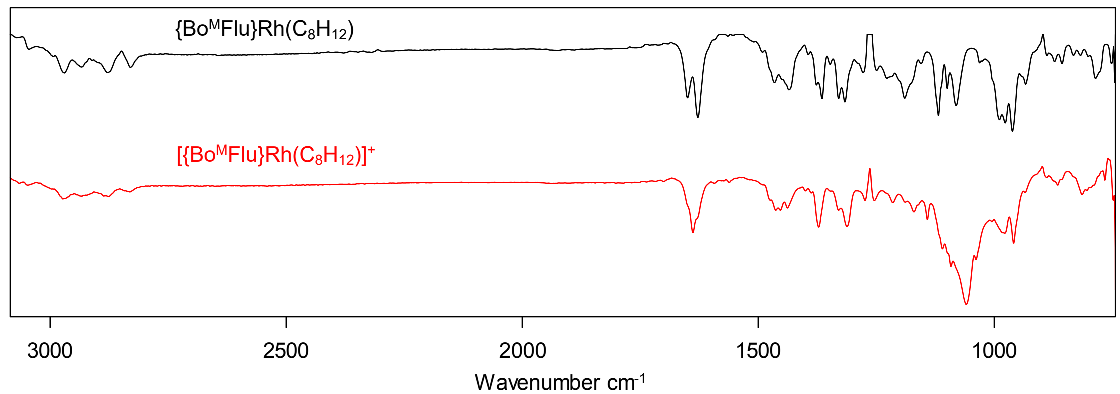

Figure S6. Solution ATR infrared spectra of $\{Bo^{M}Flu\}Rh(\eta^4\text{-}C_8H_{12})$ (Black) and $[\{Bo^{M}Flu\}Rh(C_8H_{12})][BF_4]$ (Red) as 0.1 M solutions in CH_2Cl_2.

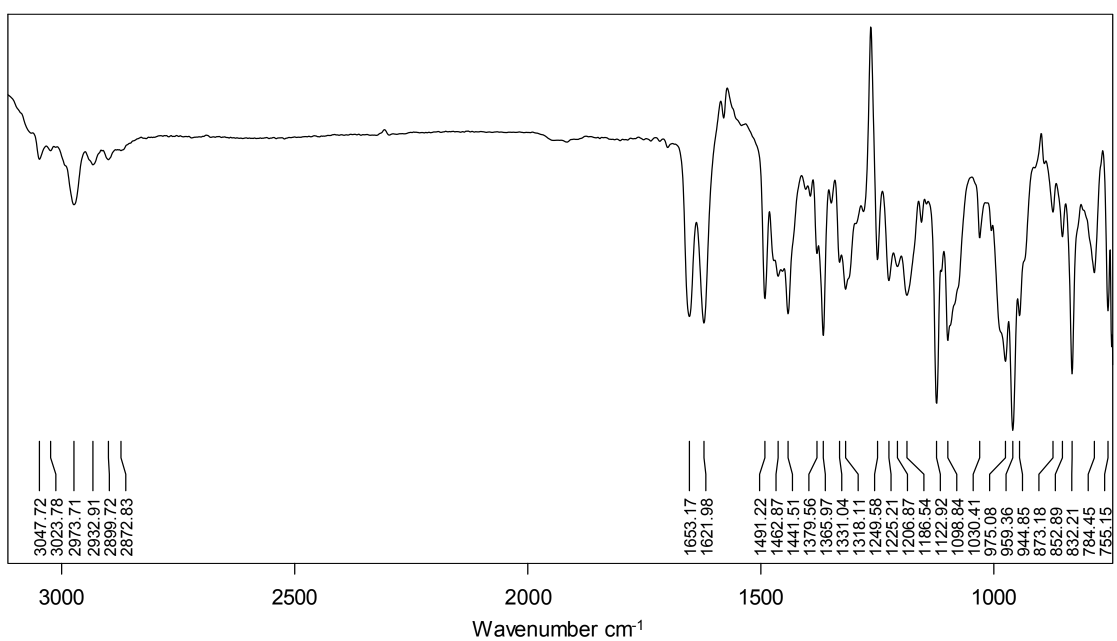

Figure S7. Solution ATR of $\{Bo^{M}Flu\}Rh(\eta^4\text{-}C_{16}H_{12})$ as a 0.1 M solution in CH_2Cl_2.

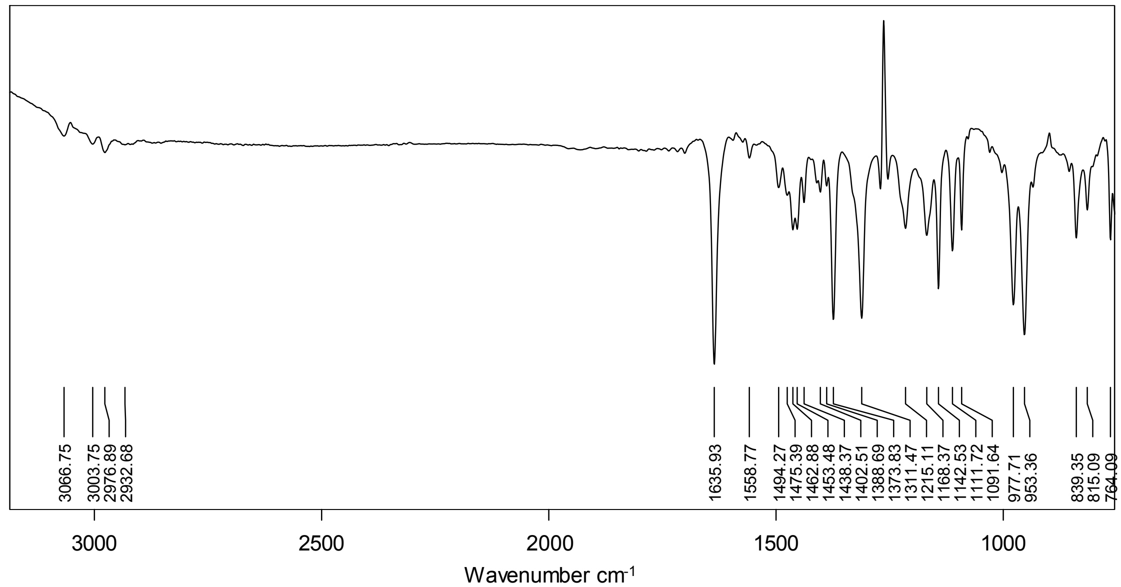

Figure S8. Solution ATR infrared spectra of the filtered reaction {Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$) + 1 eq. $AgSbF_6$ as a 0.1 M solution in CH_2Cl_2.

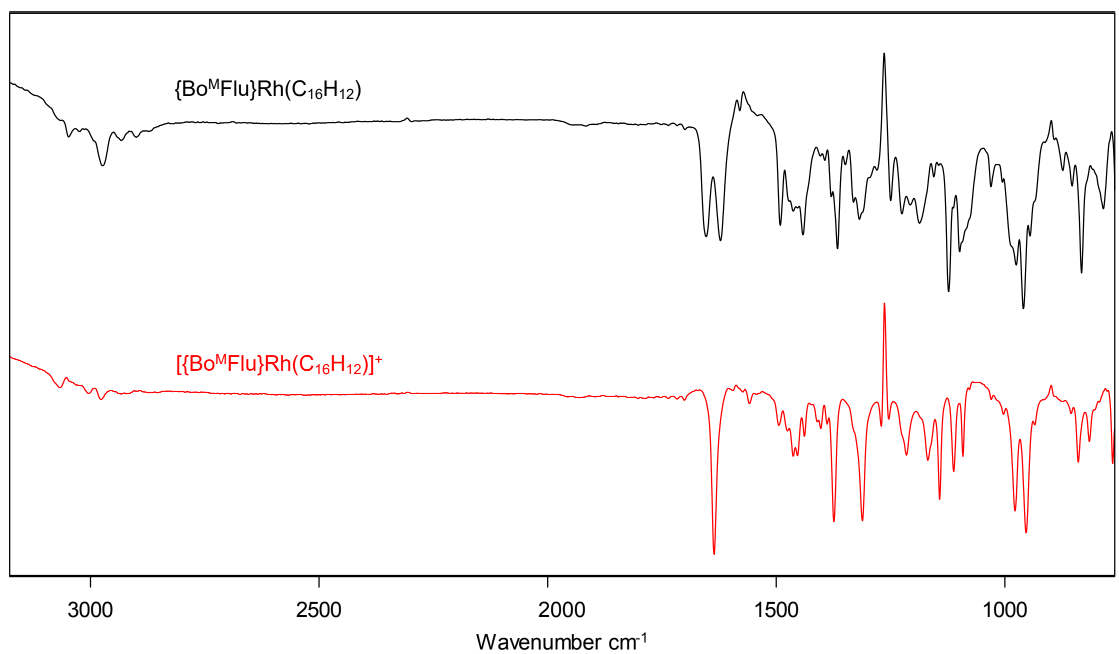

Figure S9. Solution ATR of {Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$) (Black) and [{Bo^{M}Flu}Rh($C_{16}H_{12}$)][SbF_6] (Red) as 0.1 M solutions in CH_2Cl_2.

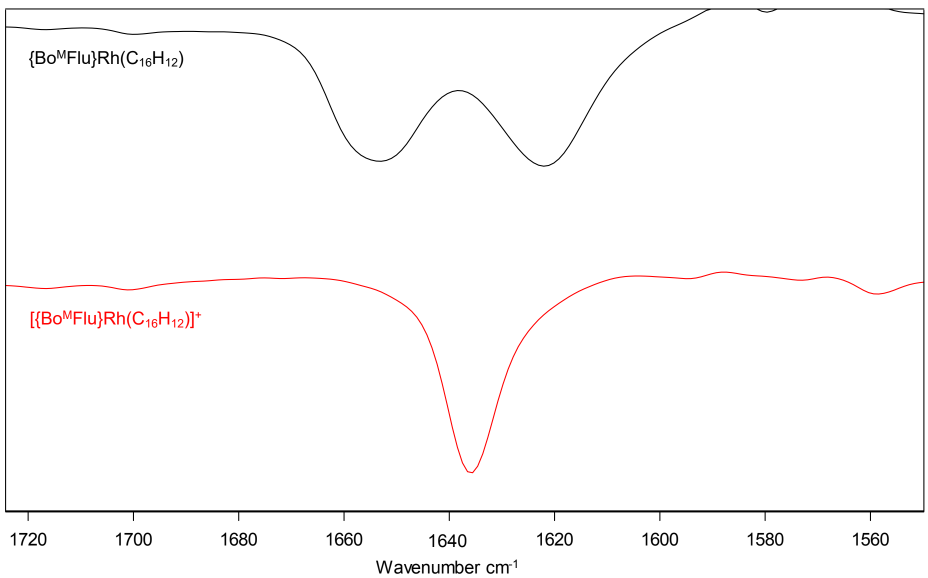

Figure S10. Solution ATR of {Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$) (Black) and [{Bo^{M}Flu}Rh($C_{16}H_{12}$)][SbF_6] (Red) as 0.1 M solutions in CH_2Cl_2 expanded region from 1550 – 1730 cm^{-1}.

III. EPR Spectra.

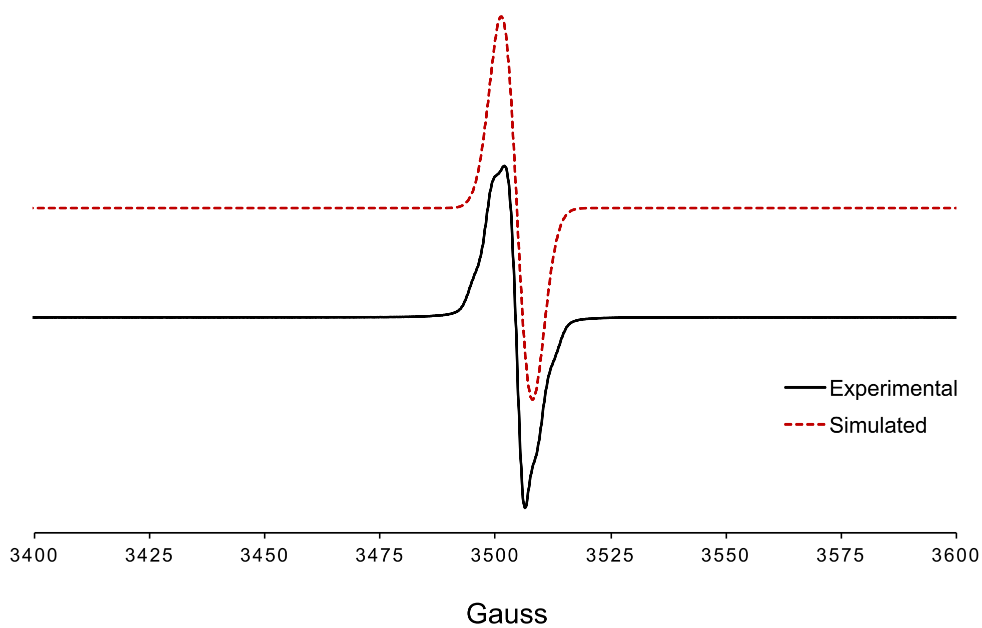

Figure S11. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-C_8H_{12})][BF_4] in 2-methyltetrahydrofuran at 298 K showing full scan window. Simulated using an isotropic model (g = 2.07).

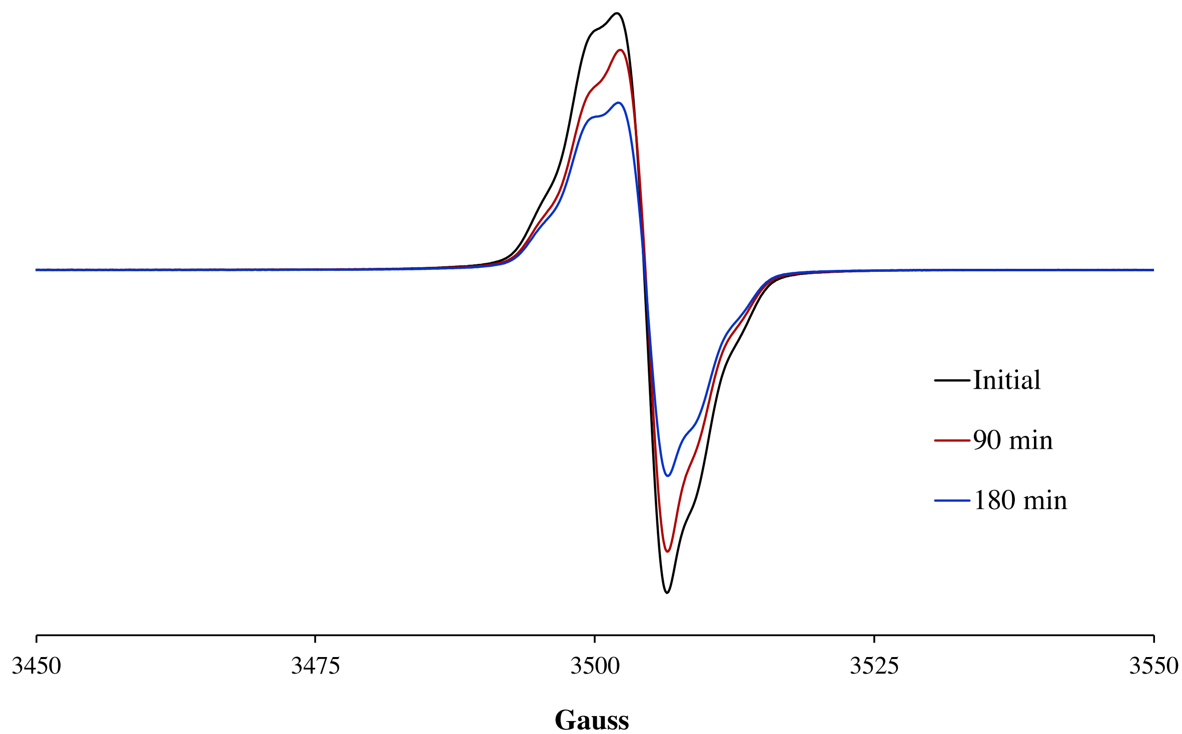

Figure S12. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-C_8H_{12})][BF_4] in 2-methyltetrahydrofuran at 298 K, measured at 0 min. (black), 90 min. (red), and 180 min. (blue) after reaction with [Ag][BF_4], showing the decay of the odd-electron species at room temperature.

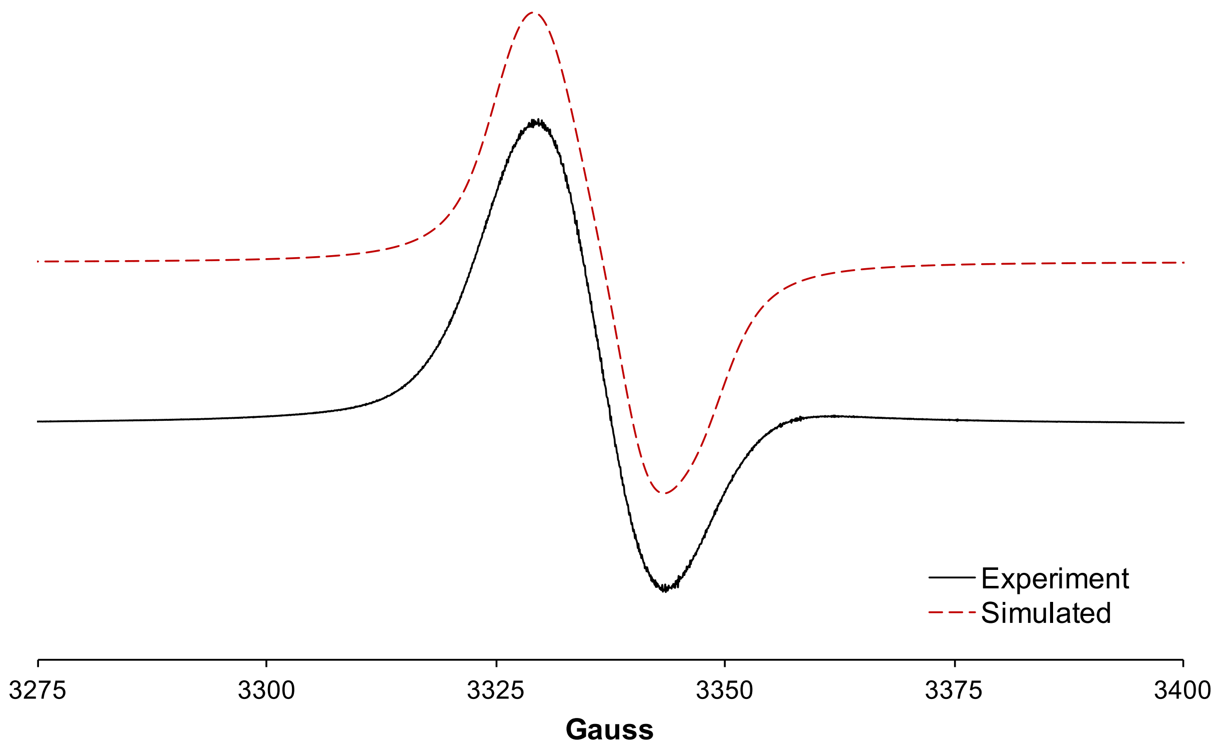

Figure S13. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-C_8H_{12})][BF_4] in 2-methyltetrahydrofuran with 0.1 M [nBu_4N]PF_6 at 20 K. g_x = 2.012 (A_{Rh} = 15.5 G) g_y = 2.004 (A_{Rh}= 16.5 G) g_z = 2.009 (A_{Rh}= 19.2 G).

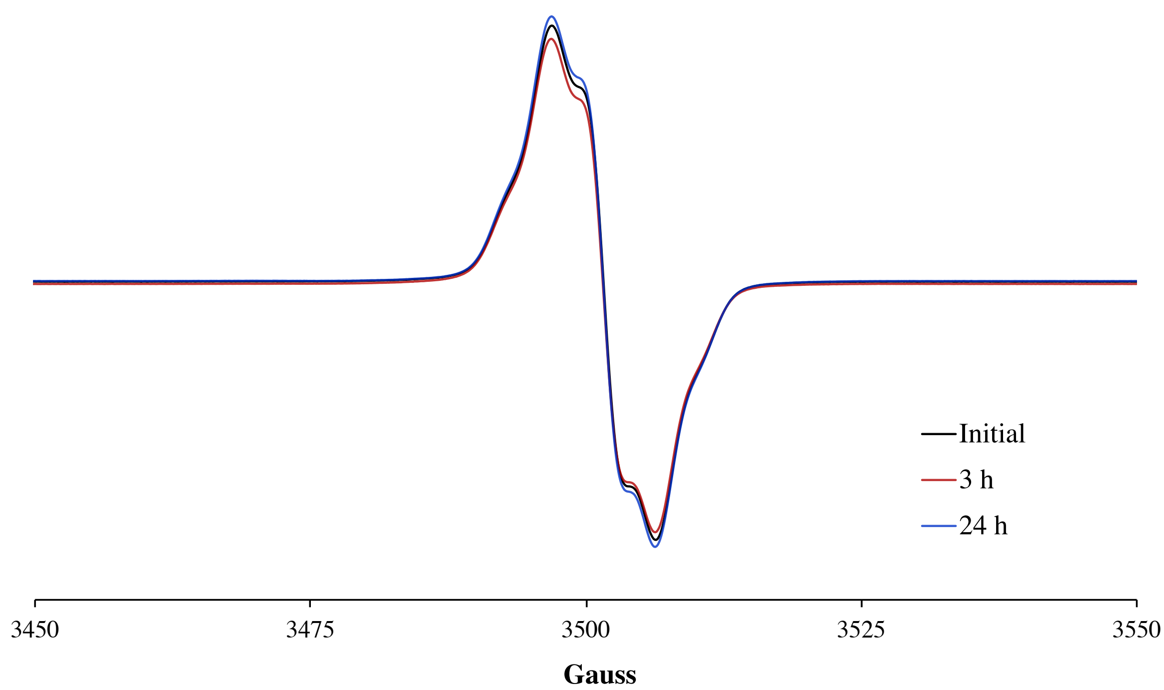

Figure S14. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$)][BF_4] in 2-MeTHF at 298 K after 0, 3 h, and 24 h showing the longer lifetime of the 1-electron oxidized species.

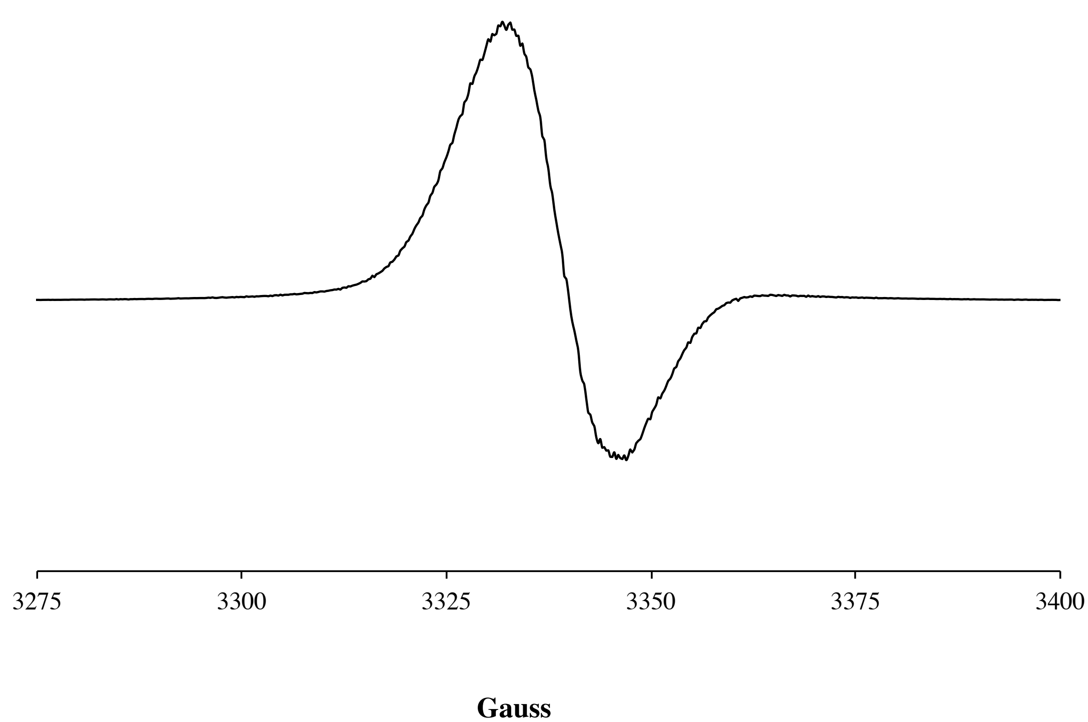

Figure S15. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$)][BF_4] in 2-methyltetrahydrofuran at 20 K.

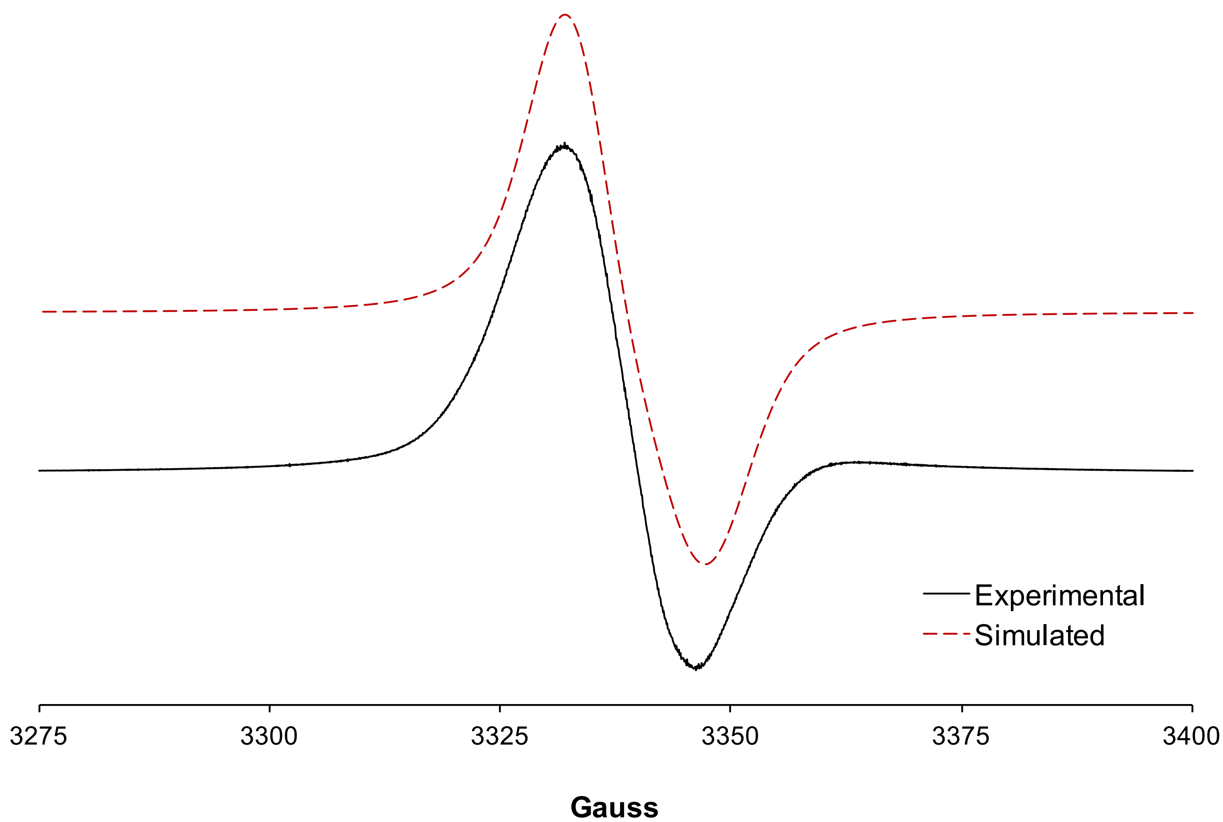

Figure S16. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$)][BF_4] in 2-methyltetrahydrofuran with 0.1 M [nBu_4N]PF_6 at 20 K. g_x = 2.004 (A_{Rh} = 25.5 G) g_y = 2.007 (A_{Rh}= 20.5 G) g_z = 2.009 (A_{Rh}= 15.2 G).

