Supporting Information

Detailed Structural and Spectroscopic Elucidation of Ferrocenium Coupled N-heterocyclic Carbene Gold(I) Complexes

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Table 1. Crystallographic data for complexes [**2**][BF_4], [**3**][BF_4]$_3$, [**5**][BF_4], and [**6**][BF_4]$_3$

compound #	[**2**][BF_4]	[**3**][BF_4]$_3$	[**5**][BF_4]
CCDC	2109471	2109472	2109473
structure code	19SW013LT_0m	19SW017LT_0m	19SW014LT_0m
solvent	none	$ClCH_2CH_2Cl$	none
formula	$C_{46}H_{48}AuFe_2N_4BF_4$	$C_{48}H_{52}AuFe_2N_4Cl_2B_3F_{12}$	$C_{50}H_{48}AuBF_4Fe_4N_4$
fw, g/mol	1052.40	1324.99	1212.13
temperature, K	173 K	173 K	173 K
wavelength	0.71073	0.71073	0.71073
2θ range, deg.	2.71 – 28.29	3.03 – 26.39	2.73 – 28.40
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$	$C2/c$
a, Å	11.798(2)	14.447(2)	18.112(5)
b, Å	23.649(4)	24.404(4)	12.733(4)
c, Å	15.577(3)	14.886(2)	19.212(5)
α, deg.	90	90	90
β, deg.	94.649(4)	99.088(4)	104.134(7)
γ, deg.	90	90	90
Volume, Å^3	4333.7(14)	5182.4(14)	4296(2)
Z	4	4	4
density, g/cm^3	1.6129	1.6980	1.8739
μ, mm^{-1}	4.092	3.561	4.781
crystal size	0.15 x 0.25 x 0.4	0.05 x 0.25 x 0.26	0.25 x 0.25 x 0.35
color, habitat	yellow, needle	blue, plate	golden, block
limiting indices, *h*	-15 ≤ h ≤ 15	-18 ≤ h ≤ 17	-24 ≤ h ≤ 24
limiting indices, *k*	-31 ≤ k ≤ 31	-30 ≤ k ≤ 30	-16 ≤ k ≤ 17
limiting indices, *l*	-20 ≤ l ≤ 20	-18 ≤ l ≤ 18	-25 ≤ l ≤ 25
ref. collected	54241	66536	42199
independent data	10721	10582	5372
restraints	0	0	0
parameters refined	529	655	294
R_{int}	0.0392	0.0659	0.0520
GooF[a]	1.0561	1.0437	1.0493
R1,[b,c] wR2[d,c]	0.0374, 0.0879	0.0394, 0.0856	0.0214, 0.0578
R1,[b,e] wR2[d,e]	0.0571, 0.0995	0.0550, 0.0955	0.0270, 0.0600

[a]GooF = {Σ[w(F_o^2–F_c^2)^2]/(n – p)}½, where n= number of reflections and p is the total number of parameters refined; [b]R1 = [a]R1 = Σ||F_o| – |F_c||/Σ|F_o|; [c]R indices for data cut off at I > 2σ(I); [d]wR2 = {[Σw(Fo 2 – Fc 2) 2 /Σw(Fo 2) 2 }1/2; w = 1/[σ2 (Fo 2) + (xP) 2 + yP], where P = (Fo 2 + 2Fc 2)/3; [e]R indices for all data. [a]R1 = Σ||F_o| – |F_c||/Σ|F_o|. [b]R_w = {[Σw(F_o^2 – F_c^2)/Σw(F_o^2)^2}$^{1/2}$; w = 1/[σ^2(F_o^2) + (xP)^2], where P = (F_o^2 + 2F_c^2)/3.

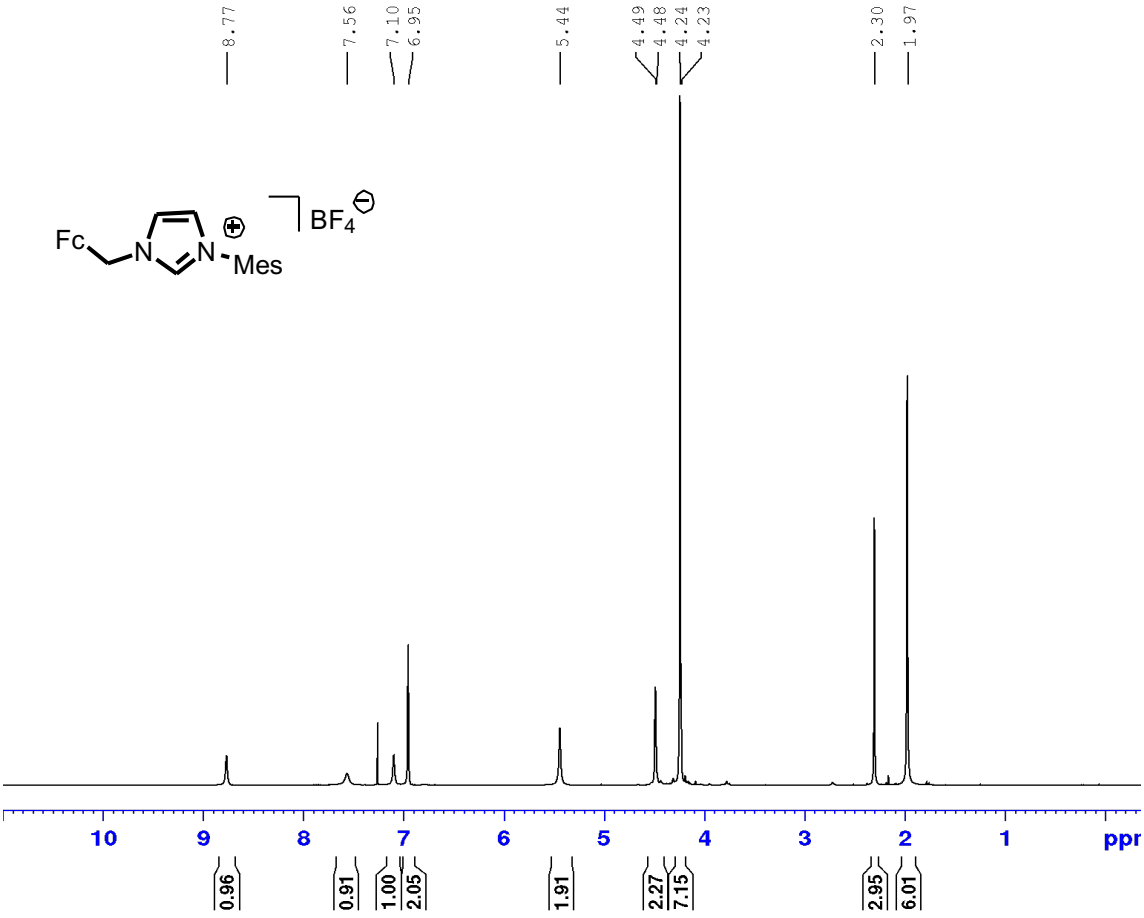

Figure S1. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