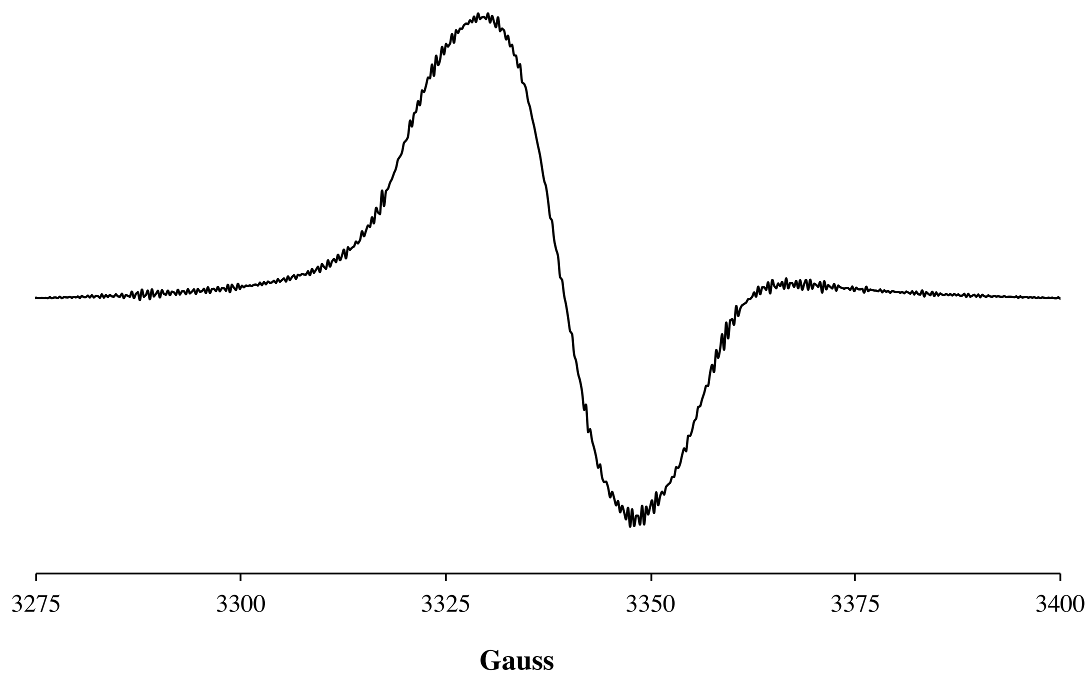

Figure S17. CW X-band EPR spectra of [{Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$)][BF_4] in 2-methyltetrahydrofuran at 10 K.

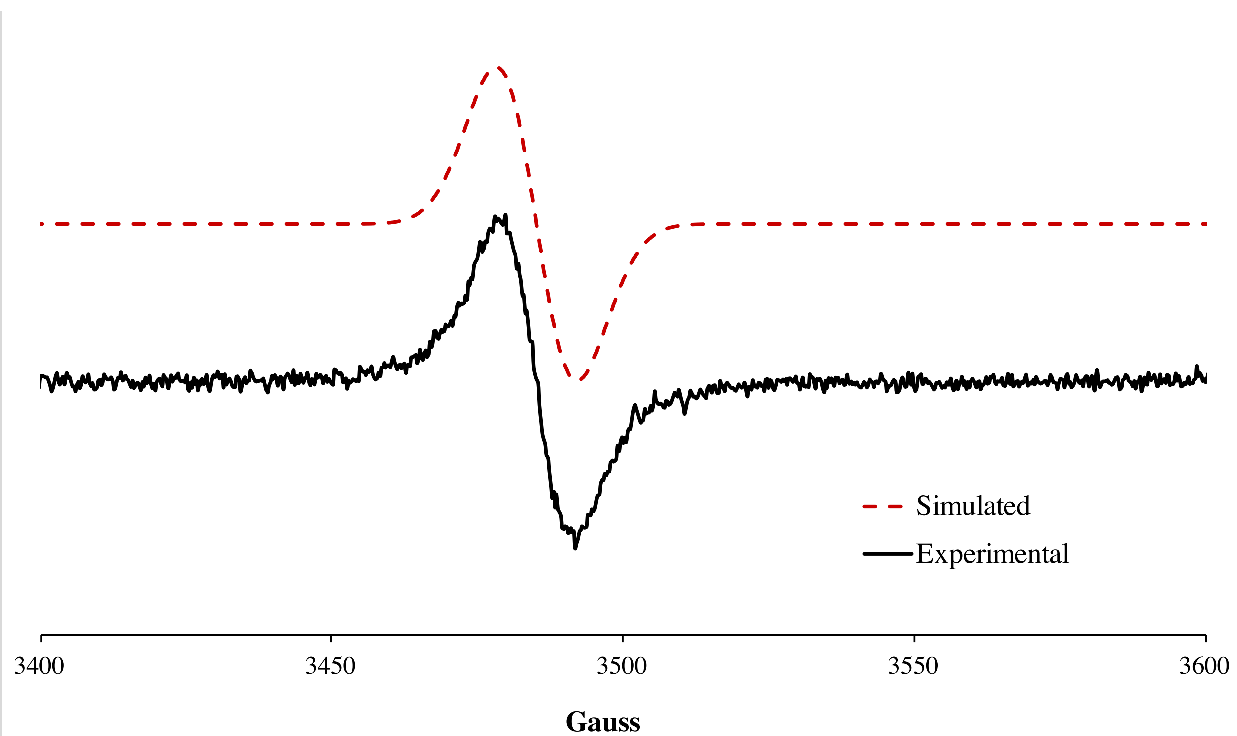

Figure S18. CW X-band EPR spectra of [{Bo^{M}Flu}Ir(η^4-$C_{16}H_{12}$)][BF_4] at a 10 mM solution in CH_2Cl_2 at 298 K. The spectrum is simulated using isotropic parameters g = 2.018 (A_{Ir} = 2.3 G).

IV. NMR and IR spectra for {Bo^{M}Cp} and {Bo^{M}Flu} Complexes.

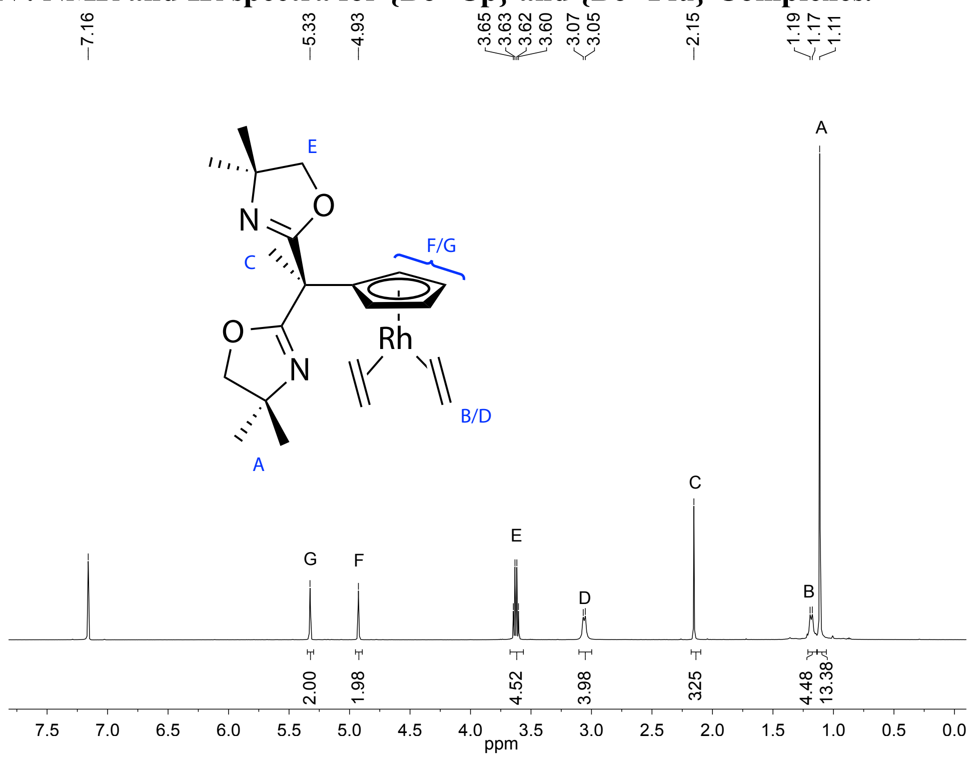

Figure S19. ^{1}H NMR spectrum of {Bo^{M}Cp}Rh(η^2-C_2H_4)$_2$ acquired at room temperature in benzene-d_6.

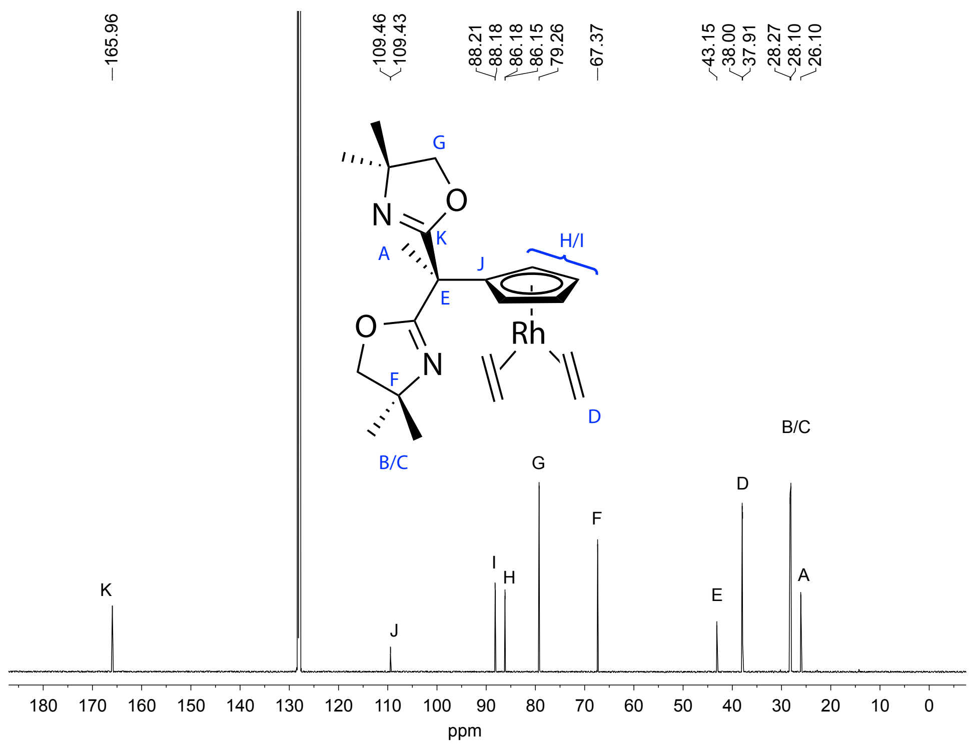

Figure S20. ^{13}C{^{1}H} NMR spectrum of {Bo^{M}Cp}Rh(η^2-C_2H_4)$_2$ acquired at room temperature in benzene-d_6.

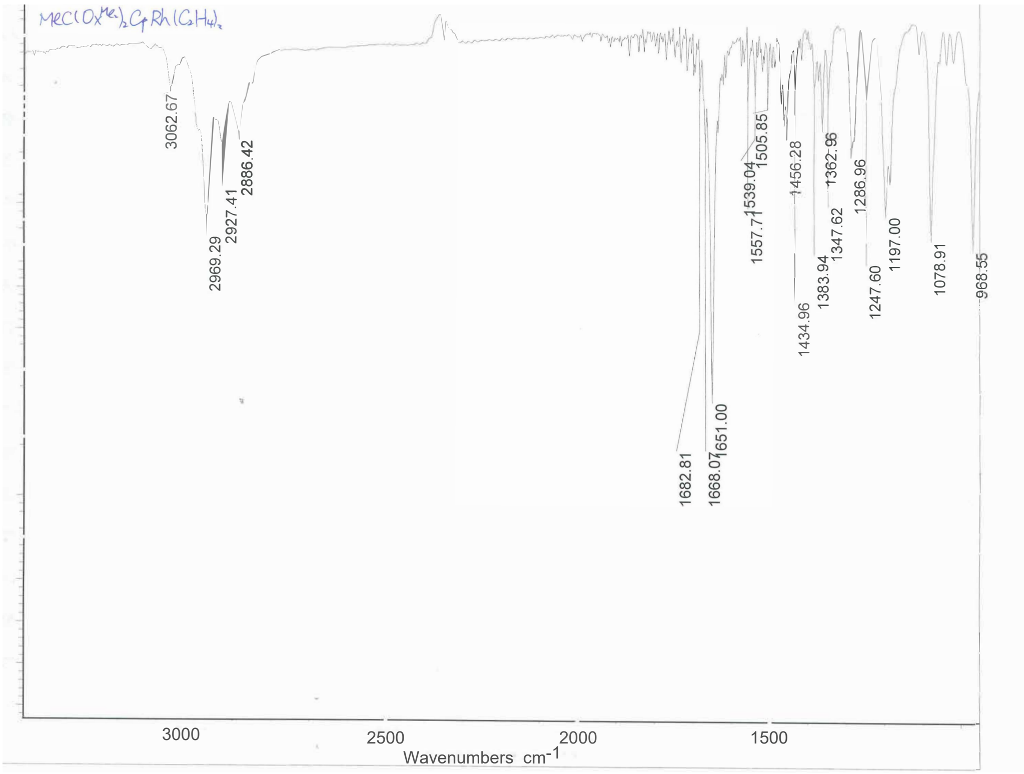

Figure S21. Infrared spectrum (KBr) of {Bo^{M}Cp}Rh(η^2-C_2H_4)$_2$.

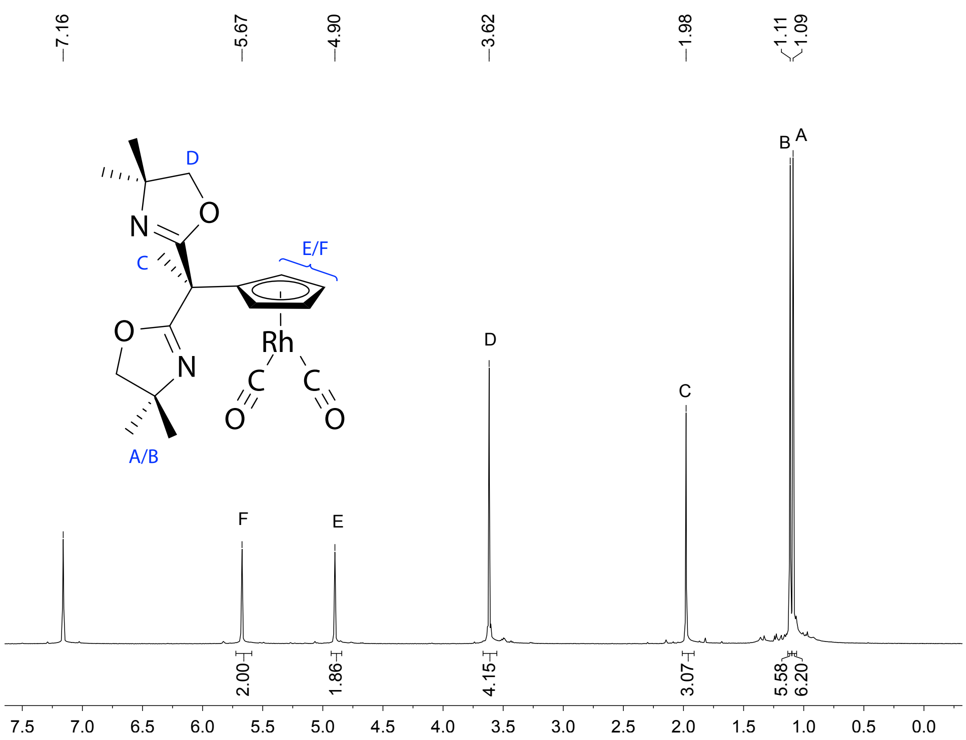

Figure S22. ^{1}H NMR spectrum of {Bo^{M}Cp}Rh(CO)$_2$ acquired at room temperature in benzene-*d*$_6$.

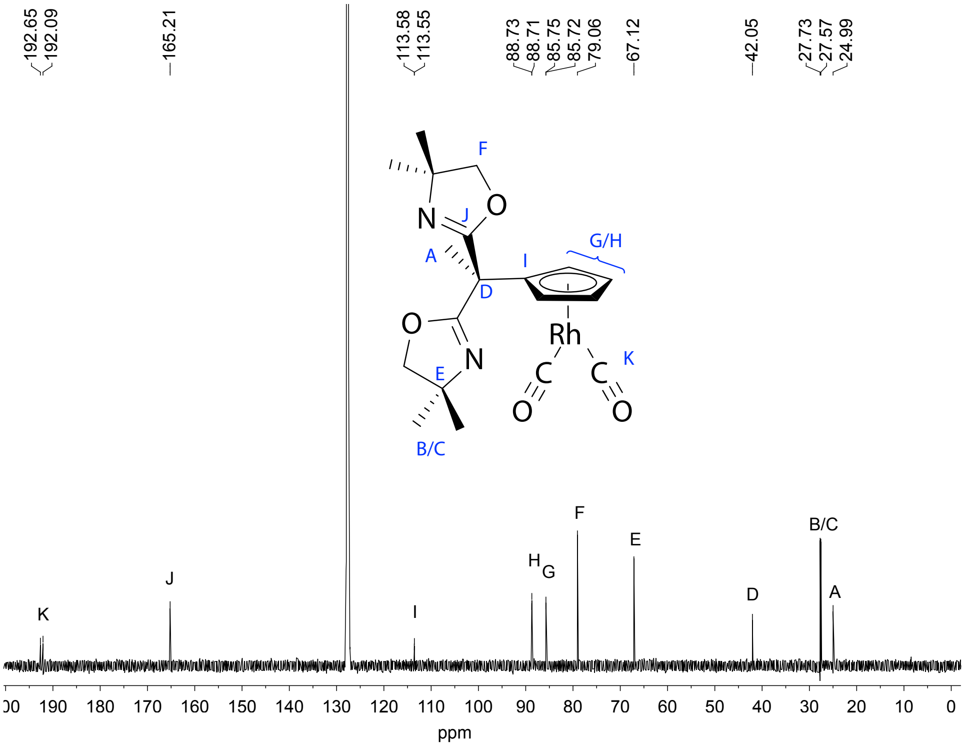

Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of $\{Bo^{M}Cp\}Rh(CO)_2$ acquired at room temperature in benzene-d_6.

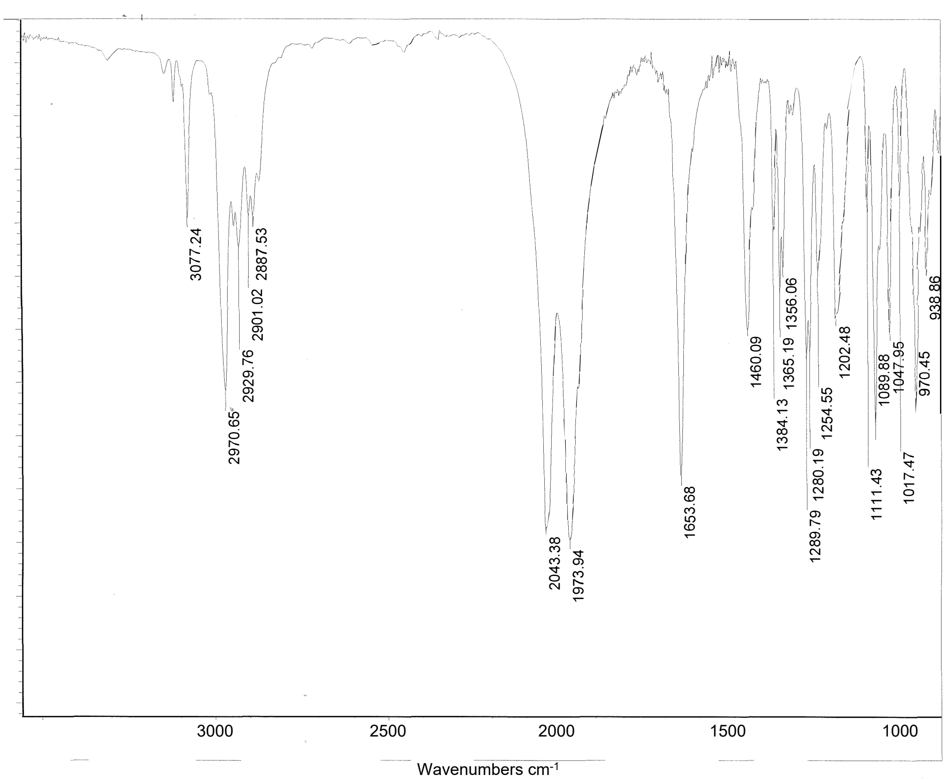

Figure S24. Infrared spectrum (KBr) of $\{Bo^{M}Cp\}Rh(CO)_2$.

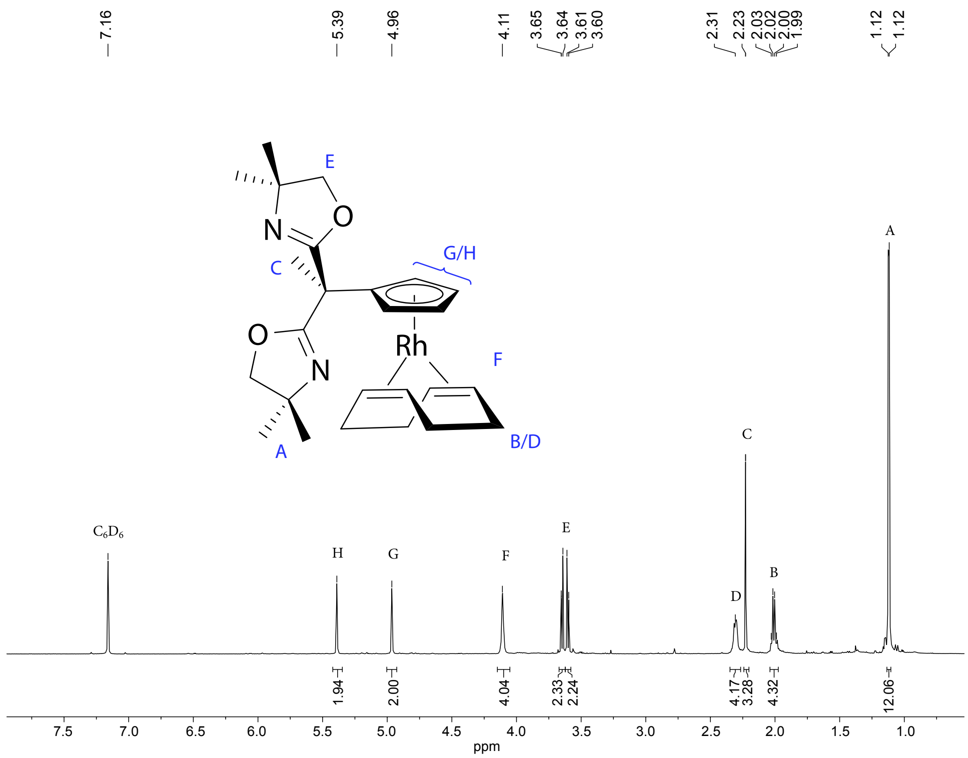

Figure S25. ^{1}H NMR spectrum of $\{Bo^{M}Cp\}Rh(\eta^4\text{-}C_8H_{12})$ acquired at room temperature in benzene-d_6.

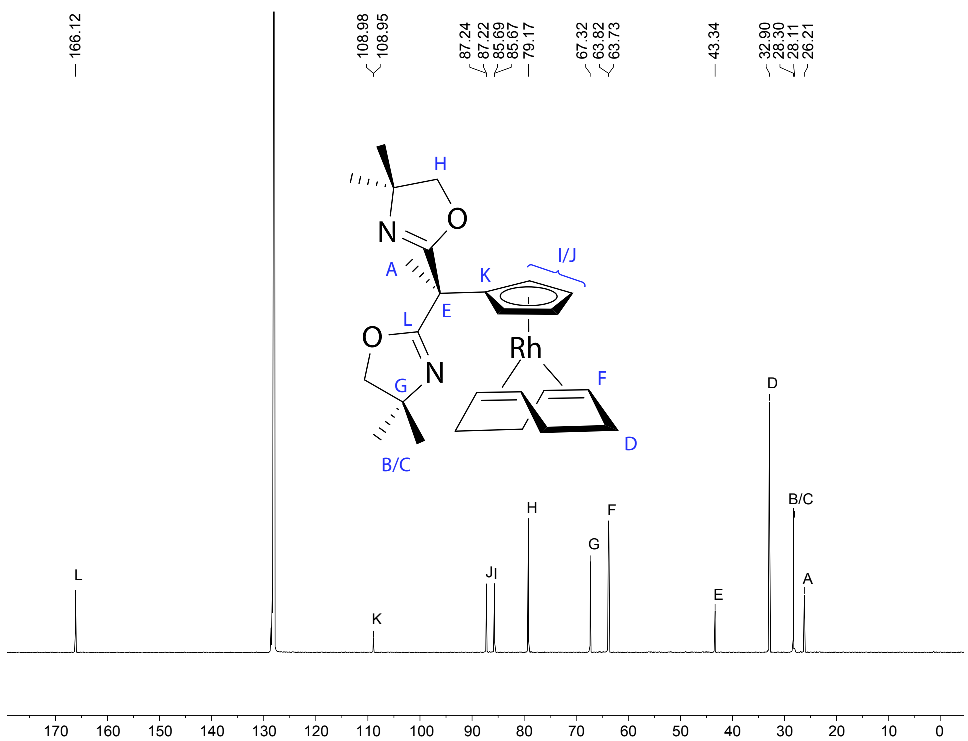

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of $\{Bo^{M}Cp\}Rh(\eta^4\text{-}C_8H_{12})$ acquired at room temperature in benzene-d_6.

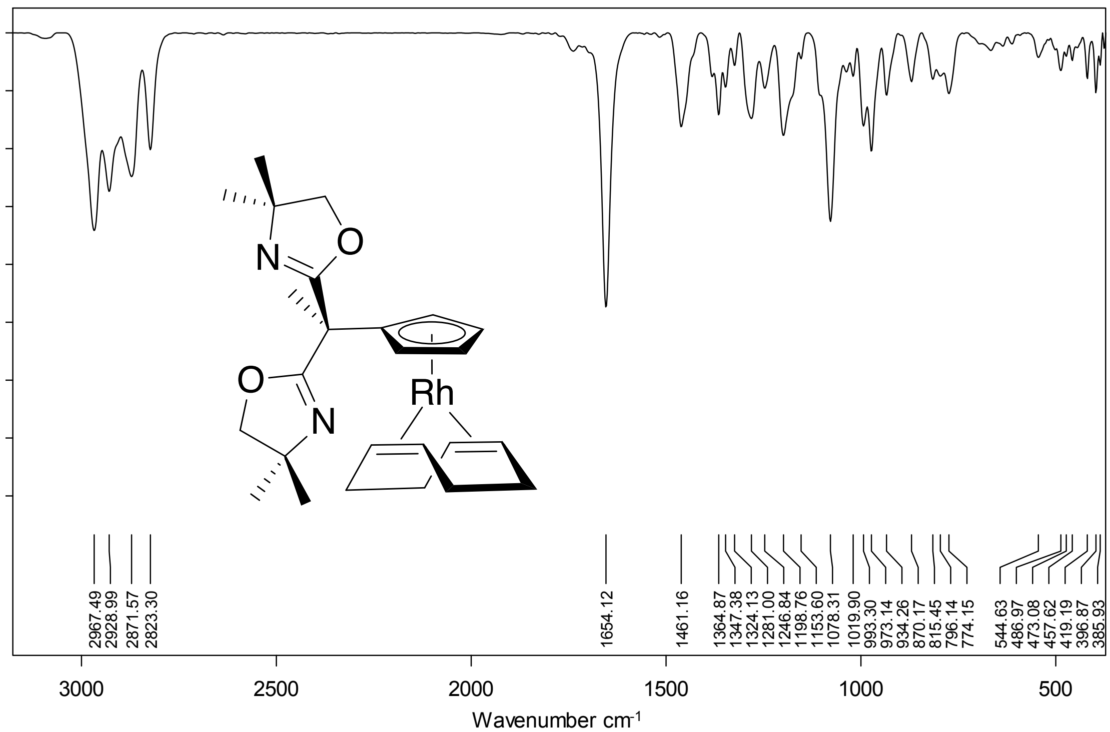

Figure S27. Infrared spectrum (KBr) of $\{Bo^MCp\}Rh(\eta^4\text{-}C_8H_{12})$.

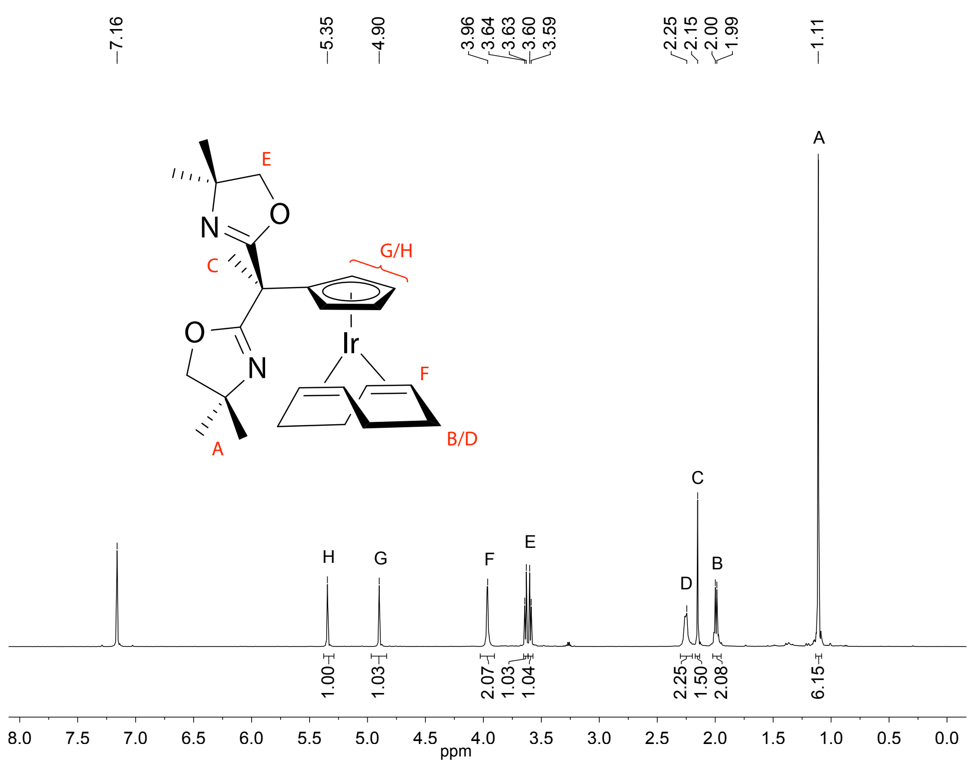

Figure S28. ^{1}H NMR spectrum of $\{Bo^MCp\}Ir(\eta^4\text{-}C_8H_{12})$ acquired at room temperature in benzene-d_6.

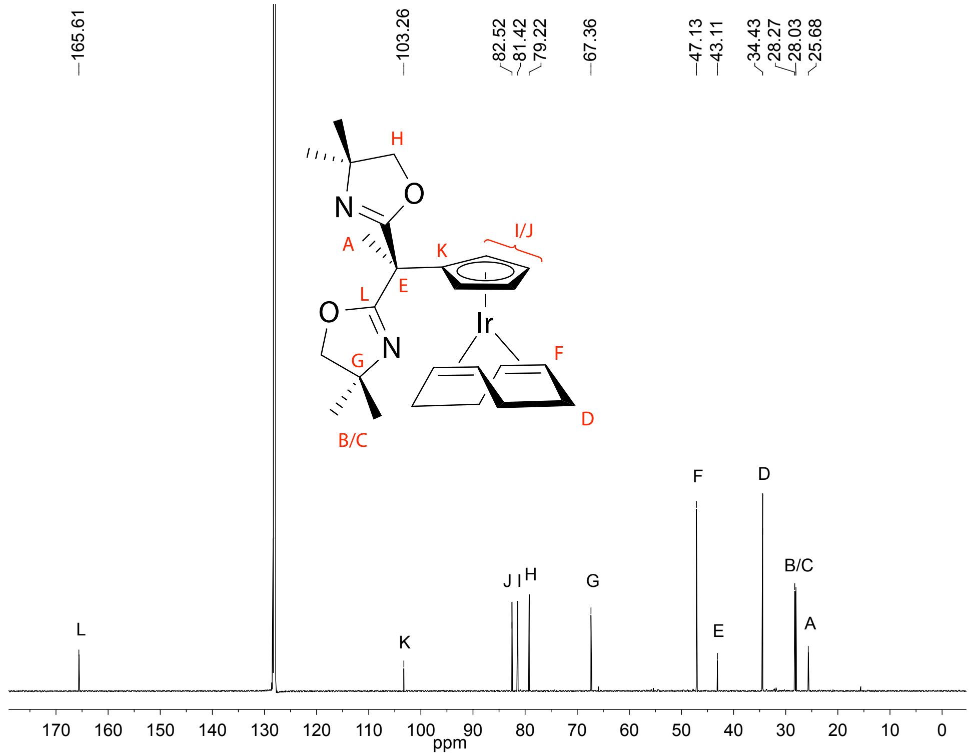

Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of $\{Bo^{M}Cp\}Ir(\eta^4\text{-}C_8H_{12})$ acquired at room temperature in benzene-d_6.

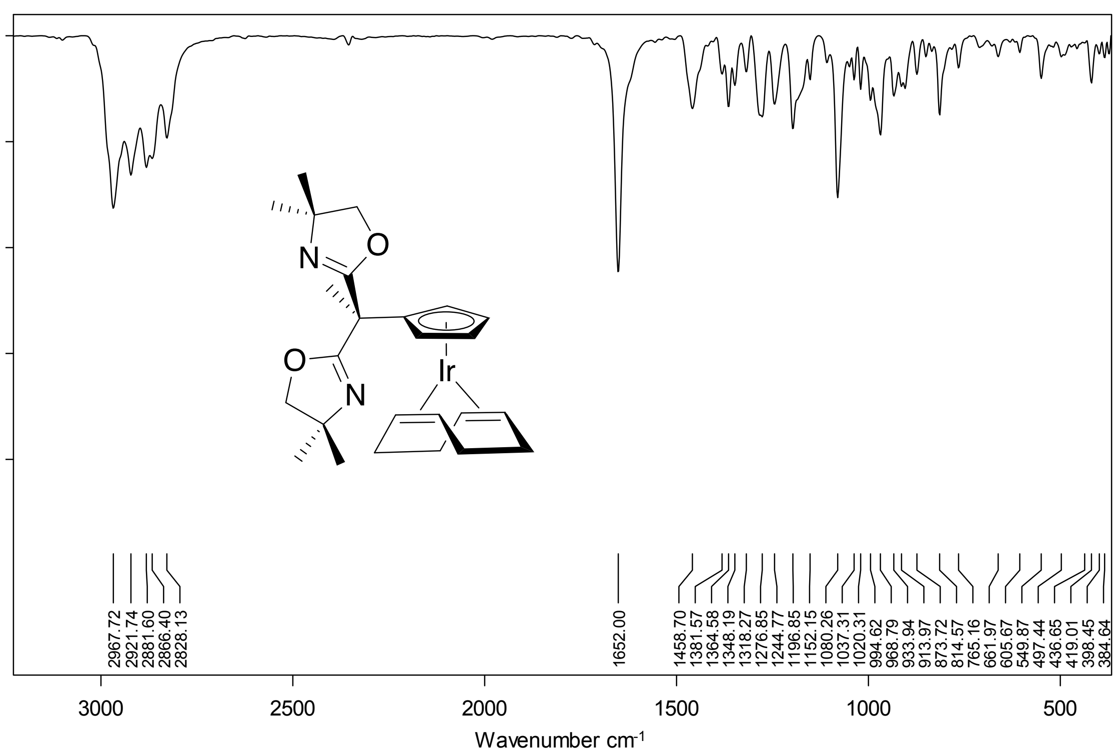

Figure S30. Infrared spectrum (KBr) of $\{Bo^{M}Cp\}Ir(\eta^4\text{-}C_8H_{12})$.

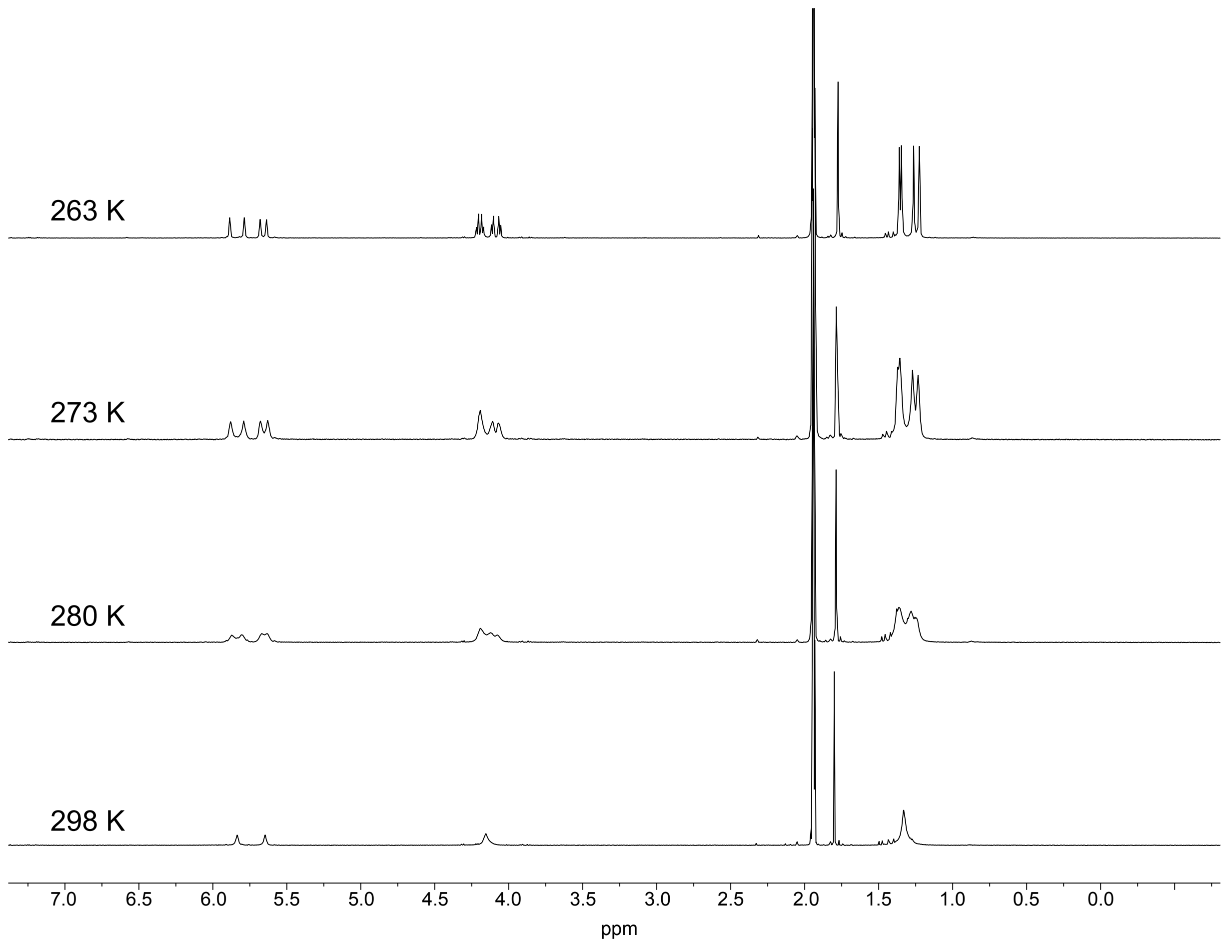

Figure S31. Variable temperature ^{1}H NMR spectra of {Bo^{M}Cp}$RhBr_2$ acquired in acetonitrile-d_3 at 298 K, 280 K, 273 K, and 263 K.

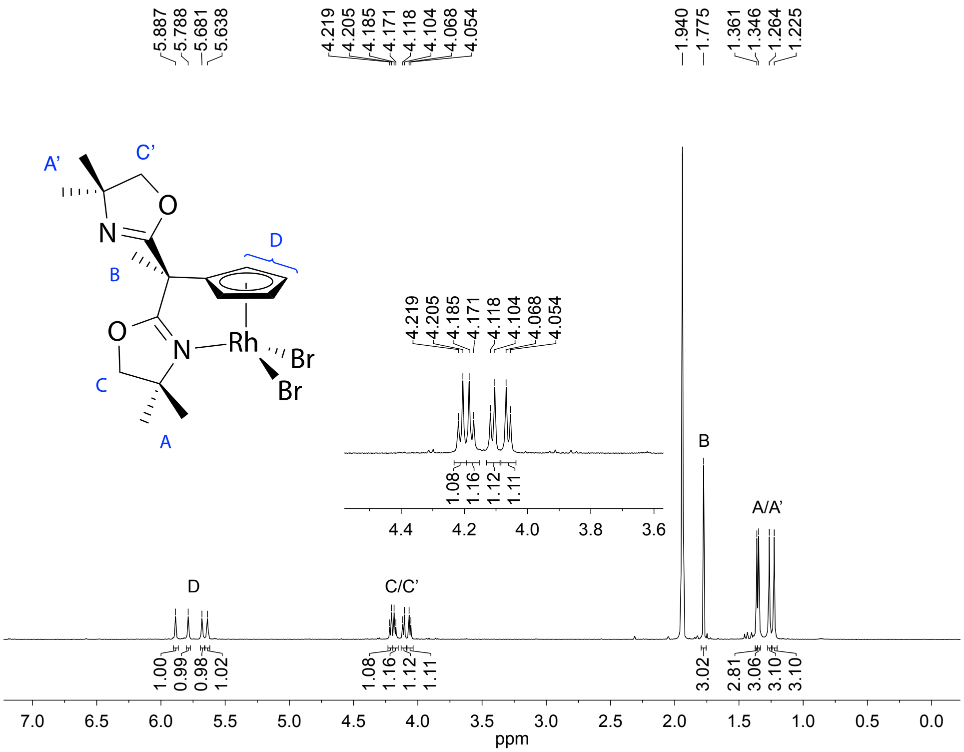

Figure S32. ^{1}H NMR spectrum of {Bo^{M}Cp}$RhBr_2$ acquired at 263 K in acetonitrile-d_3.

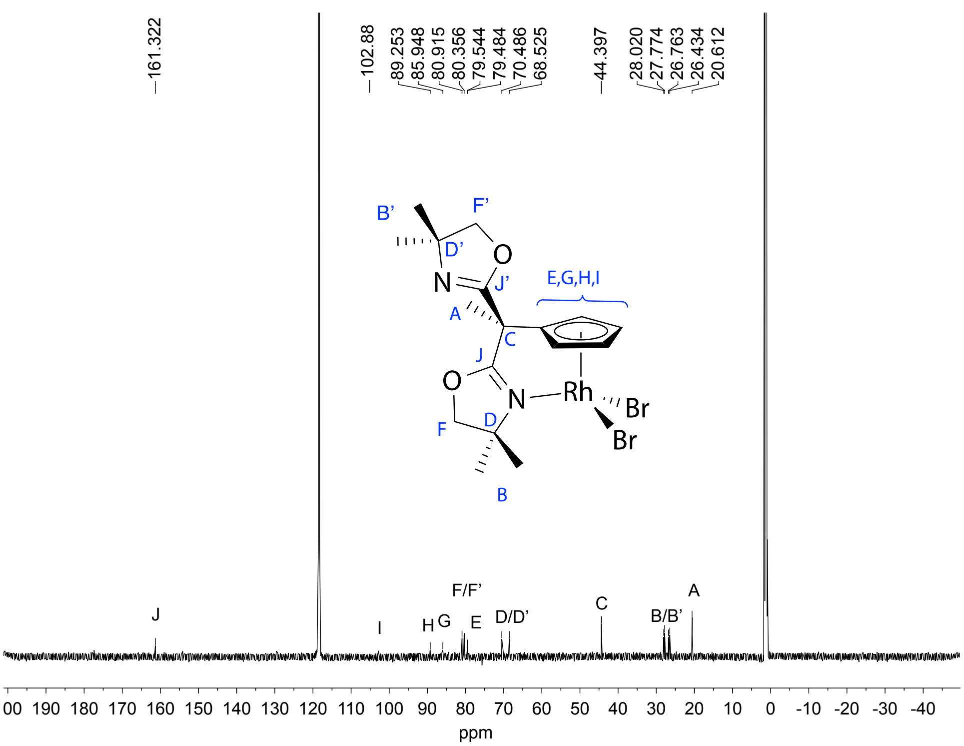

Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of {Bo^{M}Cp}$RhBr_2$ acquired at 263 K in acetonitrile-d_3.

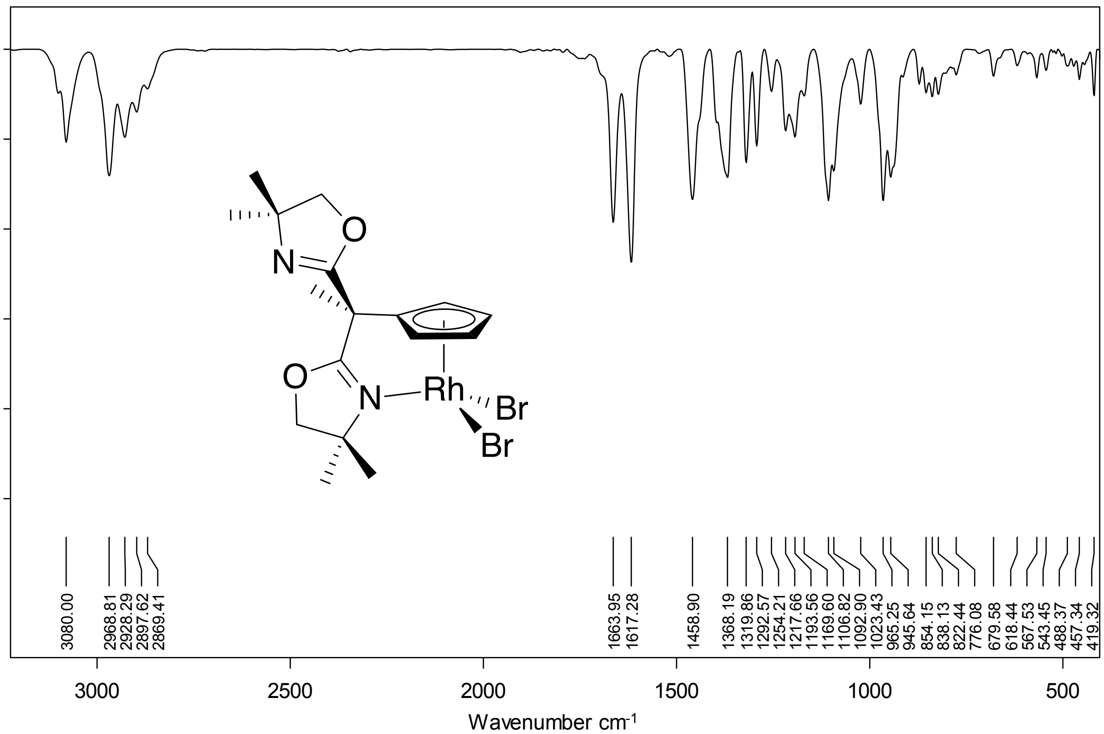

Figure S34. Infrared spectrum (KBr) of $\{Bo^{M}Cp\}RhBr_2$.

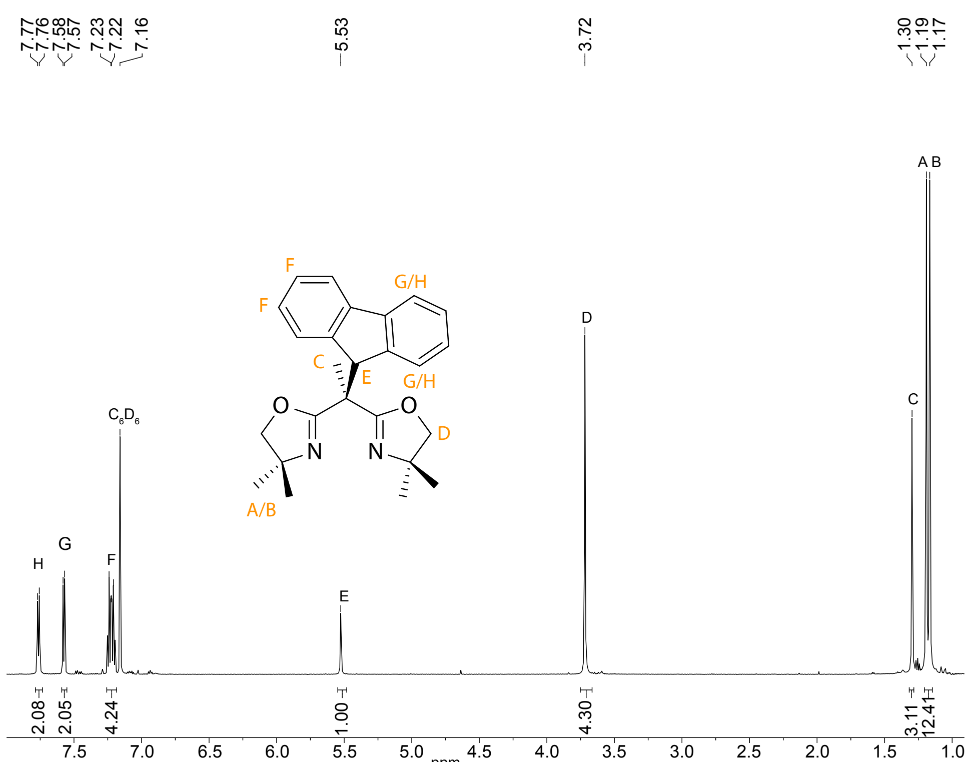

Figure S35. ^{1}H NMR spectrum of $Bo^{M}FluH$ acquired at room temperature in benzene-d_6.

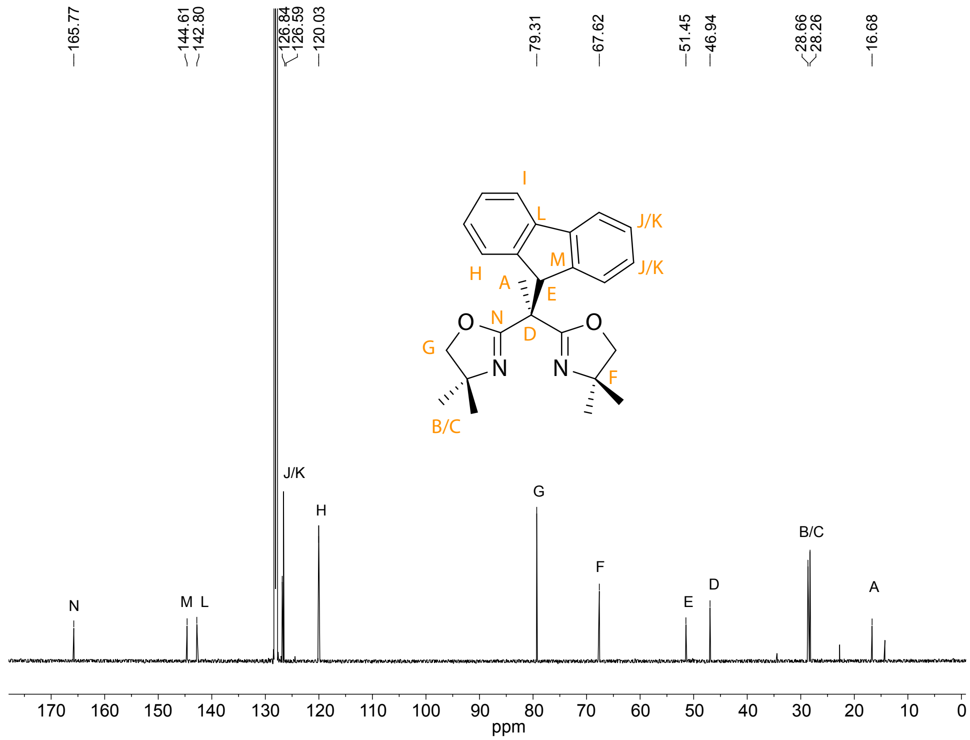

Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of Bo^{M}FluH acquired at room temperature in benzene-d_6.

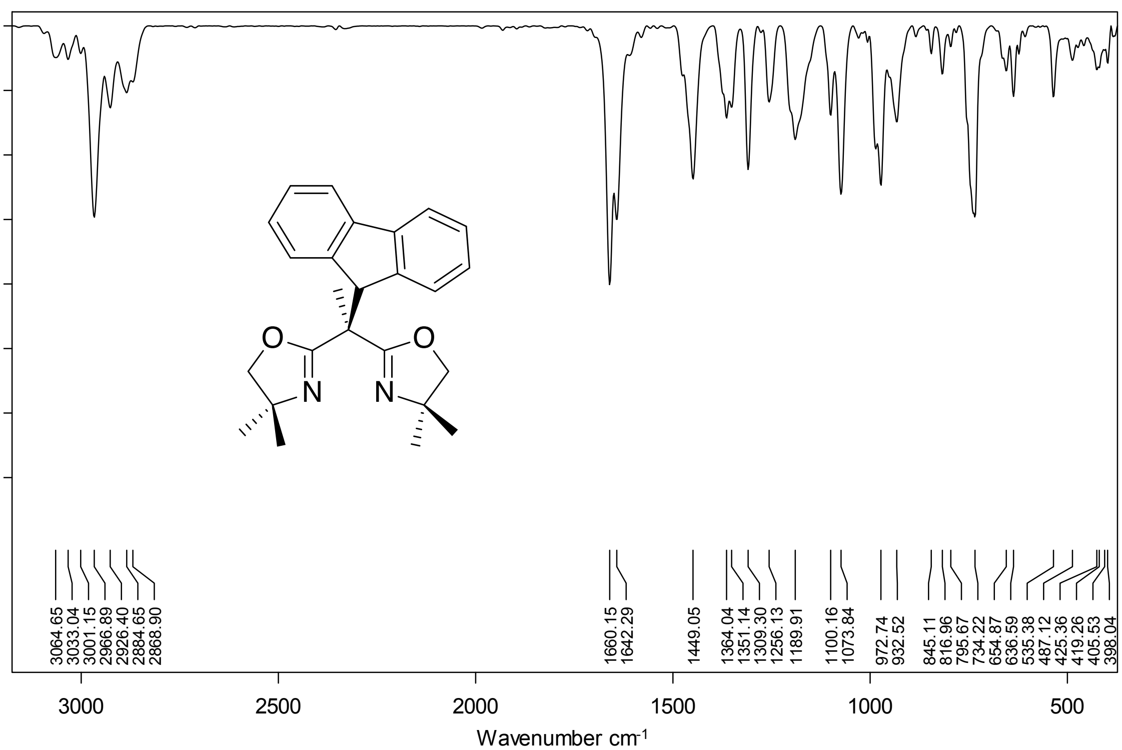

Figure S37. Infrared spectrum (KBr) of Bo^{M}FluH.

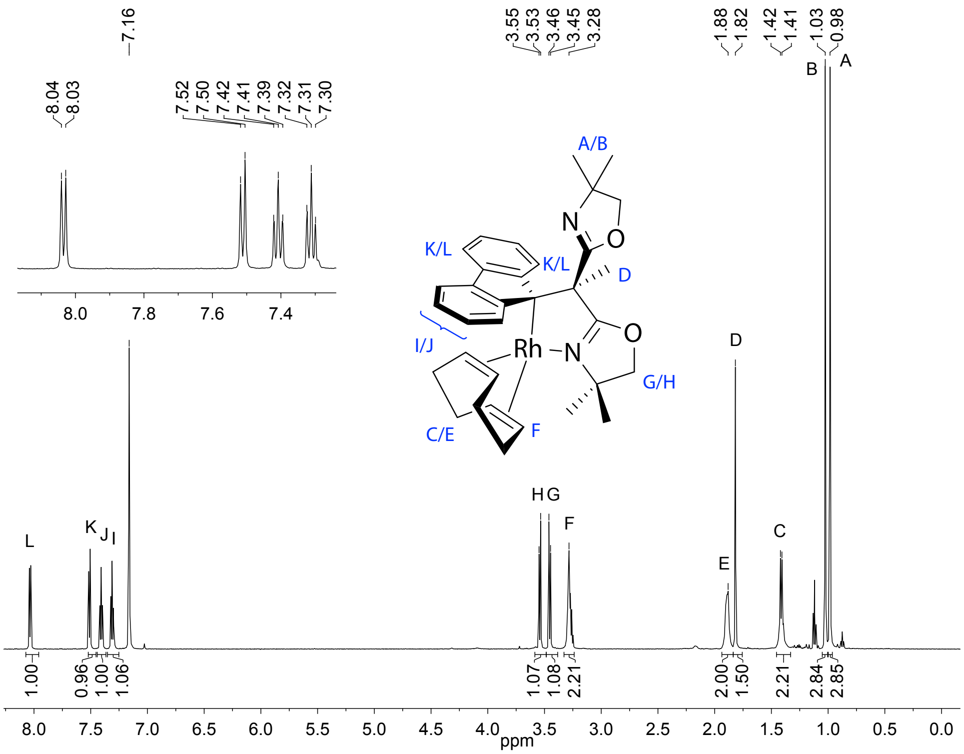

Figure S38. ^{1}H NMR spectrum of {Bo^{M}Flu}Rh(η^4-C_8H_{12}) acquired in benzene-d_6.

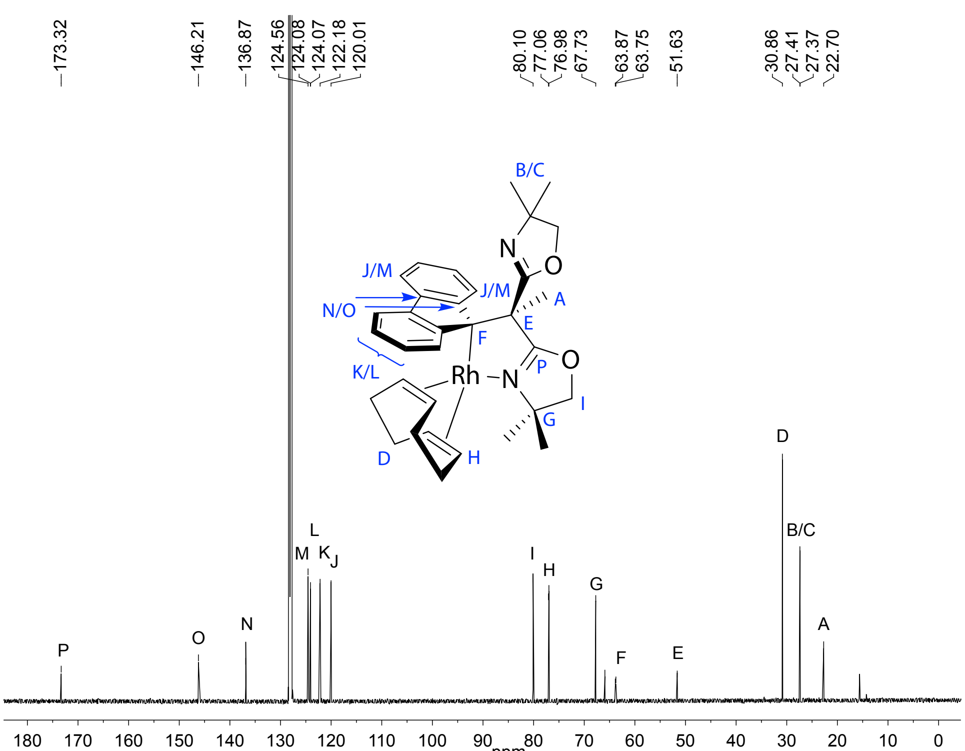

Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of {Bo^{M}Flu}Rh(η^4-C_8H_{12}) acquired in benzene-d_6.

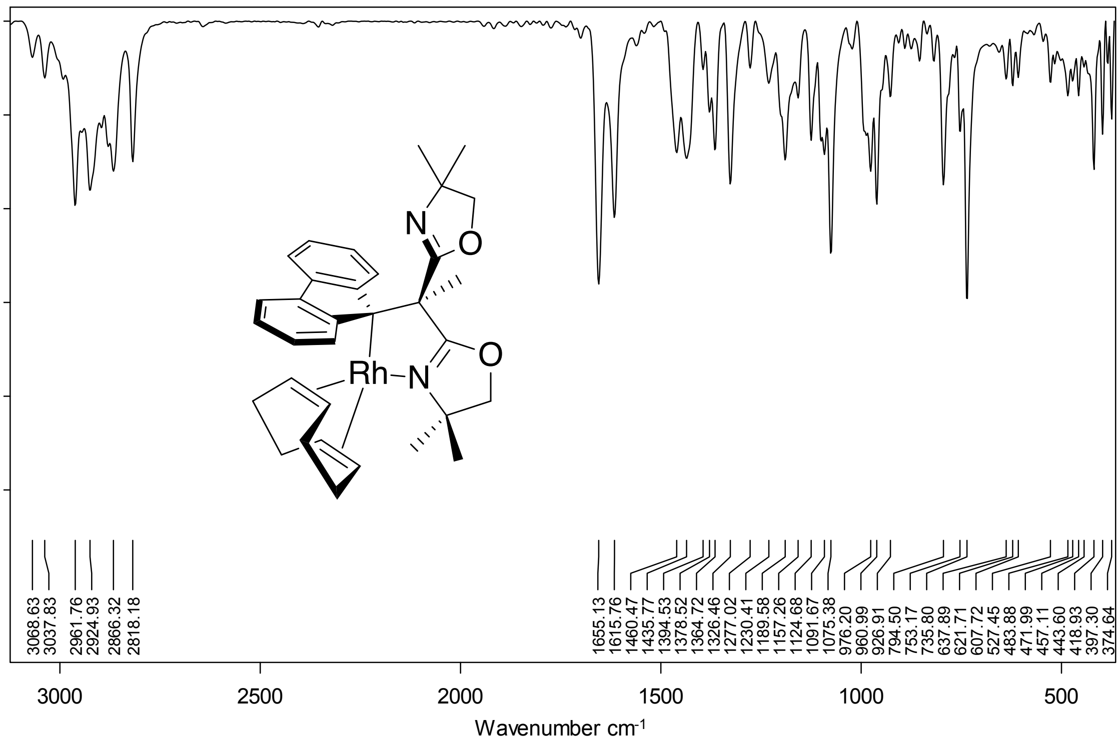

Figure S40. Infrared spectrum (KBr) of {Bo^{M}Flu}Rh(η^4-C_8H_{12}).

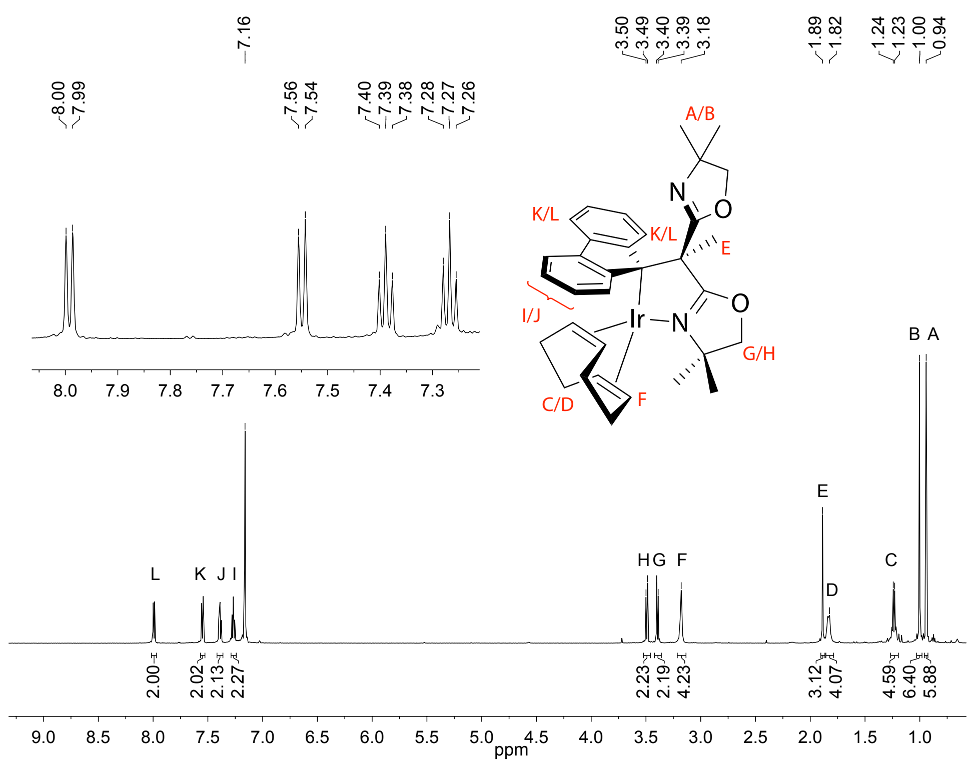

Figure S41. ^{1}H NMR spectrum of {Bo^{M}Flu}Ir(η^4-C_8H_{12}) acquired in benzene-d_6.

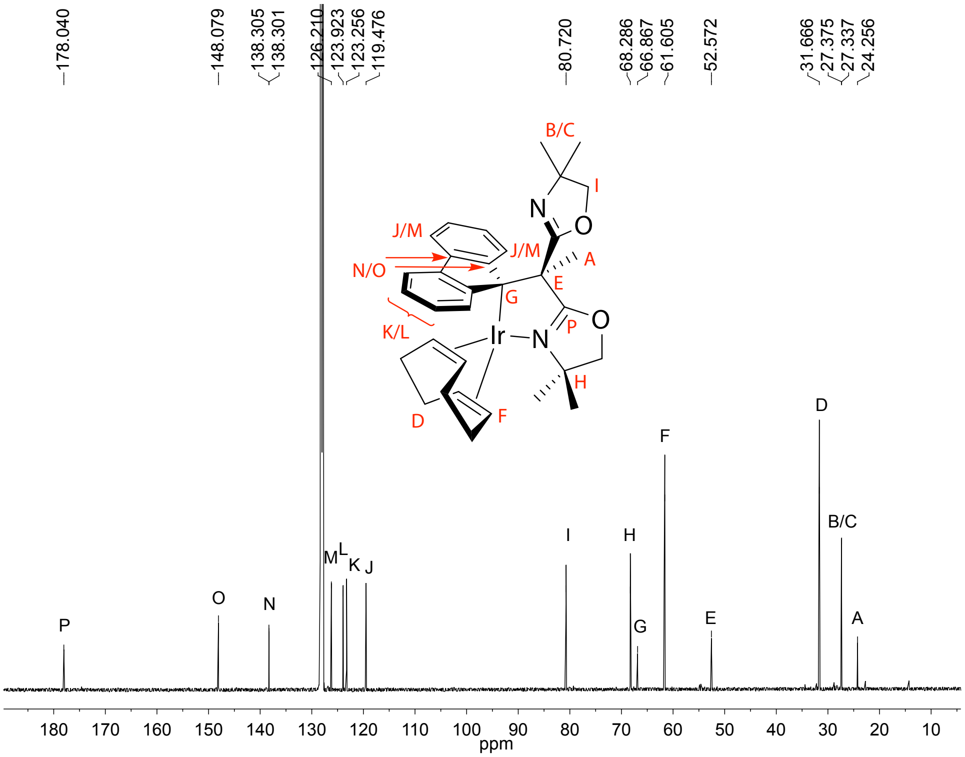

Figure S42. $^{13}C\{^1H\}$ NMR spectrum of $\{Bo^MFlu\}Ir(\eta^4\text{-}C_8H_{12})$ acquired at room temperature in benzene-d_6.

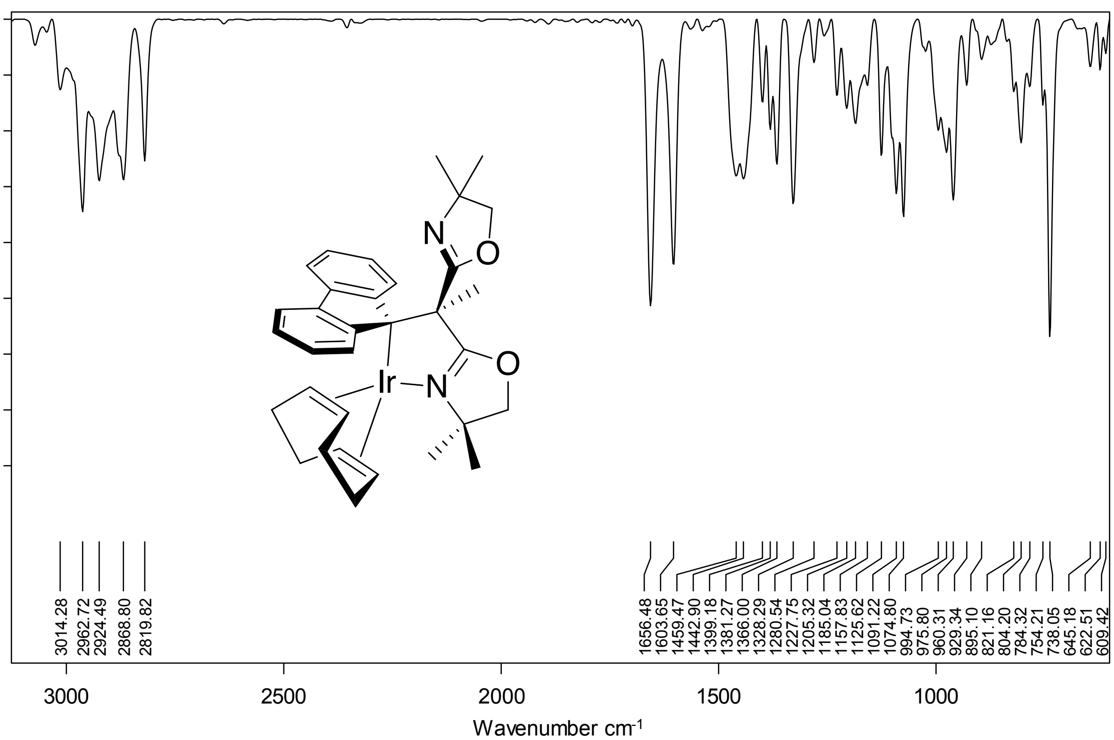

Figure S43. Infrared spectrum (KBr) of $\{Bo^MFlu\}Ir(\eta^4\text{-}C_8H_{12})$.

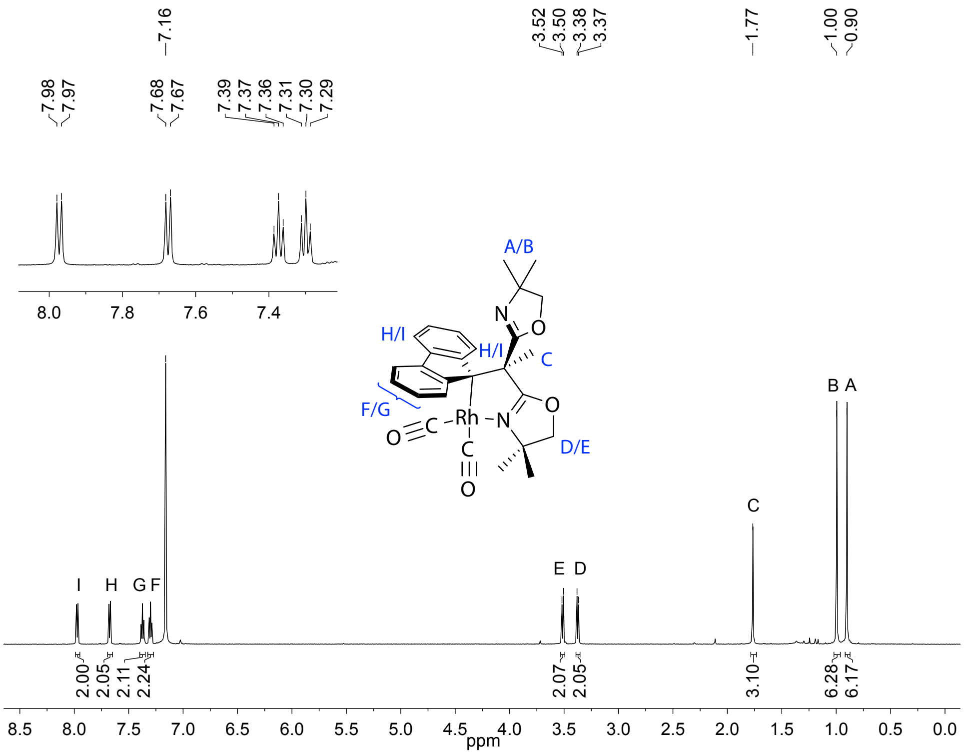

Figure S44. ^{1}H NMR spectrum of {Bo^{M}Flu}Rh(CO)$_2$ acquired in benzene-d_6.

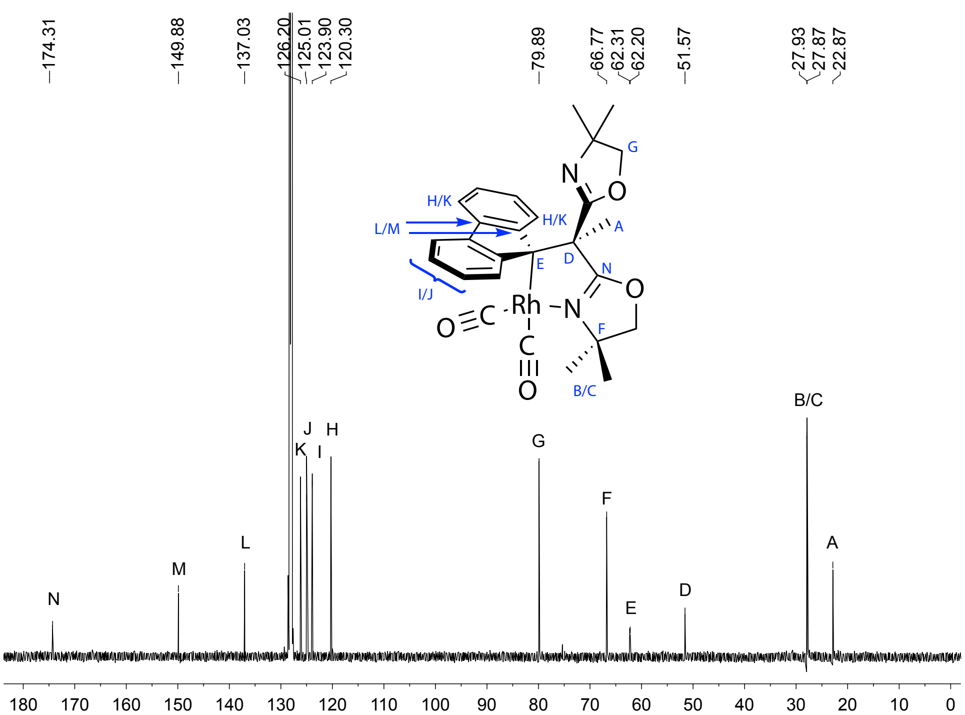

Figure S45. ^{13}C{^{1}H} NMR spectrum of {Bo^{M}Flu}Rh(CO)$_2$ acquired in benzene-d_6.

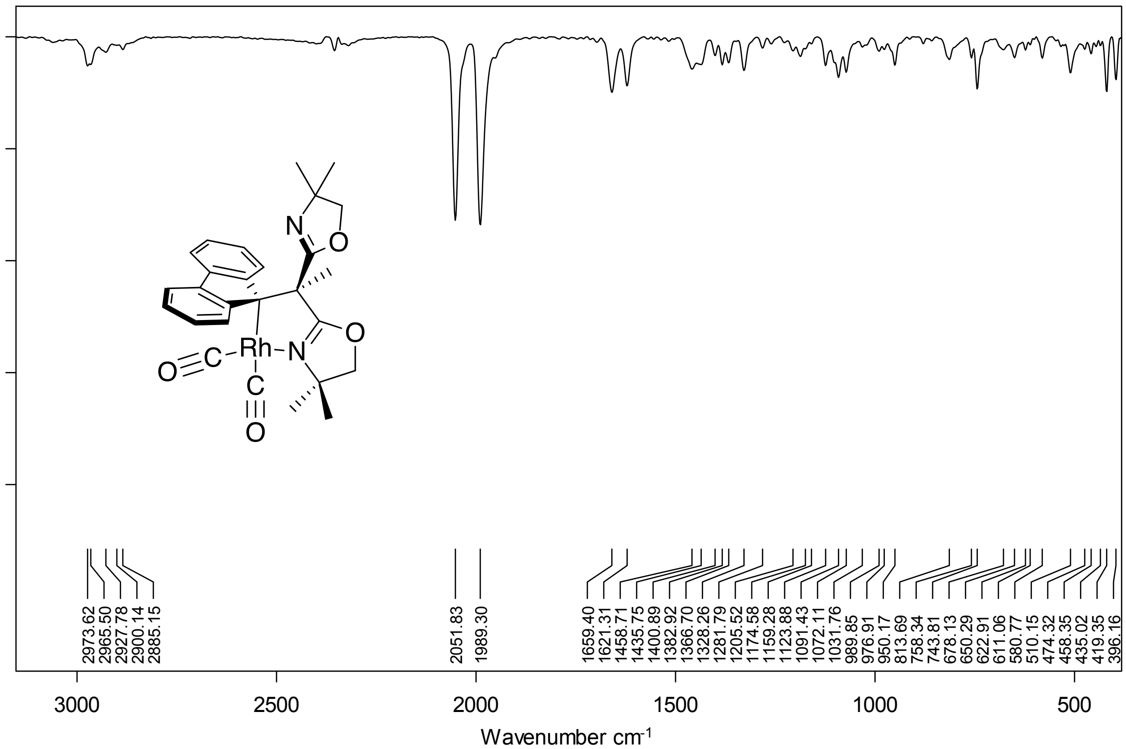

Figure S46. Infrared spectrum (KBr) of {Bo^{M}Flu}Rh(CO)$_2$.

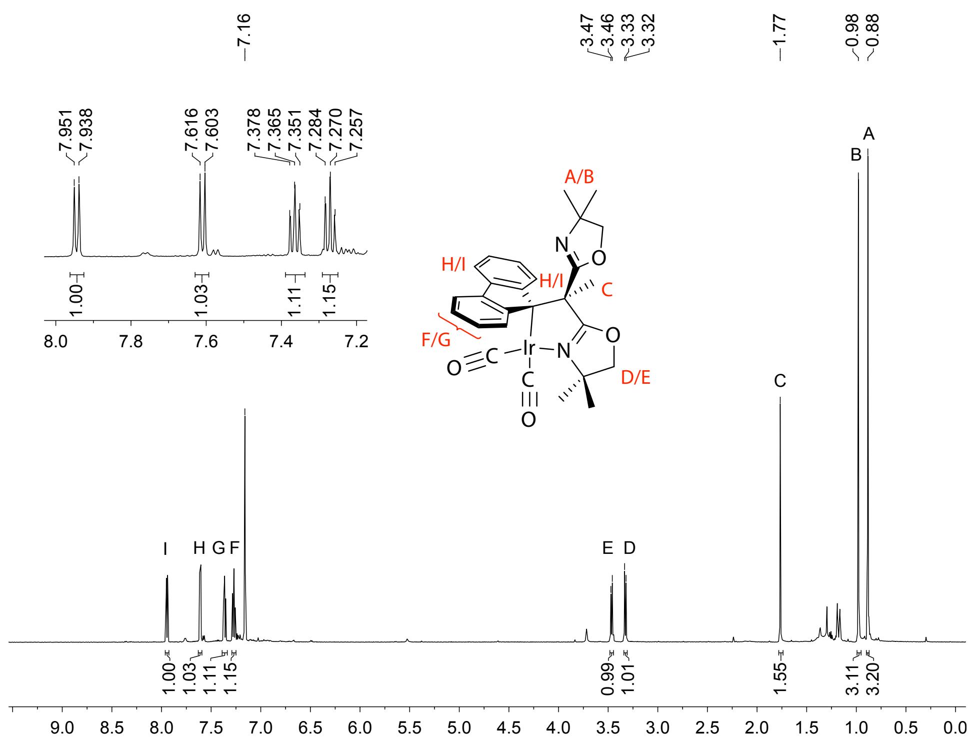

Figure S47. ^{1}H NMR spectrum of {Bo^{M}Flu}Ir(CO)$_2$ acquired in benzene-d_6.

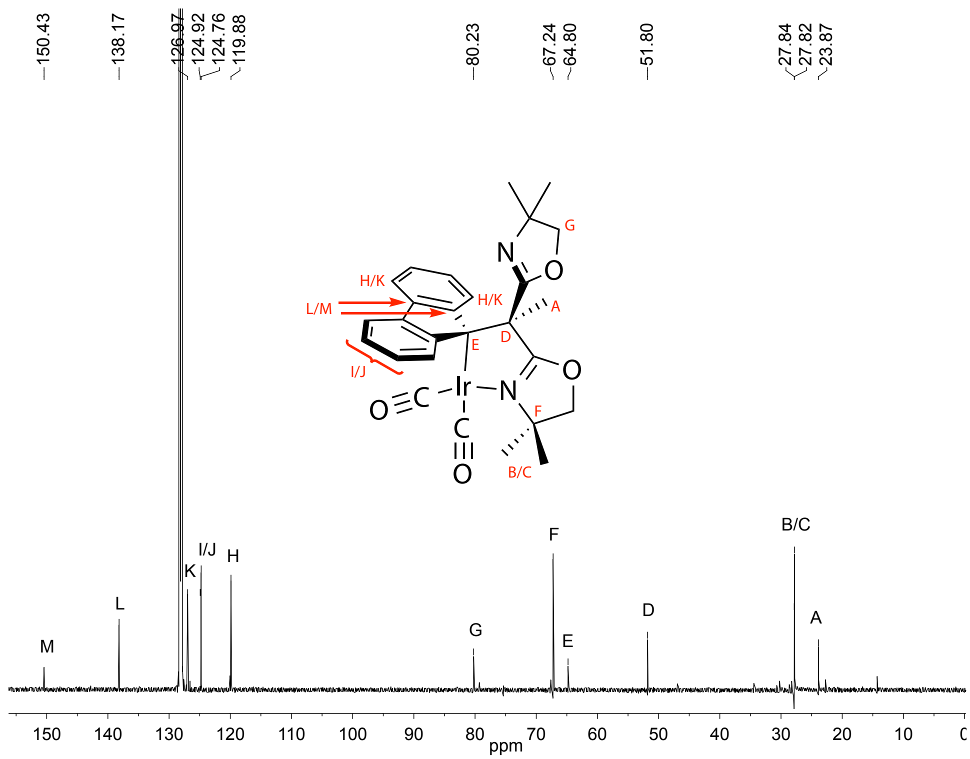

Figure S48. $^{13}C\{^{1}H\}$ NMR spectrum of $\{Bo^{M}Flu\}Ir(CO)_2$ acquired in benzene-d_6.

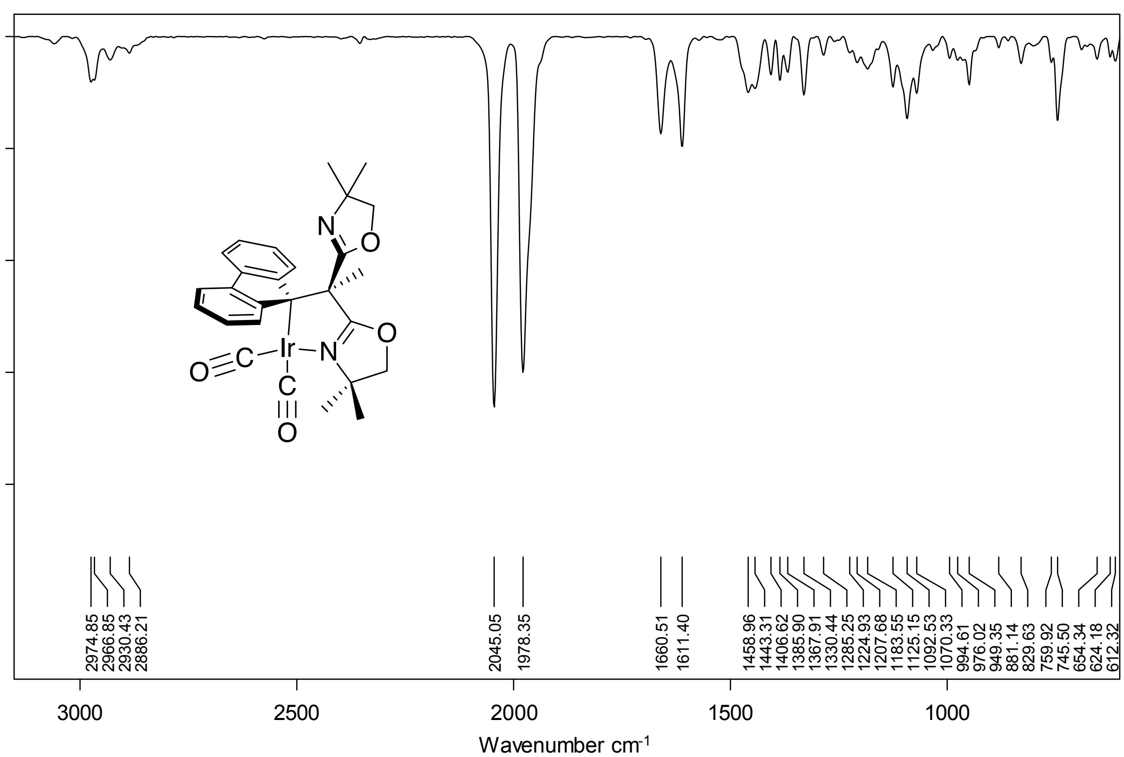

Figure S49. Infrared spectrum (KBr) of $\{Bo^{M}Flu\}Ir(CO)_2$.

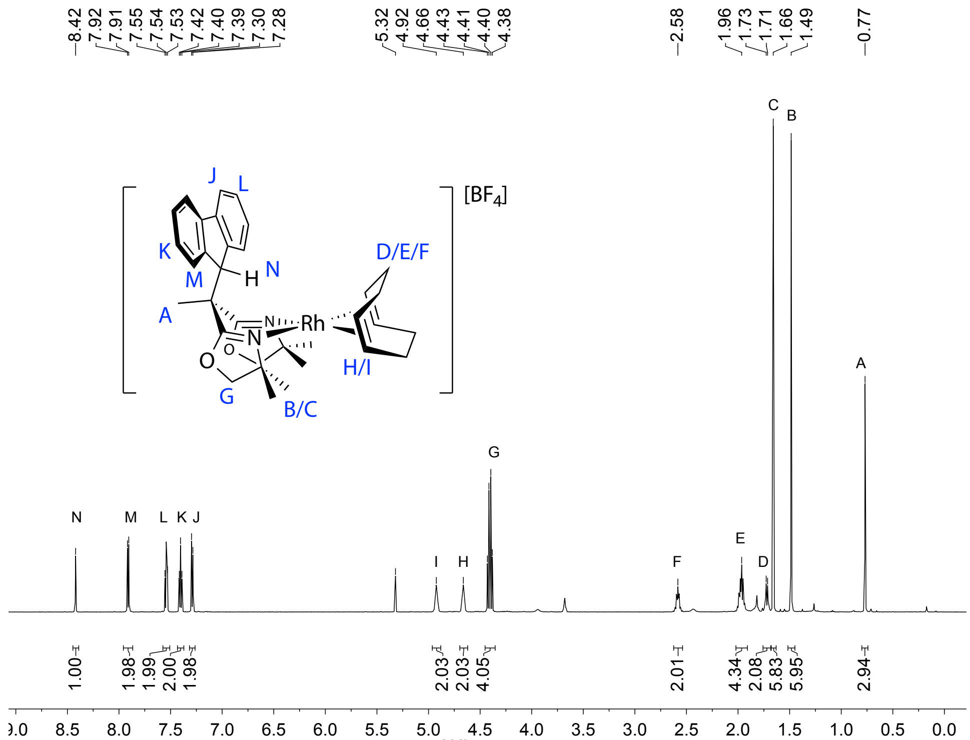

Figure S50. ^{1}H NMR spectrum of [{Bo^{M}Flu-H}Rh(η^{4}-C_8H_{12})][BF_4] acquired at room temperature in methylene chloride-d_2.

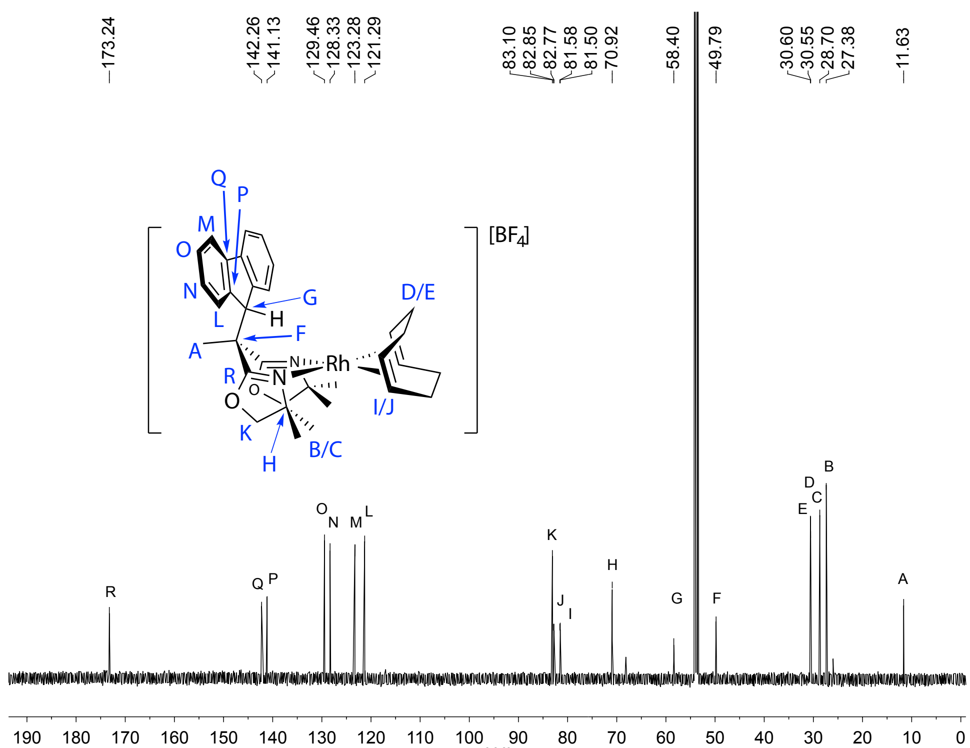

Figure S51. $^{13}C\{^{1}H\}$ NMR spectrum of [{Bo^{M}Flu-H}Rh(η^{4}-C_8H_{12})][BF_4] acquired at room temperature in methylene chloride-d_2.

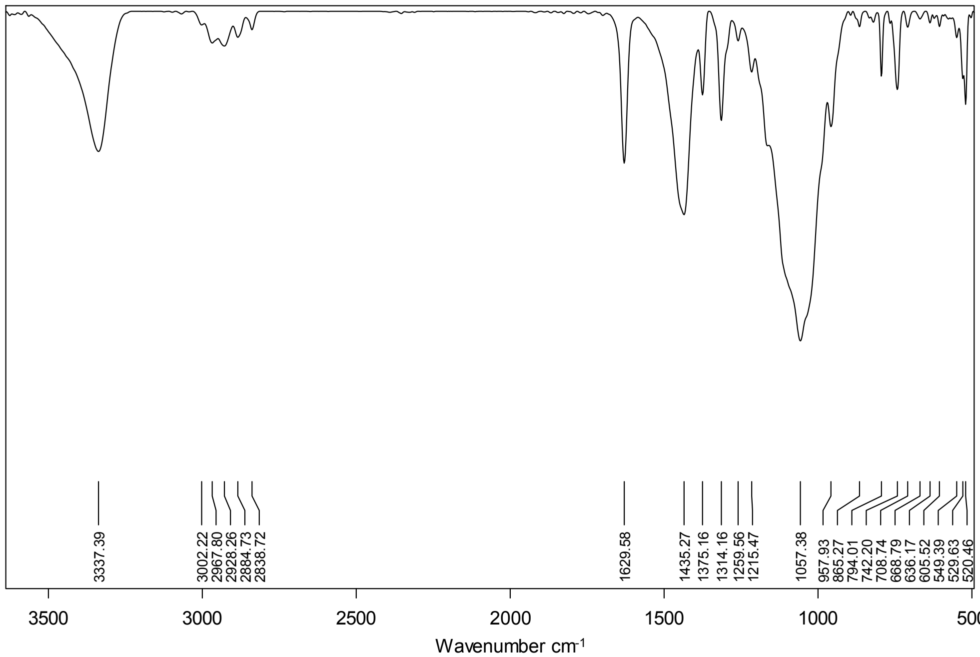

Figure S52. Infrared spectrum (KBr) of [{Bo^{M}Flu-H}Rh(η^4-C_8H_{12})][BF_4].

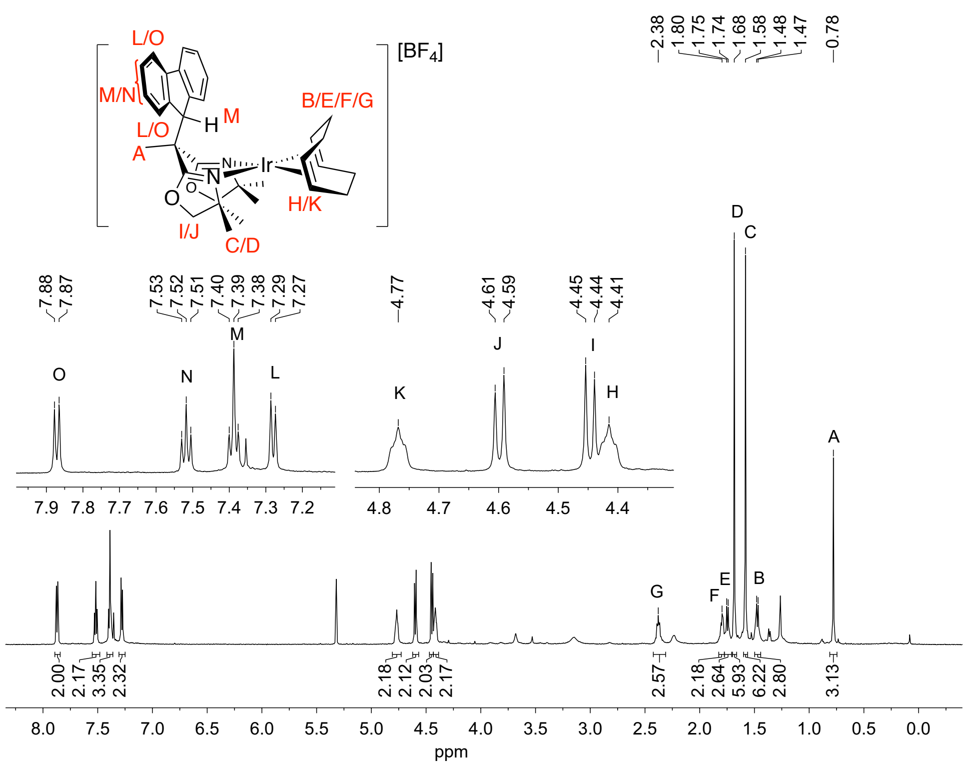

Figure S53. [1]H NMR spectrum of [{Bo^{M}Flu-H}Ir(η^4-C_8H_{12})][BF_4] acquired at room temperature in methylene chloride-d_2.

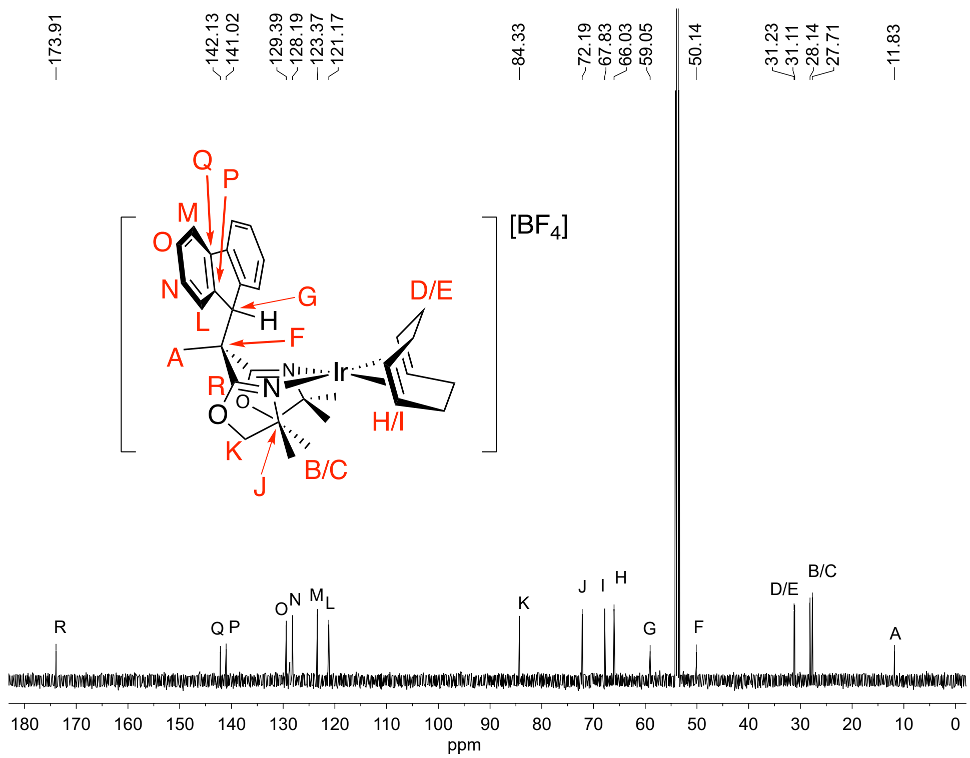

Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of [{Bo^{M}Flu-H}Ir(η^4-C_8H_{12})][BF_4] acquired at room temperature in methylene chloride-d_2.

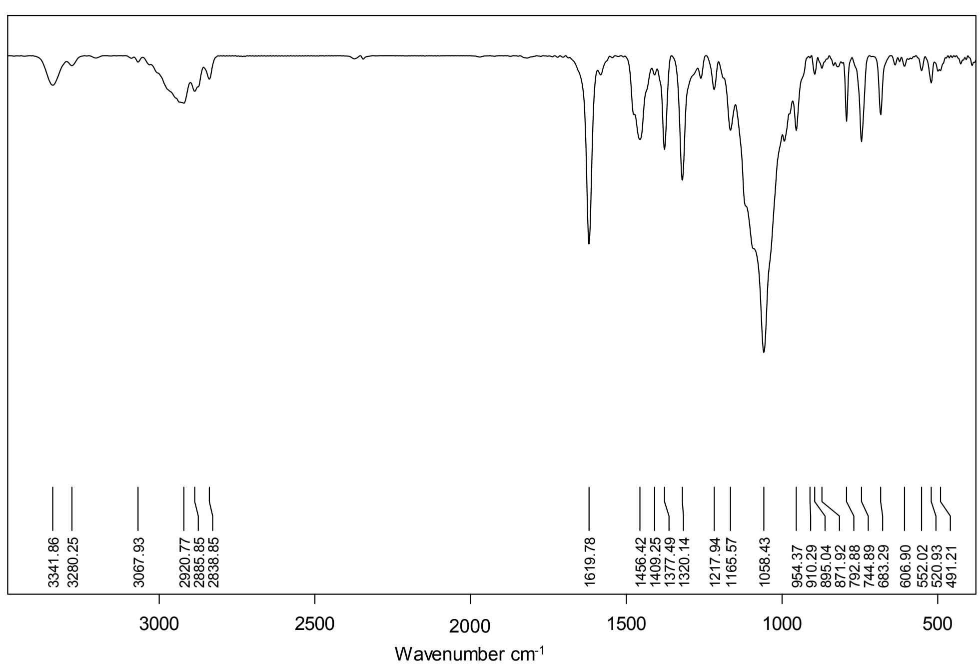

Figure S55. Infrared spectrum (KBr) of [{Bo^{M}Flu-H}Ir(η^4-C_8H_{12})][BF_4].

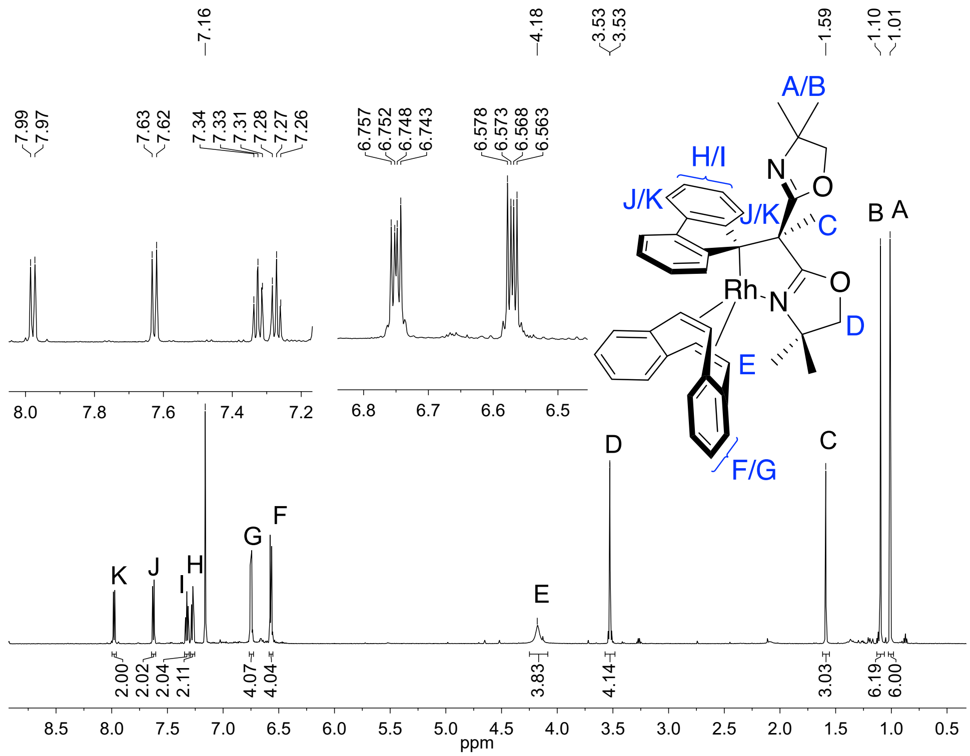

Figure S56. ^{1}H NMR spectrum of {Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$) acquired in benzene-d_6.

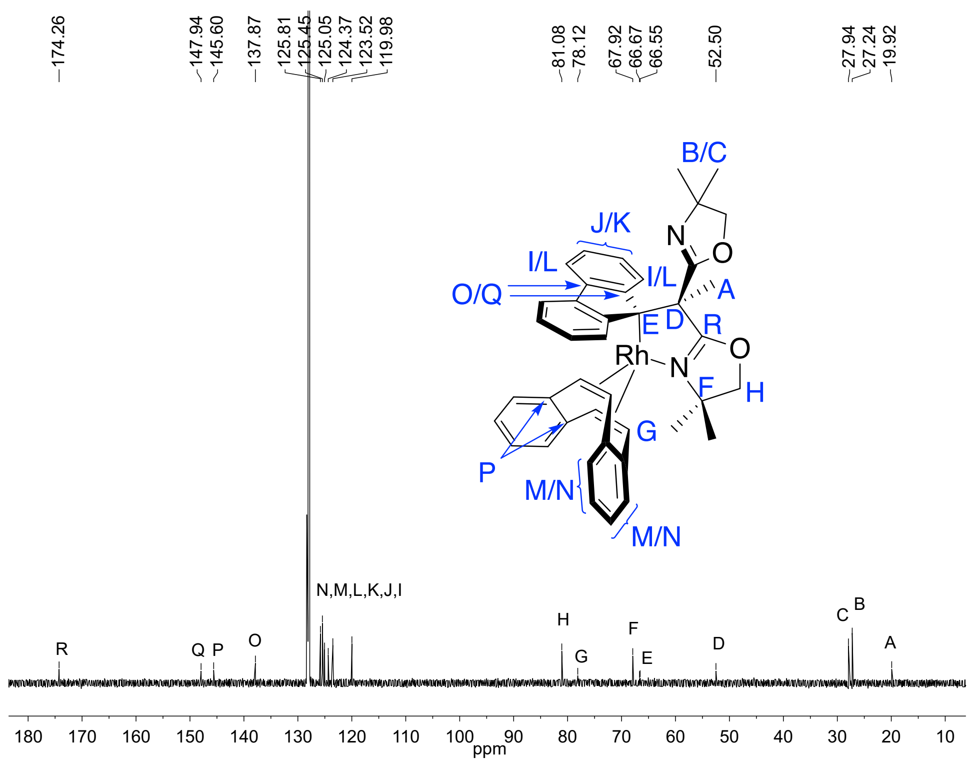

Figure S57. $^{13}C\{^{1}H\}$ NMR spectrum of {Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$) acquired in benzene-d_6.

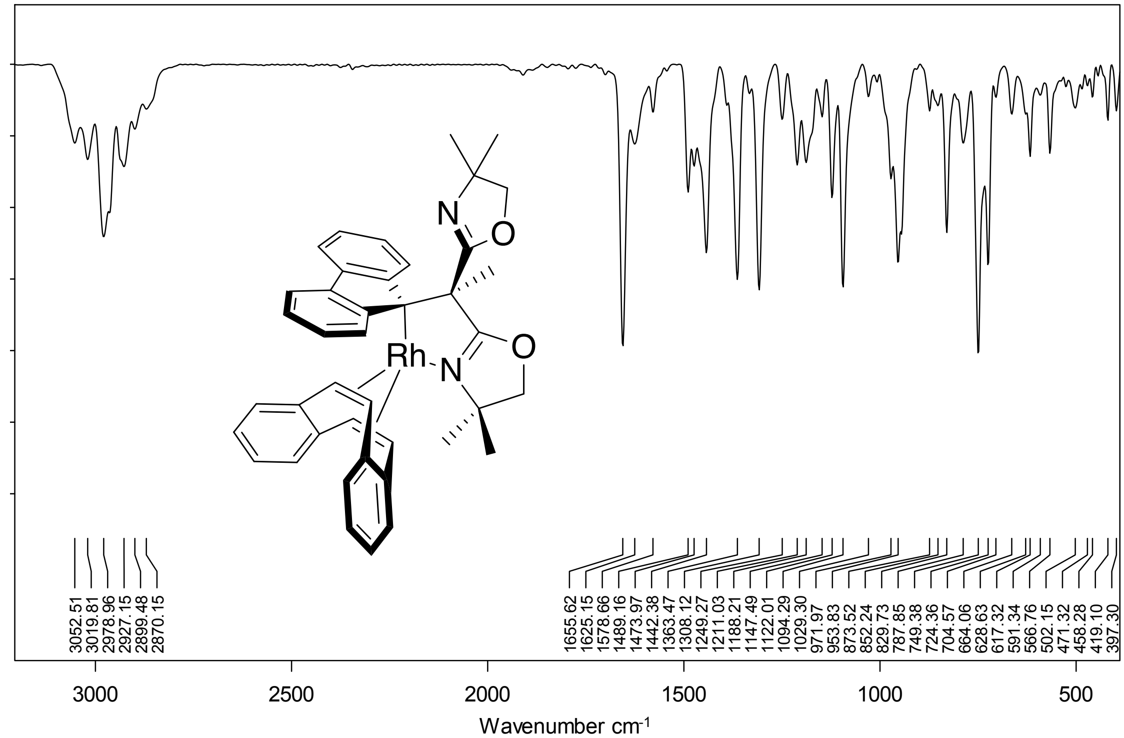

Figure S58. Infrared spectrum (KBr) of {Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$).

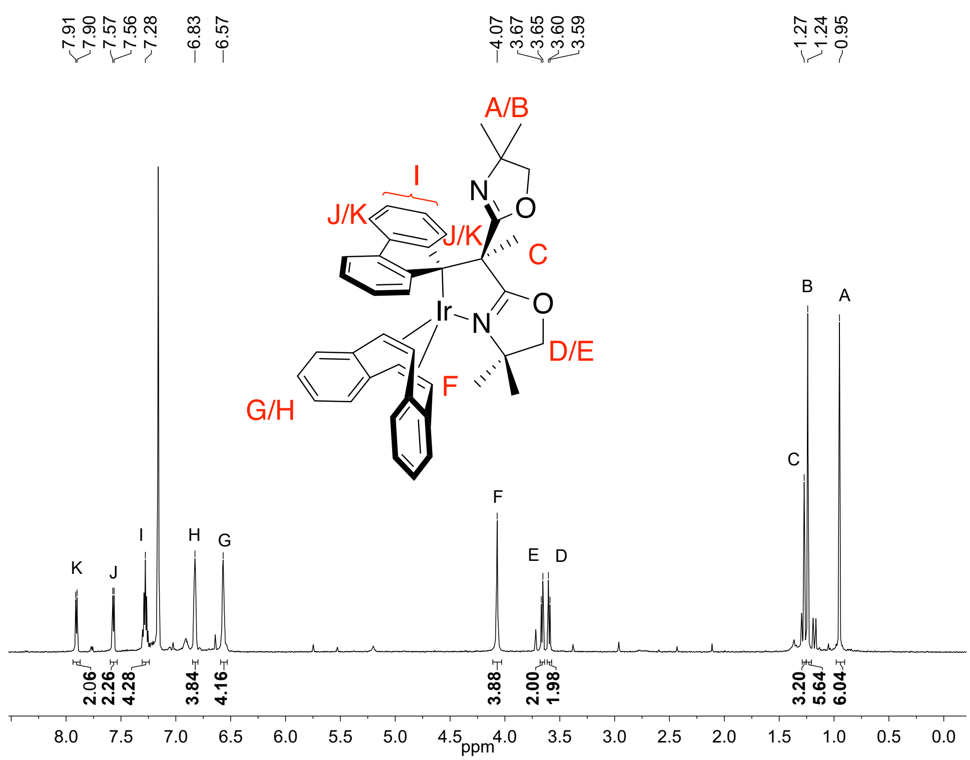

Figure S59. ^{1}H NMR spectrum of {Bo^{M}Flu}Ir(η^4-$C_{16}H_{12}$) acquired in benzene-d_6.

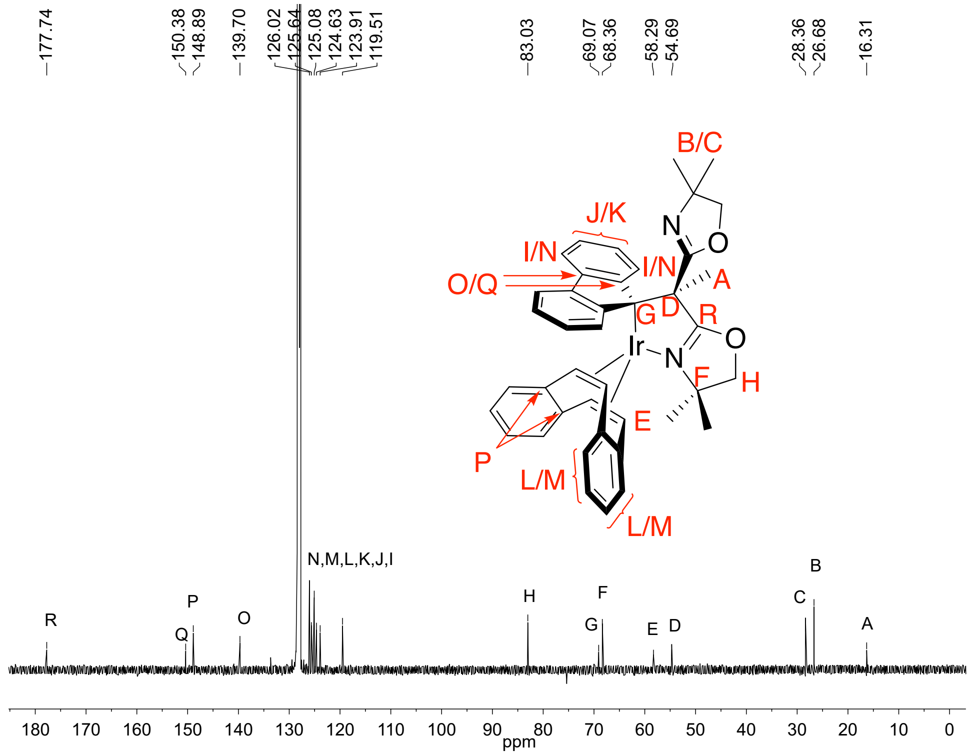

Figure S60. $^{13}C\{^{1}H\}$ NMR spectrum of $\{Bo^{M}Flu\}Ir(\eta^{4}\text{-}C_{16}H_{12})$ acquired in benzene-d_6.

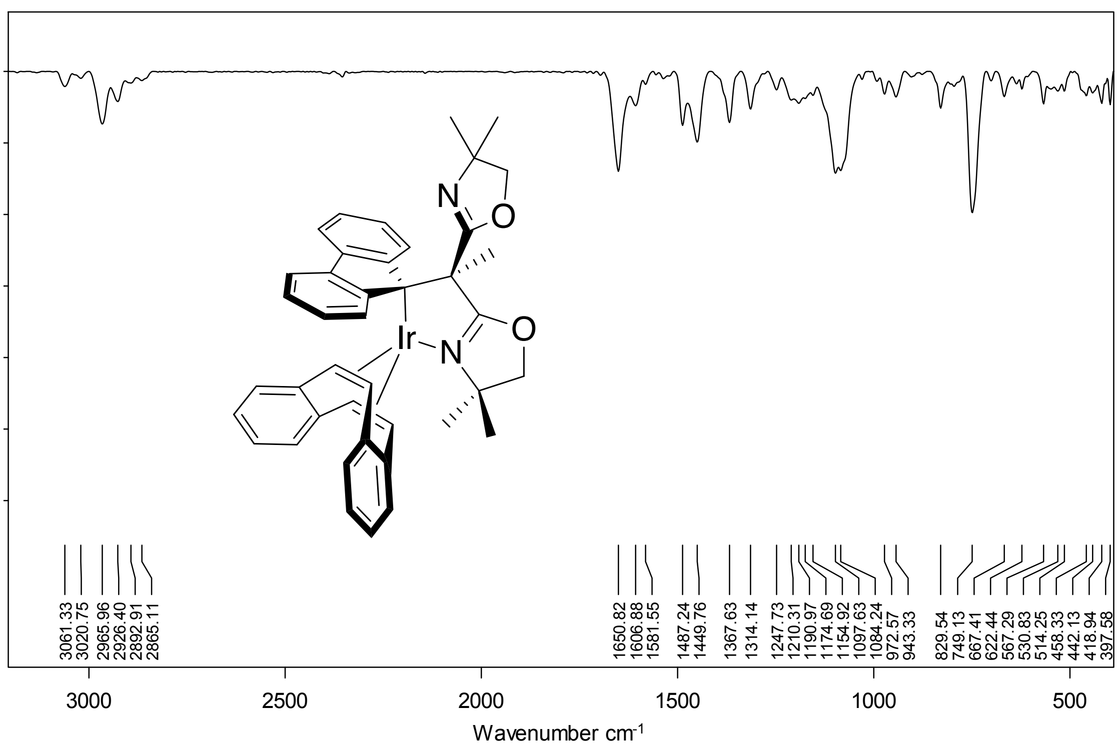

Figure S61. Infrared spectrum (KBr) of $\{Bo^{M}Flu\}Ir(\eta^{4}\text{-}C_{16}H_{12})$.

V. X-ray crystal structures.

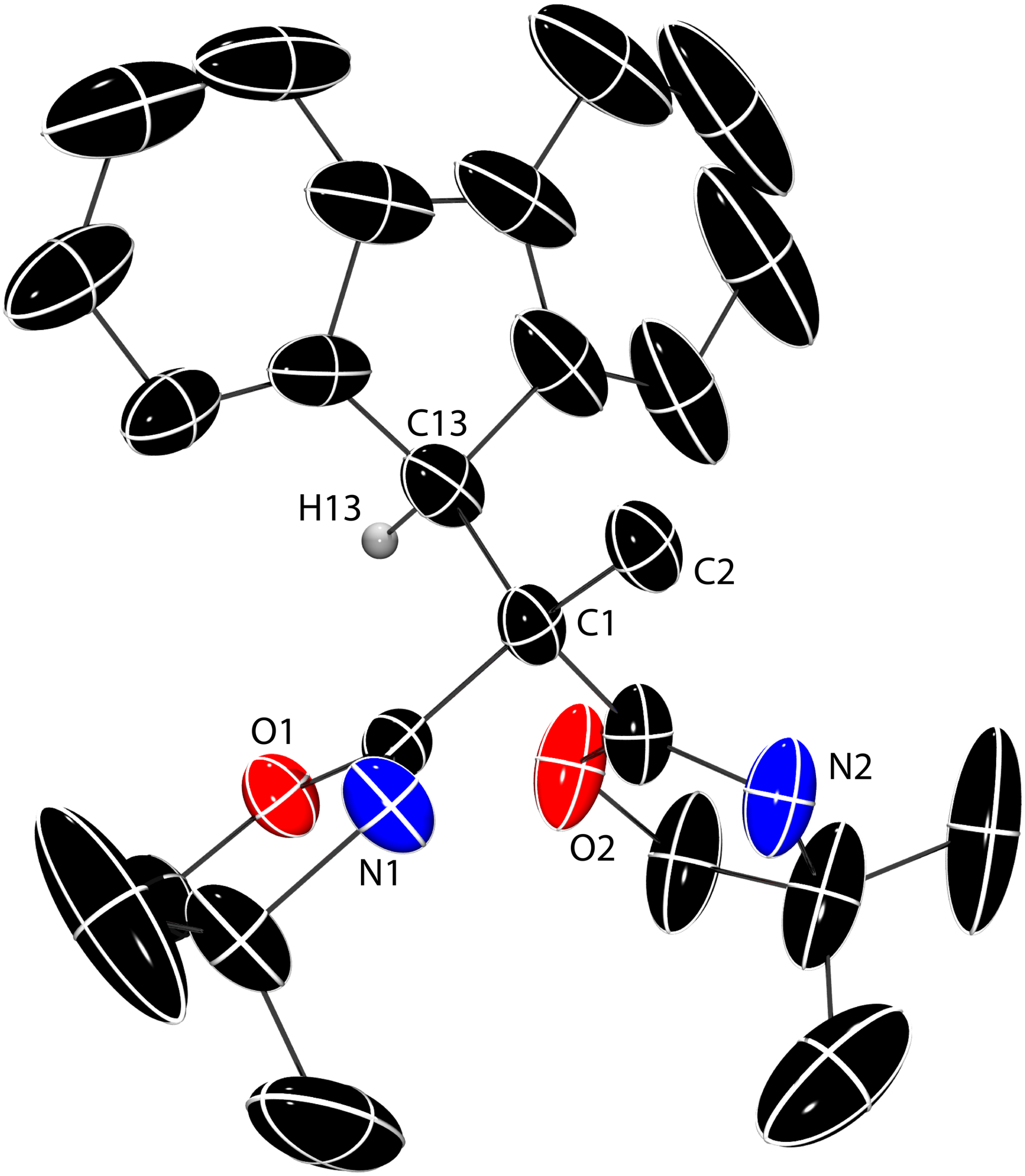

Figure S62. Rendered thermal ellipsoid diagram of 1-(fluorene)-1,1-bis(4,4-dimethyl-2-oxazolinyl)ethane (**Bo^{M}FluH**) plotted at 30% probability. Bo^{M}FluH crystallizes with two independent molecules in the unit cell with similar conformations, and only one is illustrated for clarity. In addition, H atoms, except for H13, have been omitted for clarity.

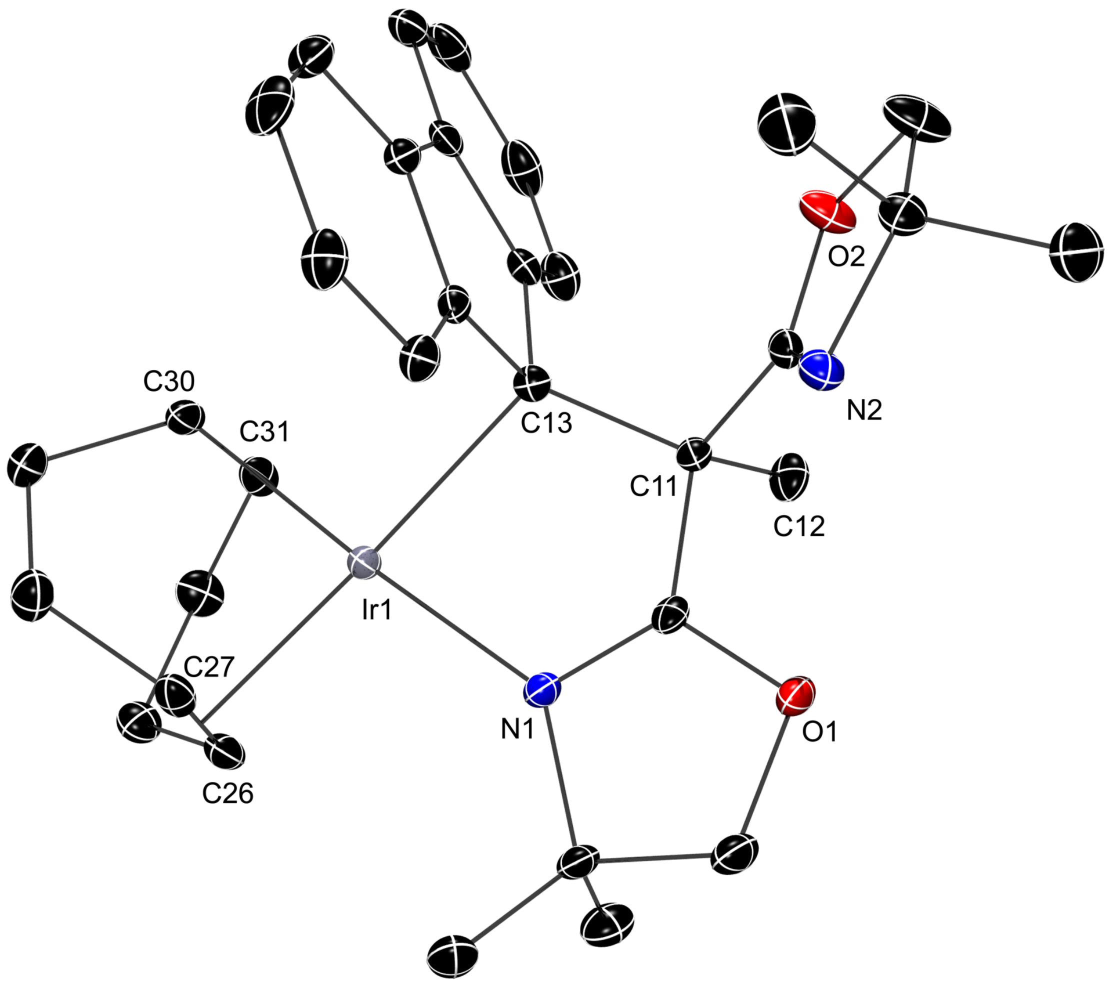

Figure S63. Rendered thermal ellipsoid diagram of {Bo^{M}Flu}Ir(η^4-C_8H_{12}) at 30% probability. H atoms have been omitted for clarity.

VI. DFT Calculations.

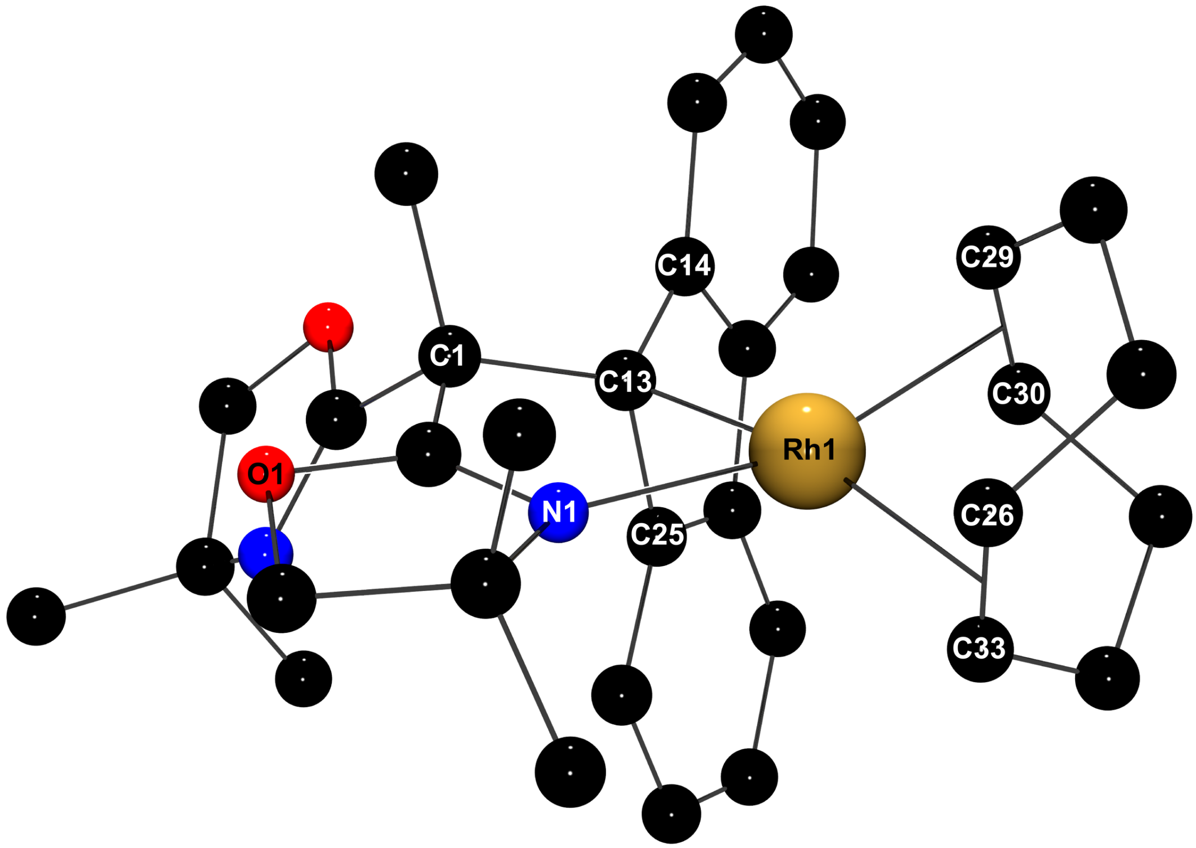

Figure S64. Geometry of {*C*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-C_8H_{12}) as determined by DFT calculations using the M06-L functional.

Table S1. Hessian calculations for {*C*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-C_8H_{12}). Calculations performed at DFT level of theory with M06-L functional.

MODE	FREQ (cm^{-1})	SYMMETRY	RED. MASS	IR INTENS.
1	2.079	A	5.455672	0.002139
2	0.667	A	7.797125	0.000049
3	0.497	A	7.746417	0.000059
4	0.141	A	7.559286	0.000187
5	3.996	A	5.238731	0.001188
6	7.595	A	4.932168	0.004031
7	24.296	A	4.481729	0.002427
8	29.985	A	4.152481	0.007066
9	38.003	A	3.36569	0.000357
10	47.829	A	4.018432	0.014942
11	54.471	A	4.599558	0.005977
12	61.603	A	3.955596	0.011379

13	66.484	A	4.877067	0.010536
14	75.657	A	5.141218	0.003195
15	97.582	A	4.387909	0.002583
16	103.993	A	3.490136	0.009037
17	109.222	A	3.760594	0.005854
18	116.641	A	4.800585	0.031346
19	124.606	A	3.920759	0.003134
20	140.868	A	3.579968	0.016096
21	146.499	A	3.533532	0.043794
22	160.404	A	4.131753	0.023751
23	166.687	A	3.90512	0.003718
24	173.862	A	2.861615	0.028194
25	177.028	A	3.805345	0.00198
26	183.57	A	4.184265	0.012712
27	193.437	A	2.638252	0.013816
28	220.872	A	4.324085	0.069318
29	227.095	A	1.796353	0.049634
30	230.648	A	1.336755	0.014076
31	231.881	A	1.245302	0.015623
32	243.619	A	2.529787	0.026433
33	251.897	A	3.424716	0.017707
34	253.371	A	1.483639	0.017397
35	266.015	A	2.058894	0.030151
36	278.969	A	2.42979	0.006188
37	291.364	A	2.835353	0.016786
38	297.01	A	1.470793	0.005761
39	306.455	A	3.140822	0.041517
40	311.642	A	3.407153	0.001387
41	327.024	A	4.439048	0.004176
42	334.67	A	2.142866	0.005188
43	339.978	A	2.941043	0.006185
44	344.924	A	1.901889	0.002424
45	350.267	A	1.800412	0.097053
46	356.996	A	3.685953	0.018949
47	362.785	A	2.80827	0.008115
48	386.697	A	2.862724	0.058999
49	389.362	A	3.783239	0.042193
50	424.5	A	3.308516	0.13478
51	430.041	A	5.163259	0.01325

52	442.833	A	3.604072	0.039637
53	453.34	A	3.893951	0.079399
54	464.12	A	3.315026	0.015831
55	475.222	A	3.409767	0.011163
56	478.276	A	3.520201	0.069899
57	479.176	A	2.919144	0.124451
58	499.72	A	4.144173	0.076302
59	509.294	A	3.076112	0.011561
60	523.91	A	4.905268	0.085248
61	530.75	A	4.445303	0.245341
62	576.706	A	3.224589	0.045208
63	579.956	A	4.012719	0.008692
64	617.399	A	4.349966	0.184026
65	619.853	A	6.454286	0.06468
66	629.601	A	4.287034	0.015276
67	635.353	A	6.223018	0.229535
68	642.247	A	5.106406	0.123279
69	663.312	A	5.861081	0.096287
70	697.707	A	1.986095	0.007727
71	703.976	A	2.609251	0.00837
72	721.648	A	6.918155	0.027254
73	733.601	A	6.401822	0.066334
74	739.736	A	1.475091	1.280908
75	747.155	A	1.50744	0.078923
76	761.1	A	5.192155	0.00227
77	765.842	A	3.370383	0.433754
78	776.962	A	1.351483	0.110134
79	790.342	A	3.2129	0.075584
80	801.869	A	3.236015	0.060845
81	805.563	A	2.591544	0.157129
82	809.166	A	2.417244	0.611865
83	839.036	A	2.137225	0.05572
84	841.549	A	4.164564	0.096765
85	849.789	A	2.95079	0.061003
86	854.24	A	1.500904	0.104326
87	859.628	A	1.678986	0.01639
88	865.778	A	1.471196	0.006224
89	880.441	A	1.650891	0.293393
90	888.193	A	2.056102	0.054674

91	893.006	A	3.073291	0.061582
92	906.084	A	4.217598	0.157777
93	909.87	A	1.444727	0.057146
94	912.403	A	2.062087	0.119123
95	919.092	A	1.417865	0.034911
96	926.374	A	2.564366	0.271249
97	940.982	A	1.91858	0.041887
98	947.078	A	1.226851	0.008569
99	948.811	A	1.728793	0.071741
100	954.464	A	1.56523	0.21346
101	956.077	A	1.303093	0.005973
102	957.084	A	1.714442	0.019071
103	969.255	A	1.606433	0.030693
104	969.896	A	1.444879	0.024564
105	981.426	A	2.432732	0.648575
106	988.064	A	3.089439	0.555629
107	993.961	A	1.532486	0.149779
108	998.062	A	1.954668	0.44731
109	1003.713	A	2.010799	0.58142
110	1009.155	A	1.777582	0.060485
111	1016.106	A	1.841444	0.171303
112	1024.567	A	5.714168	0.117943
113	1025.727	A	4.471967	0.660955
114	1028.011	A	3.808647	0.950555
115	1032.624	A	1.957679	0.110724
116	1043.043	A	1.485209	0.177027
117	1046.379	A	1.553959	0.135892
118	1062.255	A	2.159173	0.08126
119	1066.302	A	1.870989	0.115432
120	1104.745	A	1.977248	0.147079
121	1112.539	A	1.575632	0.03712
122	1114.447	A	3.072705	3.006161
123	1125.928	A	2.196175	0.588279
124	1141.166	A	3.31128	0.627463
125	1144.767	A	1.927316	0.247526
126	1153.851	A	1.846093	1.007308
127	1178.573	A	1.06082	0.158032
128	1181.085	A	1.131477	0.010234
129	1184.736	A	1.167446	0.111778

130	1199.736	A	1.760623	0.412538
131	1201.306	A	1.56191	0.154518
132	1209.539	A	1.203586	0.13999
133	1219.363	A	2.013817	0.044917
134	1220.796	A	1.235554	0.197323
135	1224.428	A	2.051443	1.181718
136	1232.769	A	2.462608	0.224272
137	1237.691	A	2.277373	1.170519
138	1248.278	A	2.07524	0.021138
139	1252.046	A	1.311784	0.167279
140	1256.696	A	2.070114	0.231038
141	1267.443	A	1.396675	0.049871
142	1275.517	A	2.773118	0.593922
143	1282.832	A	1.386747	0.025031
144	1287.33	A	2.14902	0.136467
145	1291.556	A	2.07426	0.268115
146	1317.106	A	3.770011	0.974948
147	1325.89	A	1.818056	0.242408
148	1334.859	A	1.346346	0.015543
149	1344.819	A	2.116811	0.057918
150	1346.956	A	1.392757	0.07789
151	1357.416	A	2.258768	0.699942
152	1376.225	A	1.376079	0.1285
153	1379.647	A	1.525938	0.044667
154	1382.405	A	1.597653	0.235283
155	1397.237	A	5.273769	0.344377
156	1401.885	A	1.402465	0.178797
157	1402.679	A	1.484524	0.675227
158	1407.332	A	1.356851	0.240586
159	1408.332	A	1.377545	0.325392
160	1412.657	A	3.17561	0.501826
161	1415.238	A	1.887473	0.023122
162	1420.059	A	1.550442	0.77776
163	1425.48	A	1.285202	0.122547
164	1433.894	A	1.590224	0.306539
165	1480.118	A	2.513044	1.160512
166	1483.557	A	1.172544	0.119436
167	1486.789	A	1.058566	0.000702
168	1487.764	A	1.100004	0.033297

169	1488.461	A	2.103762	0.170604
170	1488.732	A	1.1214	0.084977
171	1493.111	A	1.049145	0.018687
172	1495.454	A	1.054212	0.103711
173	1502.111	A	1.119838	0.06328
174	1504.998	A	1.139529	0.295281
175	1506.203	A	1.092276	0.195599
176	1507.231	A	1.074378	0.070148
177	1508.858	A	1.091256	0.454807
178	1512.444	A	1.058531	0.103355
179	1513.494	A	1.692662	0.062225
180	1517.099	A	1.272057	0.238267
181	1518.848	A	1.157085	0.059168
182	1522.479	A	2.527727	0.402241
183	1522.725	A	1.137433	0.064343
184	1523.736	A	3.230916	0.02057
185	1537.853	A	1.108667	0.103888
186	1545.317	A	3.541734	0.065997
187	1620.004	A	5.467202	0.012061
188	1625.561	A	6.05083	0.004999
189	1653.905	A	6.486232	0.032898
190	1666.04	A	6.375584	0.105894
191	1688.591	A	11.123246	2.429073
192	1719.358	A	11.594407	4.237128
193	2997.257	A	1.065468	1.896644
194	3000.276	A	1.066223	1.636998
195	3031.799	A	1.045196	0.836827
196	3034.171	A	1.051154	0.736399
197	3037.198	A	1.062684	0.87012
198	3040.495	A	1.039979	1.968673
199	3041.976	A	1.037932	0.584703
200	3045.069	A	1.06234	0.585231
201	3046.765	A	1.039426	0.81387
202	3051.944	A	1.037704	0.49396
203	3053.631	A	1.06427	2.783023
204	3060.706	A	1.095853	0.12942
205	3069.475	A	1.095956	0.13166
206	3094.473	A	1.102693	0.913253
207	3108.135	A	1.097599	0.366521

208	3109.212	A	1.088853	0.324231
209	3113.448	A	1.106231	0.43074
210	3123.189	A	1.08726	0.13448
211	3126.404	A	1.102626	0.587702
212	3131.695	A	1.101773	0.919677
213	3131.998	A	1.103899	0.370814
214	3132.3	A	1.103616	0.327827
215	3136.456	A	1.101743	0.925453
216	3142.5	A	1.102717	0.447129
217	3143.878	A	1.102631	0.169511
218	3145.832	A	1.101884	0.690432
219	3149.116	A	1.093885	1.30569
220	3150.558	A	1.085116	0.113426
221	3150.959	A	1.085497	0.194503
222	3153.635	A	1.10182	0.181318
223	3160.793	A	1.088942	0.466288
224	3161.074	A	1.095039	0.119184
225	3162.38	A	1.088171	0.349224
226	3173.827	A	1.087899	0.057401
227	3181.416	A	1.094732	1.486528
228	3181.809	A	1.095374	1.198833
229	3186.712	A	1.100065	0.270162
230	3196.194	A	1.094031	0.680784
231	3200.623	A	1.091992	0.292375
ZPE (hartree/molecule)	0.653503			
Total Energy (hartree/molecule)	-1650.3630992755			

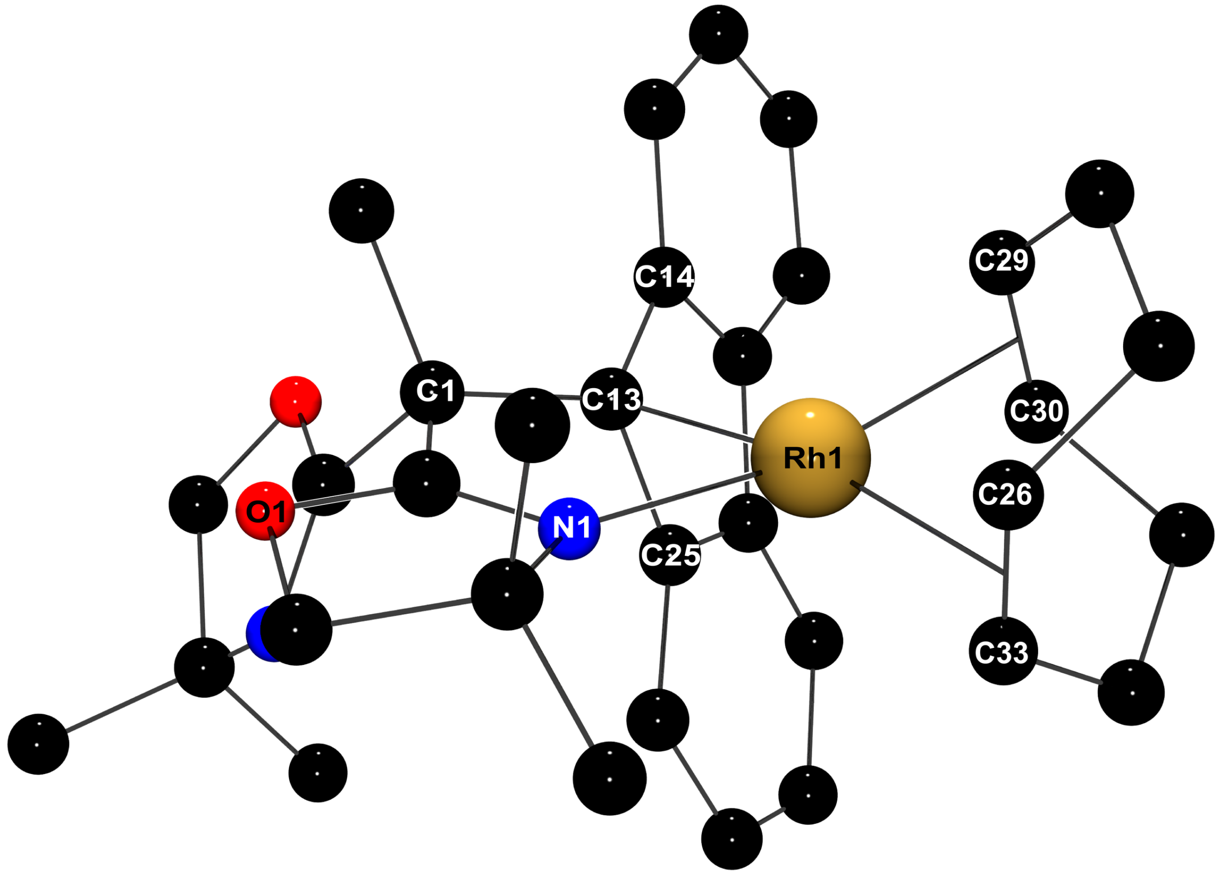

Figure S65. Geometry of [{C,N-κ^2-Bo^{M}Flu}Rh(η^4-C_8H_{12})]$^+$ as determined by DFT calculations using the M06-L functional.

Table S2. Hessian results for geometry optimized [{C,N-κ^2-Bo^{M}Flu}Rh(η^4-C_8H_{12})]$^+$. Calculations performed at DFT level of theory with M06-L functional.

MODE	FREQ (cm^{-1})	SYMMETRY	RED. MASS	IR INTENS.
1	8.133	A	4.818132	0.001863
2	4.08	A	5.461855	0.001233
3	3.193	A	5.188003	0.000614
4	0.528	A	7.773693	0.000024
5	0.372	A	7.754614	0.000002
6	0.173	A	7.765799	0.000001
7	21.066	A	4.188071	0.000939
8	25.719	A	4.299868	0.001354
9	36.725	A	3.314156	0.003115
10	41.385	A	4.346235	0.004389
11	57.423	A	5.002432	0.001539
12	62.57	A	3.984445	0.01594
13	68.898	A	4.356825	0.01075

14	74.8	A	4.782061	0.004347
15	97.487	A	4.286091	0.0043
16	101.827	A	4.030379	0.016252
17	108.752	A	3.406557	0.002659
18	122.706	A	4.354425	0.005187
19	133.029	A	3.502932	0.009264
20	144.587	A	3.003645	0.029955
21	149.928	A	3.282022	0.012028
22	152.103	A	3.639557	0.011657
23	159.404	A	3.248537	0.009958
24	176.004	A	3.569661	0.031489
25	176.736	A	3.766378	0.004483
26	180.977	A	3.799606	0.02077
27	185.524	A	3.920909	0.010139
28	214.924	A	5.354807	0.085352
29	222.995	A	4.306343	0.068294
30	229.951	A	1.125592	0.006333
31	233.982	A	1.144259	0.02335
32	243.991	A	4.388673	0.015851
33	246.397	A	3.288829	0.117322
34	250.267	A	4.373452	0.137132
35	263.411	A	1.860098	0.043649
36	278.187	A	1.259418	0.034526
37	285.832	A	2.357731	0.01421
38	291.895	A	1.677155	0.002022
39	297.806	A	2.722128	0.045639
40	304.758	A	3.887452	0.006142
41	312.811	A	3.271502	0.064686
42	316.655	A	3.97422	0.071559
43	332.259	A	2.277498	0.006895
44	339.579	A	2.952936	0.017786
45	347.051	A	2.812074	0.011786
46	356.493	A	2.916463	0.009959
47	366.831	A	2.845729	0.022638
48	369.637	A	1.340405	0.060265
49	390.977	A	2.642166	0.087242
50	398.942	A	4.503977	0.070827
51	419.806	A	3.501192	0.130497
52	428.842	A	4.656114	0.011213

53	438.135	A	3.470685	0.103246
54	451.352	A	2.938574	0.1126
55	459.273	A	3.235101	0.019813
56	467.23	A	3.135849	0.067052
57	474.083	A	3.391024	0.010301
58	495.515	A	3.967403	0.092996
59	500.425	A	2.879864	0.007142
60	521.768	A	4.873958	0.043963
61	528.975	A	4.464192	0.241921
62	556.529	A	3.10406	0.066395
63	568.205	A	3.458628	0.010395
64	606.697	A	4.440233	0.234265
65	618.033	A	7.02392	0.074976
66	628.007	A	4.618851	0.202906
67	630.3	A	5.684319	0.029275
68	631.366	A	4.714181	0.260004
69	661.406	A	5.759157	0.16775
70	691.789	A	1.667725	0.003614
71	701.453	A	3.108132	0.00339
72	718.265	A	6.505046	0.047539
73	729.422	A	6.077737	0.257551
74	738.486	A	1.553146	1.011317
75	750.781	A	1.689536	0.11413
76	761.116	A	4.417441	0.028354
77	768.778	A	3.031428	0.410462
78	774.025	A	1.360646	0.100714
79	786.957	A	2.714225	0.086543
80	797.196	A	2.022851	0.223808
81	799.918	A	3.026165	0.037197
82	804.397	A	4.174373	0.020305
83	840.248	A	4.194375	0.129555
84	847.025	A	2.089233	0.080238
85	853.339	A	3.111733	0.170345
86	864.16	A	1.790087	0.012847
87	866.503	A	1.413086	0.403265
88	869.251	A	1.598255	0.146702
89	885.535	A	1.475033	0.021206
90	890.185	A	2.054187	0.10639
91	892.734	A	2.943587	0.102378

92	908.744	A	4.278316	0.141945
93	915.329	A	2.261986	0.141314
94	923.58	A	2.699094	0.143769
95	928.285	A	1.384237	0.013101
96	941.454	A	1.880129	0.167957
97	944.762	A	1.418613	0.004159
98	949.577	A	1.74074	0.116545
99	958.387	A	2.393388	0.243546
100	968.442	A	1.36947	0.072561
101	970.096	A	1.531095	0.156757
102	977.148	A	1.338758	0.042908
103	977.922	A	1.317013	0.029709
104	983.617	A	1.388917	0.048248
105	985.298	A	2.725907	0.971032
106	988.888	A	2.6567	0.769703
107	996.252	A	1.677297	0.197949
108	1001.267	A	2.36718	0.372002
109	1005.806	A	1.986808	0.15438
110	1014.09	A	3.391131	0.721709
111	1015.347	A	1.92385	0.104469
112	1017.711	A	1.527209	0.050074
113	1020.789	A	2.875696	0.627077
114	1024.719	A	7.073093	0.018236
115	1038.308	A	1.939652	0.118521
116	1041.993	A	1.463338	0.073301
117	1046.106	A	1.567319	0.080543
118	1063.157	A	2.123142	0.038349
119	1071.873	A	1.902663	0.014275
120	1101.662	A	1.994247	0.187182
121	1118.497	A	1.568107	0.061975
122	1125.662	A	2.616939	0.580127
123	1128.351	A	2.64878	1.626692
124	1139.394	A	1.929747	0.181223
125	1151.412	A	3.20142	0.353065
126	1164.2	A	2.126193	1.320543
127	1186.113	A	1.067622	0.362532
128	1186.497	A	1.145812	0.132639
129	1192.974	A	1.53814	0.21566
130	1195.45	A	1.367951	0.377329

131	1200.781	A	1.667186	0.404397
132	1214.991	A	1.217949	0.149632
133	1218.9	A	1.872229	0.227432
134	1222.707	A	1.748686	0.75718
135	1226.604	A	1.233149	0.195014
136	1241.549	A	2.250656	1.190643
137	1243.2	A	2.425883	0.032224
138	1252.138	A	2.006041	0.055115
139	1258.347	A	2.047594	0.300614
140	1264.086	A	1.239804	0.13591
141	1274.503	A	1.323235	0.093848
142	1288.98	A	1.349992	0.249853
143	1290.76	A	2.468105	0.166039
144	1294.392	A	3.511646	0.00603
145	1296.484	A	2.025402	0.151974
146	1325.633	A	3.021892	1.215142
147	1330.545	A	2.002764	0.316681
148	1340.374	A	1.384975	0.031685
149	1341.986	A	1.920211	0.028321
150	1353.638	A	1.389718	0.14292
151	1363.25	A	2.047137	0.670807
152	1384.153	A	1.392596	0.0969
153	1388.764	A	1.533403	0.053784
154	1389.455	A	1.640484	0.374468
155	1397.63	A	6.782467	0.14339
156	1409.593	A	1.316755	0.794755
157	1413.196	A	1.368318	0.310107
158	1414.617	A	1.35032	0.165194
159	1420.029	A	1.350105	0.31821
160	1426.299	A	3.518798	0.165355
161	1428.64	A	1.676792	0.067496
162	1430.447	A	1.398815	0.714617
163	1431.5	A	1.281364	0.155763
164	1452.495	A	2.153608	0.789238
165	1467.256	A	2.515398	0.371474
166	1477.875	A	1.132973	0.436942
167	1482.099	A	1.089058	0.08694
168	1486.547	A	2.376897	1.054924
169	1489.414	A	1.056724	0.024246

170	1491.74	A	1.056534	0.068055
171	1493.368	A	1.055314	0.045495
172	1495.102	A	1.048394	0.099411
173	1501.686	A	1.11043	0.113874
174	1506.377	A	1.312323	0.131544
175	1508.364	A	1.2933	0.73011
176	1509.297	A	1.070331	0.185754
177	1512.121	A	1.376382	0.135447
178	1512.846	A	1.064245	0.201513
179	1514.518	A	1.160429	0.242586
180	1518.349	A	1.232067	0.333233
181	1521.237	A	1.168523	0.137355
182	1522.437	A	1.215046	0.038268
183	1524.562	A	1.728903	0.500954
184	1538.133	A	1.098137	0.256466
185	1552.85	A	3.635403	0.026758
186	1562.73	A	3.964865	0.02056
187	1610.179	A	4.90949	0.185342
188	1636.511	A	5.726749	0.13825
189	1649.789	A	6.456387	0.394102
190	1659.88	A	6.263375	0.703685
191	1673.777	A	10.70535	3.688229
192	1732.917	A	11.600124	3.14315
193	3022.845	A	1.063725	0.502367
194	3026.108	A	1.064148	0.576808
195	3035.991	A	1.036946	0.42024
196	3048.441	A	1.038319	0.436368
197	3050.003	A	1.037729	0.411586
198	3053.181	A	1.041421	0.203848
199	3054.924	A	1.060574	1.280596
200	3057.732	A	1.061343	0.6516
201	3059.201	A	1.038948	0.306024
202	3067.029	A	1.065176	0.366579
203	3074.426	A	1.08129	0.345257
204	3077.377	A	1.079737	0.994083
205	3081.659	A	1.098858	0.057418
206	3117.953	A	1.104223	0.395712
207	3128.196	A	1.102547	0.790399
208	3131.345	A	1.099378	0.132748

209	3132.512	A	1.108093	0.341473
210	3139.877	A	1.087988	0.103915
211	3142.026	A	1.102787	0.208198
212	3142.355	A	1.102485	0.330647
213	3143.548	A	1.101119	0.423149
214	3147.243	A	1.102187	0.39044
215	3147.612	A	1.087828	0.077777
216	3153.045	A	1.102568	0.397821
217	3154.731	A	1.102541	0.212868
218	3154.983	A	1.103828	0.143944
219	3157.956	A	1.101165	0.796637
220	3159.62	A	1.101897	0.189698
221	3173.192	A	1.088102	0.108525
222	3175.053	A	1.087326	0.078504
223	3178.703	A	1.08808	0.063119
224	3186.077	A	1.089024	0.066053
225	3186.973	A	1.090097	0.138688
226	3192.577	A	1.101532	0.095128
227	3201.009	A	1.095716	0.332152
228	3203.435	A	1.095105	0.475305
229	3213.599	A	1.087259	0.031225
230	3215.64	A	1.0939	0.314885
231	3221.972	A	1.092464	0.096454
ZPE (hartree/molecule)	0.655321			
Total Energy (hartree/molecule)	-1650.1260726161			
MP2 Total Energy (hartree/molecule)	-1644.5240528844			

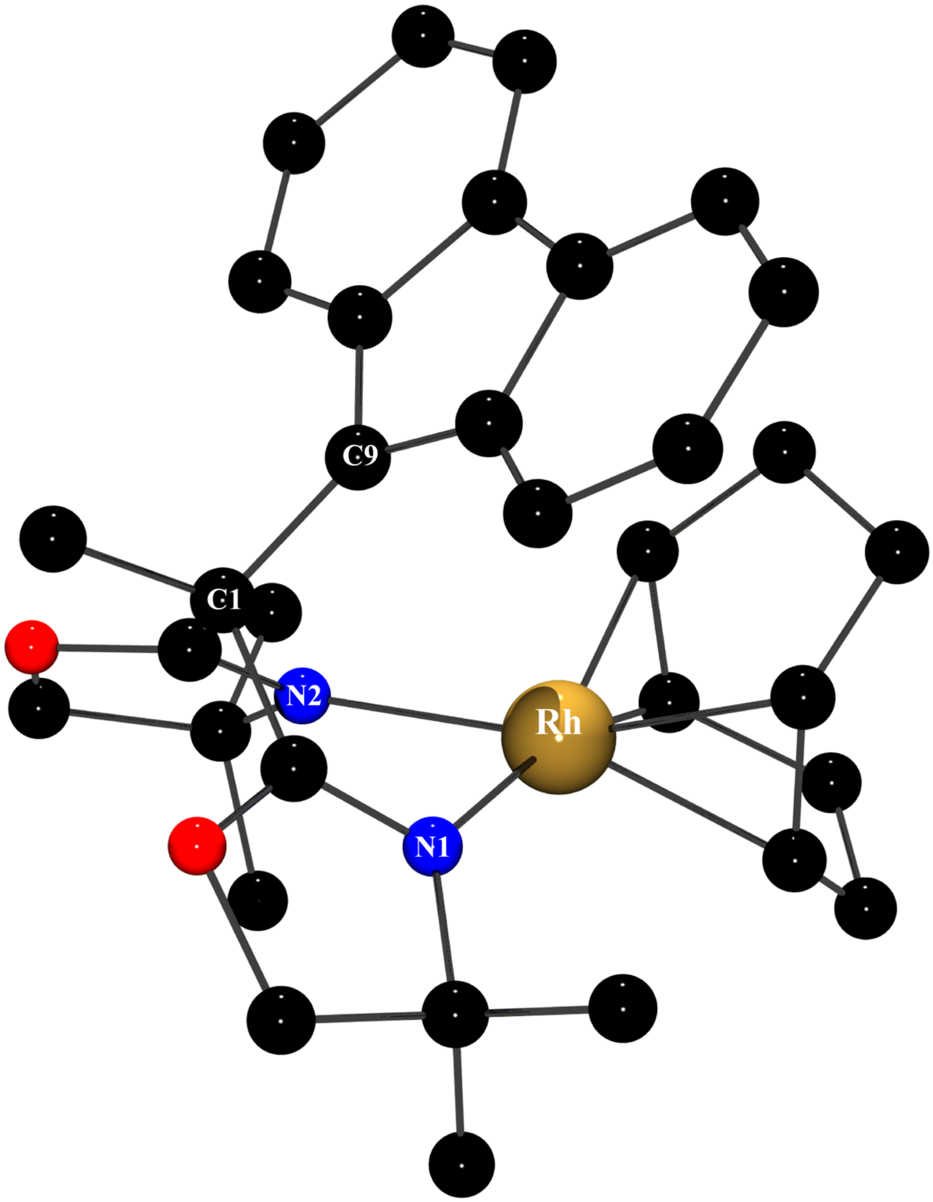

Figure S66. DFT calculation of the geometry for [{*N*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-C_8H_{12})]$^+$.

Table S3. Hessian results for geometry optimized structure [{*N*,*N*-κ^2-Bo^{M}Flu }Rh(η^4-C_8H_{12})]$^+$. Calculations performed at DFT level of theory with M06-L functional.

MODE	FREQ (cm^{-1})	SYMMETRY	RED. MASS	IR INTENS.
1	10.115	A	4.923897	0.000573
2	8.826	A	5.363993	0.002557
3	4.719	A	5.331302	0.003076
4	0.756	A	7.767782	0.000012

5	0.566	A	7.766626	0.000001
6	0.269	A	7.765180	0.000003
7	28.420	A	4.476418	0.000966
8	39.181	A	3.533645	0.004903
9	46.036	A	5.382967	0.001275
10	56.823	A	4.032562	0.001544
11	57.400	A	3.959147	0.017027
12	70.994	A	3.167258	0.005305
13	71.266	A	3.583417	0.003154
14	83.021	A	3.564171	0.001723
15	98.540	A	5.065810	0.001768
16	105.398	A	3.852008	0.008877
17	117.285	A	4.177871	0.015232
18	122.671	A	5.604563	0.005146
19	138.322	A	4.865650	0.026952
20	144.935	A	4.851631	0.004323
21	151.697	A	4.446160	0.035338
22	162.287	A	4.148572	0.002931
23	166.493	A	3.905553	0.003563
24	168.701	A	2.522572	0.000955
25	175.022	A	3.074484	0.033557
26	184.426	A	2.823011	0.006508
27	191.873	A	2.300866	0.009837
28	203.687	A	2.349502	0.041039
29	211.702	A	2.200501	0.007212
30	224.809	A	1.740995	0.002551
31	233.044	A	1.416440	0.007691
32	247.275	A	1.298886	0.005147
33	253.849	A	2.477004	0.035751
34	254.985	A	3.031874	0.032957
35	262.260	A	2.367566	0.001117
36	267.866	A	1.329304	0.007417
37	277.728	A	1.102680	0.000762
38	284.209	A	3.251268	0.027055
39	287.112	A	4.095703	0.005464
40	294.544	A	3.281245	0.020498
41	308.342	A	3.945491	0.016248
42	332.599	A	5.373706	0.098354
43	337.619	A	2.878124	0.040725

44	345.357	A	2.675274	0.022928
45	357.587	A	3.944259	0.019086
46	360.834	A	2.382326	0.035510
47	369.198	A	2.662122	0.016063
48	385.363	A	4.265201	0.026542
49	393.616	A	3.063974	0.034028
50	420.838	A	3.360052	0.035024
51	439.930	A	4.389416	0.014446
52	445.468	A	4.445952	0.064267
53	446.272	A	3.384625	0.022966
54	460.344	A	4.463647	0.111563
55	464.771	A	3.556807	0.042042
56	473.266	A	2.855806	0.027068
57	483.492	A	2.700299	0.105227
58	497.090	A	4.269125	0.079326
59	515.865	A	3.084564	0.037774
60	521.208	A	5.357592	0.001050
61	549.360	A	3.851910	0.270496
62	570.606	A	3.576516	0.000327
63	578.114	A	3.061742	0.016663
64	601.067	A	6.169978	0.000687
65	615.443	A	4.762384	0.198191
66	624.364	A	4.986103	0.151816
67	626.827	A	5.430360	0.026049
68	630.999	A	5.488402	0.026387
69	651.331	A	1.72322	0.0229349
70	664.448	A	7.475391	0.057806
71	699.647	A	2.838329	0.009343
72	708.259	A	1.906361	0.006574
73	715.317	A	6.183767	0.003764
74	733.960	A	1.916805	1.191300
75	749.559	A	1.477615	0.007626
76	768.559	A	2.956900	0.617049
77	771.627	A	3.418861	0.523046
78	781.155	A	2.969067	0.000765
79	784.206	A	2.186665	0.094745
80	785.449	A	2.106740	0.037150
81	805.932	A	1.545326	0.049151
82	833.095	A	5.204903	0.328163

83	841.402	A	1.888348	0.065490
84	856.666	A	3.313305	0.081727
85	857.385	A	1.944357	0.109283
86	859.596	A	3.853463	0.137521
87	866.558	A	1.328325	0.007589
88	874.180	A	1.432542	0.003383
89	893.528	A	2.639204	0.066670
90	896.581	A	1.989617	0.407255
91	899.114	A	1.923211	0.031961
92	906.919	A	2.980522	0.028420
93	920.149	A	2.179054	0.116256
94	929.410	A	1.370251	0.021703
95	932.910	A	1.370188	0.021406
96	941.177	A	1.667046	0.034857
97	944.605	A	1.670985	0.025158
98	955.808	A	4.141418	0.016188
99	962.125	A	1.508726	0.171169
100	964.274	A	1.326727	0.239295
101	967.671	A	1.339005	0.100158
102	970.395	A	1.302631	0.006579
103	973.084	A	2.614336	0.632196
104	973.741	A	1.342065	0.143875
105	975.151	A	3.046212	0.688268
106	994.045	A	1.492302	0.175192
107	996.877	A	2.954291	0.799260
108	1007.774	A	3.362563	0.605395
109	1008.307	A	1.884073	0.045921
110	1012.313	A	3.141738	0.562150
111	1013.009	A	2.279038	0.233620
112	1018.349	A	1.836670	0.097238
113	1021.375	A	2.463373	0.134537
114	1022.946	A	6.397129	0.005438
115	1035.188	A	1.434858	0.052558
116	1038.551	A	1.422165	0.068808
117	1043.265	A	2.008187	0.046100
118	1064.173	A	2.147866	0.013904
119	1068.740	A	1.792958	0.010381
120	1102.957	A	2.073383	0.086020
121	1121.514	A	1.638504	0.035416

122	1133.111	A	2.160343	0.190861
123	1135.464	A	2.169607	1.173862
124	1144.958	A	2.047425	0.636458
125	1151.970	A	5.722250	0.469448
126	1173.370	A	2.117908	1.313469
127	1184.977	A	1.132481	0.063522
128	1185.704	A	1.057237	0.245094
129	1192.819	A	1.253557	0.159400
130	1198.164	A	2.213330	0.736391
131	1202.692	A	2.293931	0.746669
132	1206.654	A	1.209335	0.017942
133	1212.446	A	1.404852	0.036425
134	1213.488	A	1.405958	0.180353
135	1222.554	A	1.208228	0.129518
136	1240.124	A	2.159361	0.622595
137	1241.323	A	2.205384	0.352699
138	1248.661	A	2.150595	0.128749
139	1253.624	A	1.232338	0.187087
140	1261.858	A	2.092192	0.003362
141	1271.667	A	1.357224	0.076567
142	1283.401	A	1.426585	0.088074
143	1293.365	A	1.974910	0.084347
144	1295.025	A	2.069806	0.087767
145	1336.031	A	1.327253	0.007834
146	1338.801	A	2.549702	0.475057
147	1339.376	A	2.008987	0.613465
148	1342.652	A	2.355691	1.437551
149	1348.933	A	1.392159	0.206387
150	1349.847	A	1.999419	0.211791
151	1374.038	A	3.919670	0.424701
152	1375.810	A	1.415048	0.032843
153	1386.144	A	1.511623	0.104734
154	1397.968	A	6.567102	0.145046
155	1402.605	A	1.437826	0.016509
156	1410.855	A	1.760801	1.387839
157	1411.335	A	1.871356	1.637561
158	1414.658	A	1.397382	0.092487
159	1419.546	A	1.297081	0.458397
160	1421.632	A	1.473428	0.190660

161	1426.806	A	2.072419	0.231554
162	1432.335	A	1.682519	0.209615
163	1437.328	A	1.316120	0.111629
164	1443.815	A	1.604620	0.329648
165	1485.149	A	1.291724	0.260796
166	1485.562	A	1.445400	0.206336
167	1487.339	A	1.211301	0.208408
168	1489.359	A	1.122679	0.032078
169	1490.771	A	1.073702	0.035056
170	1491.226	A	1.061985	0.012669
171	1492.501	A	1.101855	0.030776
172	1494.041	A	2.350913	0.195159
173	1499.311	A	1.106910	0.537007
174	1502.708	A	1.086501	0.167997
175	1506.949	A	1.077400	0.206028
176	1508.112	A	1.114799	0.018306
177	1509.802	A	1.074101	0.484608
178	1510.122	A	1.068275	0.419777
179	1512.113	A	1.062088	0.461527
180	1514.693	A	2.605022	0.120011
181	1522.814	A	1.115504	0.082992
182	1523.640	A	1.166455	0.039489
183	1529.423	A	3.170132	0.017312
184	1536.508	A	1.222848	0.280879
185	1538.069	A	2.627693	0.057679
186	1546.502	A	3.360643	0.005901
187	1627.859	A	5.603378	0.106783
188	1628.631	A	5.379089	0.072136
189	1645.946	A	6.420686	0.348823
190	1658.235	A	6.263897	0.358605
191	1671.520	A	10.826536	0.064255
192	1703.681	A	11.172947	5.656422
193	3023.675	A	1.063279	0.891404
194	3028.621	A	1.070531	0.399643
195	3047.157	A	1.037023	0.200912
196	3051.360	A	1.037283	0.475424
197	3054.762	A	1.038993	0.299974
198	3058.691	A	1.064086	0.336859
199	3061.291	A	1.040346	0.295875

200	3067.513	A	1.064236	1.104350
201	3069.629	A	1.060348	0.771332
202	3071.735	A	1.059792	0.757546
203	3075.387	A	1.035646	0.255730
204	3077.966	A	1.097611	0.280130
205	3107.546	A	1.098495	0.189314
206	3116.263	A	1.090335	0.097579
207	3119.986	A	1.098183	0.152811
208	3126.009	A	1.091395	0.070005
209	3136.141	A	1.092860	0.082853
210	3140.801	A	1.109227	0.034568
211	3142.118	A	1.110220	0.100582
212	3143.452	A	1.104600	0.318991
213	3144.102	A	1.103215	0.398222
214	3146.882	A	1.102759	0.303586
215	3148.407	A	1.101974	0.456435
216	3149.391	A	1.101550	0.317667
217	3153.380	A	1.101583	0.485249
218	3157.187	A	1.092288	0.314845
219	3170.985	A	1.086095	0.080702
220	3171.432	A	1.088881	0.172758
221	3171.748	A	1.095608	0.114346
222	3172.720	A	1.094874	0.319819
223	3175.477	A	1.088716	0.013112
224	3177.526	A	1.088184	0.017085
225	3178.842	A	1.103857	0.130703
226	3180.648	A	1.104072	0.161584
227	3187.767	A	1.089166	0.081427
228	3189.309	A	1.092473	0.252648
229	3190.623	A	1.092405	0.631006
230	3203.665	A	1.097601	0.291261
231	3204.460	A	1.097425	0.714126
ZPE (hartree/molecule)	0.655860			
Total Energy (hartree/molecule)	-1650.1513159565			
MP2 Total Energy (hartree/molecule)	-1644.5329091690			

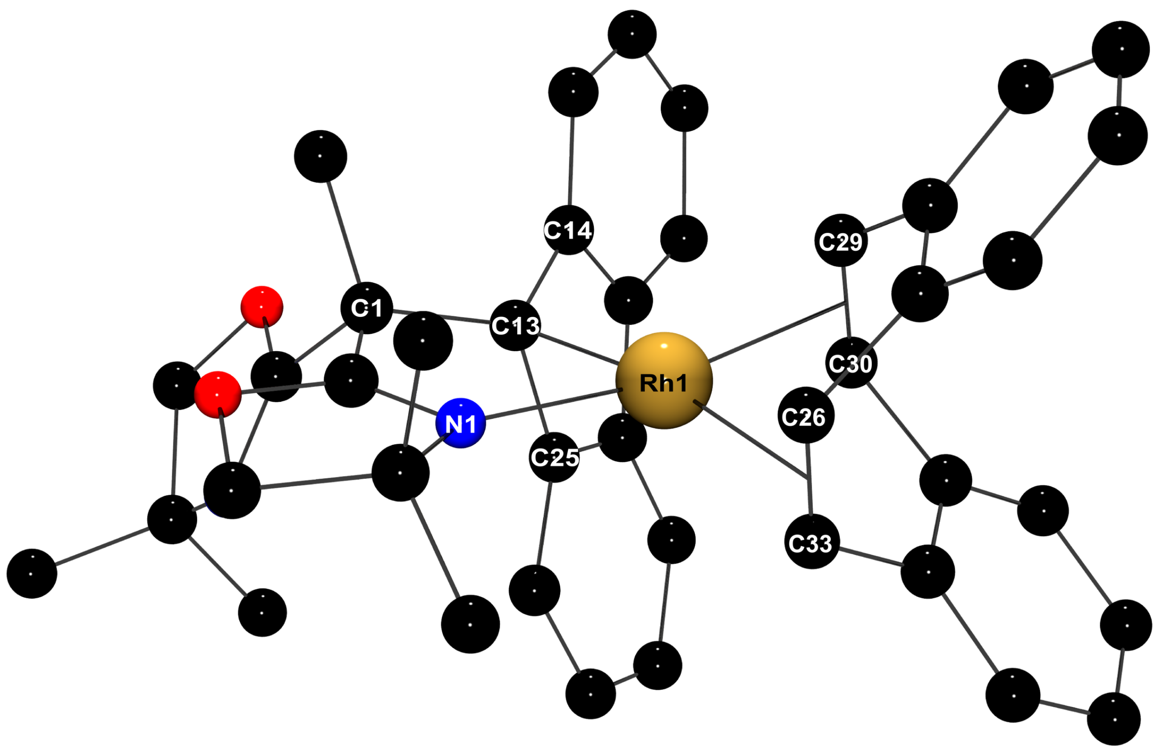

Figure S67. DFT calculation of the geometry for {*C*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$).

Table S4. Hessian results for geometry optimized structure {*C*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$). Calculations performed at DFT level of theory with M06-L functional.

MODE	FREQ(cm^{-1})	SYMMETRY	RED. MASS	IR INTENS.
1	9.271	A	6.186594	0.00125
2	7.458	A	5.810653	0.001469
3	6.927	A	6.254326	0.001448
4	5.086	A	6.262547	0.000459
5	4.053	A	7.594176	0.000713
6	3.709	A	7.98757	0.000171
7	16.04	A	5.358979	0.000763
8	16.505	A	5.236373	0.000738
9	31.265	A	5.101853	0.004117
10	43.593	A	4.980721	0.003309
11	45.695	A	4.24142	0.007731
12	49.971	A	5.857629	0.003406
13	56.052	A	4.225694	0.002325

14	57.366	A	4.494126	0.009822
15	69.871	A	4.382902	0.008313
16	80.627	A	4.533478	0.01545
17	85.163	A	4.157675	0.000218
18	100.239	A	4.094721	0.013401
19	104.659	A	3.73858	0.008159
20	111.478	A	4.151562	0.007797
21	118.203	A	4.38642	0.00463
22	122.887	A	4.333037	0.017093
23	144.93	A	6.707319	0.010203
24	149.39	A	3.814762	0.003283
25	153.843	A	5.008518	0.021063
26	162.705	A	4.599976	0.000647
27	168.503	A	4.670962	0.121711
28	181.99	A	4.40024	0.015249
29	188.299	A	3.759432	0.005575
30	213.798	A	4.077502	0.008553
31	228.619	A	4.940093	0.057856
32	236.307	A	1.240125	0.006091
33	236.641	A	4.246657	0.068108
34	243.994	A	2.438664	0.010843
35	250.632	A	1.180048	0.008281
36	255.06	A	4.175723	0.004013
37	264.591	A	1.743128	0.03163
38	268.442	A	5.534297	0.003854
39	274.489	A	3.434093	0.02726
40	283.143	A	2.59606	0.010491
41	286.786	A	1.913299	0.057791
42	289.912	A	3.106583	0.054834
43	297.634	A	1.599676	0.019244
44	310.381	A	3.10637	0.001906
45	317.774	A	2.960235	0.025189
46	336.719	A	3.02178	0.011043
47	343.344	A	1.534203	0.017798
48	355.281	A	2.158241	0.064851
49	363.027	A	2.393564	0.004869
50	369.935	A	2.655798	0.025066
51	379.512	A	4.959807	0.007542
52	393.167	A	3.483144	0.062122

53	394.856	A	2.747757	0.090302
54	402.632	A	4.34851	0.021396
55	424.001	A	5.079896	0.074757
56	430.725	A	3.372765	0.044939
57	439.606	A	4.574907	0.150949
58	442.049	A	3.561738	0.024531
59	467.078	A	3.105259	0.020284
60	472.83	A	3.603156	0.131754
61	478.409	A	3.272691	0.004001
62	488.127	A	3.618105	0.094416
63	503.821	A	3.979649	0.059853
64	510.156	A	3.651097	0.047757
65	517.549	A	4.905133	0.031454
66	519.566	A	4.664573	0.00611
67	531.076	A	4.268797	0.231377
68	537.806	A	3.712646	0.01124
69	570.133	A	5.570414	0.39645
70	574.967	A	3.868835	0.023442
71	585.219	A	6.094834	0.031225
72	593.721	A	4.152132	0.100492
73	609.696	A	4.620442	0.12371
74	615.434	A	6.851962	0.093902
75	622.253	A	3.969881	0.09833
76	630.709	A	6.622719	0.144485
77	632.619	A	4.188753	0.022094
78	651.888	A	5.094529	0.299123
79	663.06	A	6.143638	0.062063
80	673.667	A	3.39008	0.026577
81	680.819	A	4.417834	0.01574
82	729.119	A	6.520454	0.198213
83	735.647	A	3.218198	0.006718
84	743.244	A	3.008981	0.289778
85	746.243	A	1.909438	0.866766
86	747.995	A	2.858271	0.16586
87	751.262	A	1.526075	0.060312
88	755.345	A	1.304434	0.784327
89	759.652	A	1.450842	0.68903
90	761.006	A	5.057484	0.022796
91	775.536	A	3.70297	0.198454

92	790.195	A	3.909823	0.005048
93	793.902	A	2.813045	0.038004
94	801.861	A	1.664604	0.048709
95	805.284	A	4.091572	0.033591
96	823.445	A	3.655198	0.097096
97	827.473	A	3.236526	0.7145
98	841.736	A	3.937041	0.224917
99	847.68	A	3.068447	0.45491
100	852.825	A	2.74437	0.137726
101	863.072	A	1.606161	0.113804
102	866.617	A	1.610525	0.018355
103	868.954	A	1.384425	0.147675
104	875.144	A	1.447224	0.078079
105	888.077	A	1.417393	0.191491
106	890.114	A	4.221359	0.006439
107	906.799	A	3.152886	0.175086
108	912.281	A	2.740789	0.017137
109	916.734	A	1.426941	0.032058
110	929.967	A	1.678345	0.043637
111	933.69	A	1.853258	0.21901
112	937.296	A	1.377638	0.016983
113	939.427	A	1.434742	0.124738
114	942.681	A	1.577825	0.024502
115	947.85	A	1.677198	0.081639
116	955.991	A	1.676335	0.048826
117	957.226	A	1.279871	0.016495
118	961.75	A	1.437711	0.221261
119	964.244	A	1.264066	0.009706
120	965.727	A	1.816952	0.015114
121	971.419	A	1.318014	0.008414
122	972.439	A	1.440384	0.004442
123	973.44	A	1.311643	0.001284
124	981.744	A	2.492774	0.265138
125	995.423	A	2.394377	0.621679
126	1001.298	A	2.012278	0.26435
127	1006.946	A	1.844349	0.218451
128	1017.874	A	2.833845	0.026149
129	1020.07	A	1.747751	0.145413
130	1032.295	A	1.452405	0.07202

131	1038.938	A	1.56758	0.128287
132	1053.297	A	1.964801	0.102453
133	1056.223	A	4.007515	0.95839
134	1060.973	A	1.83026	0.140836
135	1064.934	A	4.99502	0.694214
136	1065.404	A	2.177977	0.058331
137	1066.762	A	2.05552	0.070994
138	1089.865	A	2.537645	0.0443
139	1115.164	A	2.199308	0.151285
140	1127.348	A	1.570998	0.00518
141	1129.817	A	2.778693	1.779333
142	1132.765	A	1.766558	0.50243
143	1140.982	A	2.765639	1.568313
144	1142.205	A	1.538584	0.17472
145	1149.956	A	1.435942	0.022084
146	1153.531	A	1.765219	1.264732
147	1163.084	A	1.16798	0.005988
148	1163.224	A	1.077615	0.017739
149	1167.47	A	1.080047	0.011342
150	1169.168	A	1.311231	0.401793
151	1195.734	A	1.598649	0.221631
152	1206.613	A	1.544689	0.273132
153	1207.36	A	2.060071	0.057143
154	1213.413	A	2.60911	0.113591
155	1222.537	A	2.317385	0.108316
156	1227.875	A	2.315187	1.302906
157	1229.716	A	1.803071	0.057829
158	1236.641	A	2.299607	0.182741
159	1244.788	A	2.249571	0.609257
160	1245.732	A	1.688484	0.394099
161	1250.823	A	1.659135	0.049581
162	1257.149	A	2.085463	0.373505
163	1262.264	A	2.444931	0.498288
164	1269.562	A	1.468828	0.012252
165	1272.914	A	1.500489	0.30813
166	1289.064	A	2.118652	0.373014
167	1289.4	A	2.163464	0.188531
168	1309.675	A	1.756263	0.04286
169	1330.192	A	3.546083	0.78075

170	1331.701	A	2.347448	0.155421
171	1362.725	A	1.96205	0.52611
172	1366.472	A	7.359258	0.00886
173	1370.481	A	7.505401	0.09087
174	1376.097	A	6.93713	0.377896
175	1384.918	A	1.643173	0.01615
176	1386.692	A	1.559367	0.577414
177	1396.138	A	4.331089	0.166796
178	1399.364	A	1.404079	0.172599
179	1403.804	A	1.374627	0.134444
180	1404.168	A	1.447365	0.777724
181	1407.004	A	1.764151	0.582206
182	1415.211	A	1.337287	0.50339
183	1417.244	A	1.365727	0.401399
184	1444.562	A	2.316639	1.266449
185	1449.527	A	2.455249	0.162027
186	1469.186	A	1.054453	0.044795
187	1469.884	A	1.051905	0.020899
188	1475.1	A	2.506455	1.129503
189	1476.489	A	1.065401	0.090451
190	1477.62	A	1.065502	0.056268
191	1482.216	A	2.532288	0.340254
192	1488.123	A	1.082764	0.431749
193	1490.252	A	1.103196	0.251773
194	1491.446	A	1.074564	0.05737
195	1491.749	A	2.482248	0.008638
196	1494.596	A	1.103949	0.335539
197	1495.011	A	1.059969	0.155804
198	1497.022	A	1.082809	0.241748
199	1504.398	A	1.257014	0.409015
200	1506.748	A	3.076257	0.083133
201	1511.456	A	2.747513	0.174825
202	1516.283	A	1.120166	0.102263
203	1522.606	A	3.707604	0.374877
204	1536.769	A	3.324343	0.236965
205	1541.667	A	4.37364	0.210905
206	1558.456	A	5.800046	0.526302
207	1633.812	A	6.248057	0.012112
208	1640.109	A	6.801764	0.011521

209	1652.875	A	7.289642	0.055992
210	1655.388	A	7.055944	0.1105
211	1668.054	A	7.222049	0.006514
212	1672.142	A	6.648035	0.0093
213	1673.416	A	6.727768	0.039607
214	1678.3	A	7.074202	0.071153
215	1700.287	A	11.34157	3.46808
216	1749.935	A	11.840458	5.087365
217	3019.604	A	1.036417	0.710465
218	3025.105	A	1.038881	0.43687
219	3031.35	A	1.060405	0.862706
220	3031.839	A	1.037603	0.39818
221	3032.909	A	1.05218	0.337394
222	3036.48	A	1.051076	0.881279
223	3037.535	A	1.038326	0.28283
224	3103.761	A	1.106039	0.640878
225	3107.743	A	1.102958	1.108216
226	3108.357	A	1.102802	0.079134
227	3112.388	A	1.102717	0.309375
228	3115.806	A	1.101542	0.61175
229	3117.735	A	1.08566	0.083873
230	3122.343	A	1.103397	0.392411
231	3126.998	A	1.102061	0.488317
232	3127.672	A	1.102781	0.204964
233	3128.397	A	1.103133	0.364438
234	3128.938	A	1.084833	0.012942
235	3133.552	A	1.101677	0.23006
236	3137.765	A	1.09138	0.916137
237	3140.349	A	1.089936	0.034321
238	3147.309	A	1.097081	0.069064
239	3151.333	A	1.088146	0.192882
240	3156.592	A	1.087175	0.063885
241	3156.964	A	1.086677	0.348873
242	3158.745	A	1.086072	0.126761
243	3161.957	A	1.08853	0.016196
244	3162.786	A	1.088208	0.032411
245	3166.316	A	1.088932	0.194088
246	3169.112	A	1.087609	0.045916
247	3171.619	A	1.099276	0.194685

248	3175.803	A	1.092552	0.502138
249	3177.944	A	1.092216	0.406474
250	3178.469	A	1.091541	0.533291
251	3182.405	A	1.092889	0.681362
252	3187.837	A	1.097604	1.020239
253	3189.727	A	1.098649	1.085888
254	3190.424	A	1.097358	0.58498
255	3193.085	A	1.098173	1.160645
ZPE (hartree/molecule)	0.698404			
Total Energy (hartree/molecule)	-1954.9574610021			

Table S5. Hessian results for geometry optimized structure [{*C*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-$C_{16}H_{12}$)]$^+$. Calculations performed at DFT level of theory with M06-L functional.

MODE	FREQ (cm^{-1})	SYMMETRY	RED. MASS	IR INTENS.
1	6.333	A	7.600986	0.003809
2	5.156	A	6.084888	0.000845
3	4.455	A	5.479901	0.00029
4	2.616	A	5.905935	0.000171
5	0.517	A	8.143717	0.000005
6	0.219	A	8.161951	0.000001
7	21.524	A	5.212326	0.000328
8	26.867	A	5.009934	0.00084
9	30.423	A	5.392409	0.001079
10	39.405	A	4.706193	0.005538
11	41.155	A	4.729674	0.004416
12	48.32	A	3.779961	0.003784
13	54.977	A	5.135937	0.004734
14	58.161	A	4.262304	0.024361
15	61.424	A	4.575183	0.009957
16	78.024	A	4.6775	0.000541
17	81.721	A	4.296617	0.001445
18	101.378	A	4.215228	0.004925
19	104.4	A	4.31906	0.008377
20	109.147	A	3.497614	0.003085
21	117.04	A	4.251824	0.020692
22	122.615	A	4.417064	0.02464

23	145.623	A	4.25271	0.013229
24	152.229	A	4.917256	0.019353
25	155.605	A	4.437455	0.062612
26	161.073	A	5.479636	0.029229
27	168.632	A	4.261439	0.008997
28	181.218	A	3.947099	0.008281
29	182.897	A	4.51748	0.000966
30	204.68	A	7.886485	0.143761
31	213.99	A	4.932125	0.040236
32	226.986	A	4.595431	0.059858
33	231.172	A	1.169092	0.012868
34	235.877	A	2.356663	0.022481
35	237.165	A	1.625351	0.01186
36	243.426	A	3.294407	0.029628
37	245.529	A	3.955327	0.004128
38	254.13	A	4.680008	0.028425
39	260.988	A	1.304129	0.035301
40	265.3	A	1.873839	0.021581
41	283.253	A	2.477925	0.005355
42	288.366	A	4.689724	0.245055
43	294.627	A	1.391897	0.010365
44	306.336	A	3.959333	0.006874
45	309.213	A	3.249966	0.072428
46	331.482	A	2.339457	0.006788
47	340.22	A	2.942622	0.012272
48	352.059	A	2.829137	0.139923
49	360.428	A	2.739767	0.032352
50	362.469	A	3.780184	0.223983
51	376.929	A	1.364155	0.025938
52	383.215	A	3.622132	0.173987
53	384.596	A	4.086362	0.298947
54	393.965	A	2.748769	0.112898
55	400.695	A	4.12993	0.135437
56	418.045	A	3.667359	0.14069
57	428.52	A	4.280853	0.010234
58	441.122	A	3.614967	0.108206
59	457.05	A	3.448403	0.020761
60	463.687	A	3.449417	0.06576
61	466.636	A	3.279362	0.023581

62	474.213	A	3.385014	0.014403
63	495.394	A	3.995084	0.093203
64	511.081	A	3.797638	0.013424
65	512.821	A	4.451139	0.020786
66	521.485	A	4.698774	0.084123
67	527.035	A	3.692243	0.104626
68	528.751	A	4.328978	0.158448
69	566.808	A	4.24107	0.128172
70	567.682	A	4.287065	0.294602
71	582.552	A	5.983119	0.024995
72	589.326	A	3.957514	0.001384
73	597.619	A	5.148035	0.528908
74	609.735	A	4.407525	0.284631
75	619.253	A	6.881133	0.076506
76	628.359	A	4.654327	0.211291
77	630.704	A	5.460591	0.103062
78	633.983	A	5.051698	0.321024
79	662.958	A	5.84861	0.151704
80	680.211	A	3.423209	0.070715
81	690.451	A	4.484214	0.019398
82	718.357	A	6.273661	0.02932
83	729.489	A	5.972864	0.243923
84	736.804	A	3.12458	0.030428
85	739.405	A	1.63713	1.026947
86	745.294	A	2.981802	0.008719
87	751.431	A	1.717657	0.203196
88	759.709	A	1.572042	0.503581
89	761.483	A	2.740588	0.352297
90	766.555	A	1.490357	0.550123
91	767.862	A	3.139954	0.406825
92	787.524	A	2.811489	0.101538
93	796.002	A	2.855446	0.135996
94	800.274	A	3.461193	0.119933
95	804.211	A	3.976393	0.058706
96	809.906	A	2.0442	0.086388
97	826.776	A	4.767163	0.009103
98	839.932	A	4.163271	0.151162
99	852.654	A	2.162777	0.31495
100	853.096	A	3.065813	0.408333

101	859.601	A	1.560633	0.334722
102	869.985	A	1.331902	0.058541
103	874.032	A	1.572148	0.012272
104	884.797	A	1.422809	0.02911
105	888.951	A	1.421092	0.033169
106	892.678	A	2.905948	0.127971
107	911.643	A	5.083887	0.149099
108	918.411	A	2.519215	0.032753
109	923.915	A	2.73884	0.120626
110	929.728	A	1.405245	0.023895
111	941.607	A	1.838744	0.209016
112	944.502	A	1.454502	0.014351
113	946.693	A	1.377569	0.01138
114	948.604	A	1.508983	0.045967
115	949.076	A	1.568164	0.113358
116	959.1	A	2.321459	0.247651
117	967.984	A	1.41629	0.08345
118	970.01	A	1.542752	0.114738
119	976.507	A	1.485965	0.028861
120	978.057	A	1.317851	0.027616
121	983.46	A	1.303149	0.013286
122	985.827	A	2.689699	0.909389
123	986.45	A	1.355677	0.135665
124	987.609	A	1.292948	0.033682
125	988.131	A	2.564685	0.888752
126	1000.7	A	2.515647	0.438802
127	1005.727	A	1.951376	0.0878
128	1009.651	A	1.311479	0.059613
129	1014.268	A	3.418248	0.719001
130	1020.464	A	2.883868	0.636154
131	1024.914	A	7.256456	0.02744
132	1042.249	A	1.463069	0.089836
133	1046.493	A	1.562981	0.104055
134	1062.631	A	2.108572	0.038327
135	1070.848	A	1.886685	0.014466
136	1071.375	A	2.392437	0.006326
137	1073.961	A	2.215175	0.002529
138	1105.095	A	2.787362	0.014058
139	1125.407	A	2.84651	0.791396

140	1127.689	A	2.440105	1.522499
141	1138.242	A	1.871941	0.14157
142	1144.502	A	1.693447	0.000436
143	1151.892	A	3.210693	0.29121
144	1157.81	A	1.663891	0.317221
145	1165.061	A	2.141136	1.356212
146	1168.38	A	1.556355	0.200411
147	1186.689	A	1.147071	0.147139
148	1190.869	A	1.079119	0.020742
149	1191.916	A	1.15517	0.037886
150	1192.243	A	1.452402	0.218713
151	1194.782	A	1.36166	0.36331
152	1200.778	A	1.667241	0.432355
153	1219.43	A	1.874112	0.146405
154	1220.49	A	2.175938	0.139881
155	1223.19	A	1.783045	0.675642
156	1240.917	A	2.003603	0.230286
157	1241.47	A	2.272998	0.808447
158	1242.763	A	2.18898	0.603643
159	1251.21	A	2.044905	0.050015
160	1257.577	A	2.103422	0.225338
161	1261.973	A	1.518514	0.092947
162	1265.768	A	1.500071	0.295164
163	1287.244	A	4.002504	0.068843
164	1289.329	A	1.482915	0.008438
165	1292.103	A	2.301323	0.061279
166	1293.201	A	1.61472	0.497638
167	1296.302	A	1.967975	0.093112
168	1325.645	A	2.986043	1.312935
169	1330.062	A	2.016993	0.433623
170	1340.572	A	1.996919	0.052814
171	1363.244	A	2.01231	0.641607
172	1388.568	A	1.655451	0.463329
173	1395.147	A	6.55408	0.033161
174	1398.657	A	6.983196	0.200154
175	1400.477	A	7.504945	0.01709
176	1410.044	A	1.341439	0.669497
177	1410.559	A	1.489643	0.025867
178	1413.36	A	1.365333	0.38182

179	1418.188	A	1.341886	0.283165
180	1426.588	A	3.525437	0.207788
181	1429.38	A	1.451476	0.728175
182	1431.041	A	1.284393	0.11621
183	1434.965	A	1.730159	0.625968
184	1454.272	A	2.23546	0.89348
185	1460.996	A	2.275939	0.156868
186	1466.367	A	2.560723	0.370768
187	1486.017	A	2.409418	0.933725
188	1489.677	A	1.051832	0.031065
189	1491.811	A	1.070059	0.03372
190	1493.2	A	1.079387	0.074854
191	1495.06	A	1.05007	0.114285
192	1499.146	A	2.279526	0.008375
193	1506.716	A	1.288647	0.181106
194	1508.714	A	1.259375	0.627645
195	1510.093	A	1.090359	0.118482
196	1510.421	A	1.22964	0.366127
197	1512.946	A	1.076531	0.218554
198	1513.059	A	1.397871	0.185555
199	1518.709	A	2.494267	0.18835
200	1519.557	A	1.416488	0.121893
201	1521.838	A	1.256571	0.181747
202	1522.75	A	1.326672	0.074941
203	1526.801	A	1.279001	0.647221
204	1542.676	A	3.222933	0.058492
205	1547.885	A	4.246827	0.051588
206	1558.019	A	4.53654	0.166858
207	1611.027	A	4.94358	0.201979
208	1637.03	A	5.775637	0.129317
209	1646.152	A	6.760801	0.017969
210	1649.462	A	6.52876	0.215935
211	1651.076	A	6.523086	0.381064
212	1660.01	A	6.286559	0.688056
213	1662.962	A	5.977739	0.265013
214	1665.065	A	6.010198	0.084625
215	1676.045	A	10.737058	4.256624
216	1731.761	A	11.60224	3.318802
217	3035.182	A	1.037057	0.392246

218	3048.481	A	1.038336	0.465074
219	3050.969	A	1.037949	0.411693
220	3053.56	A	1.042161	0.18635
221	3054.958	A	1.060806	1.39255
222	3057.789	A	1.061108	0.678768
223	3060.797	A	1.038395	0.241925
224	3125.829	A	1.087646	0.151384
225	3127.645	A	1.102401	0.822874
226	3133.649	A	1.108039	0.299721
227	3135.697	A	1.086321	0.098587
228	3142.122	A	1.102864	0.14884
229	3142.406	A	1.10251	0.353406
230	3144.029	A	1.101966	0.481902
231	3147.881	A	1.102343	0.343591
232	3153.346	A	1.10254	0.402059
233	3154.982	A	1.102426	0.281346
234	3155.545	A	1.104604	0.094138
235	3158.05	A	1.097273	0.834944
236	3160.725	A	1.101459	0.157993
237	3168.223	A	1.086911	0.07504
238	3169.473	A	1.087536	0.171997
239	3171.912	A	1.089617	0.016641
240	3172.182	A	1.089657	0.0305
241	3172.963	A	1.08792	0.096437
242	3174.061	A	1.089137	0.002055
243	3175.504	A	1.087646	0.088579
244	3185.687	A	1.088948	0.072108
245	3188.45	A	1.09006	0.060681
246	3189.471	A	1.092271	0.195367
247	3190.641	A	1.092373	0.402748
248	3193.185	A	1.101256	0.116827
249	3201.561	A	1.08658	0.04481
250	3202.03	A	1.094742	0.323142
251	3202.607	A	1.094237	0.397735
252	3204.21	A	1.09855	0.59475
253	3205.35	A	1.098521	0.678534
254	3213.305	A	1.094768	0.319447
255	3220.209	A	1.093078	0.137433

ZPE (hartree/molecule)	0.698404			
Total Energy (hartree/molecule)	-1953.9659908776			

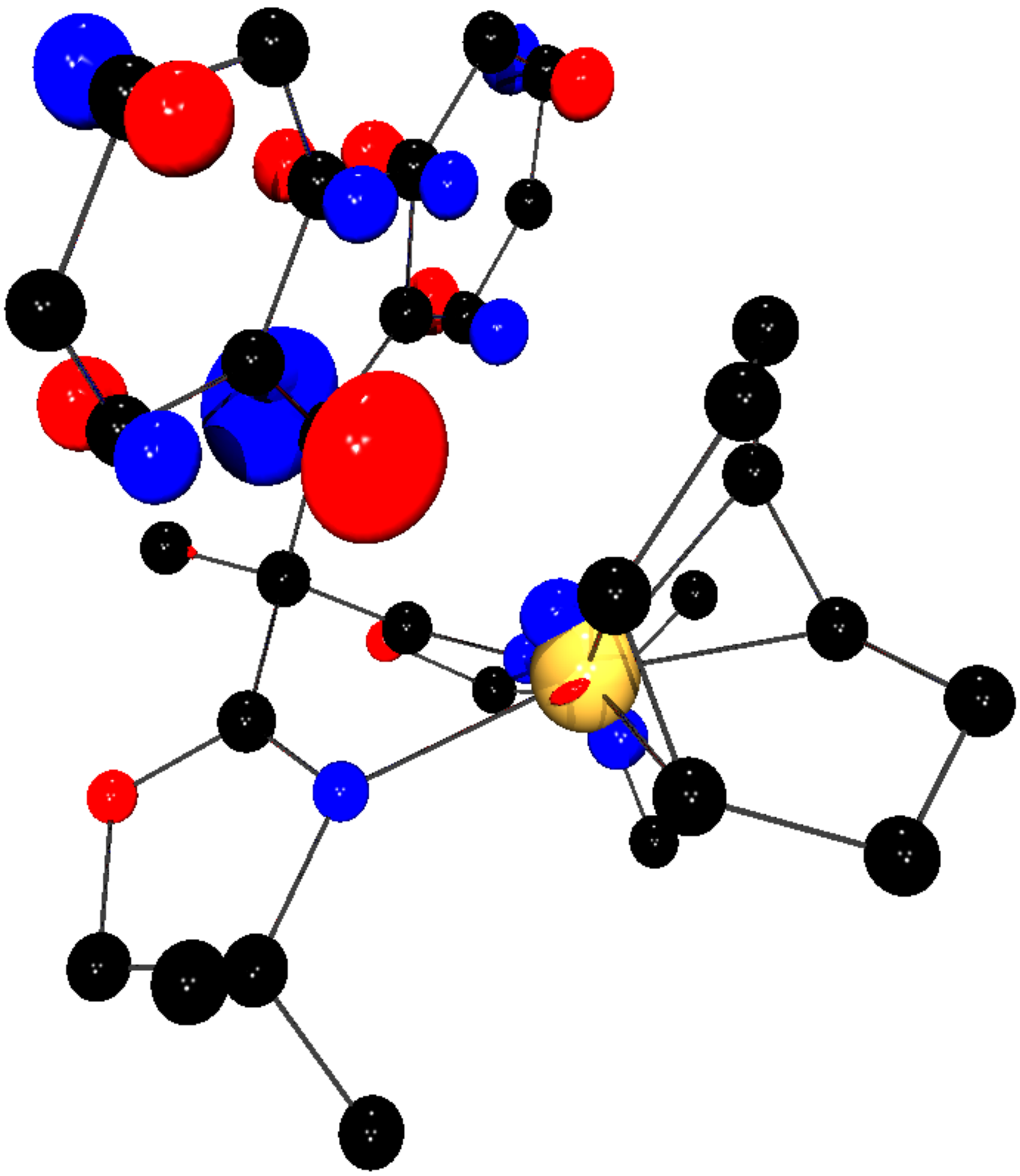

Figure S68. SOMO of {*N*,*N*-κ^2-Bo^{M}Flu}Rh(η^4-C_8H_{12})$^+$ showing localization of the unpaired electron on the fluorenyl group. The atomic coordinates are equivalent to the structure depicted in Figure S66.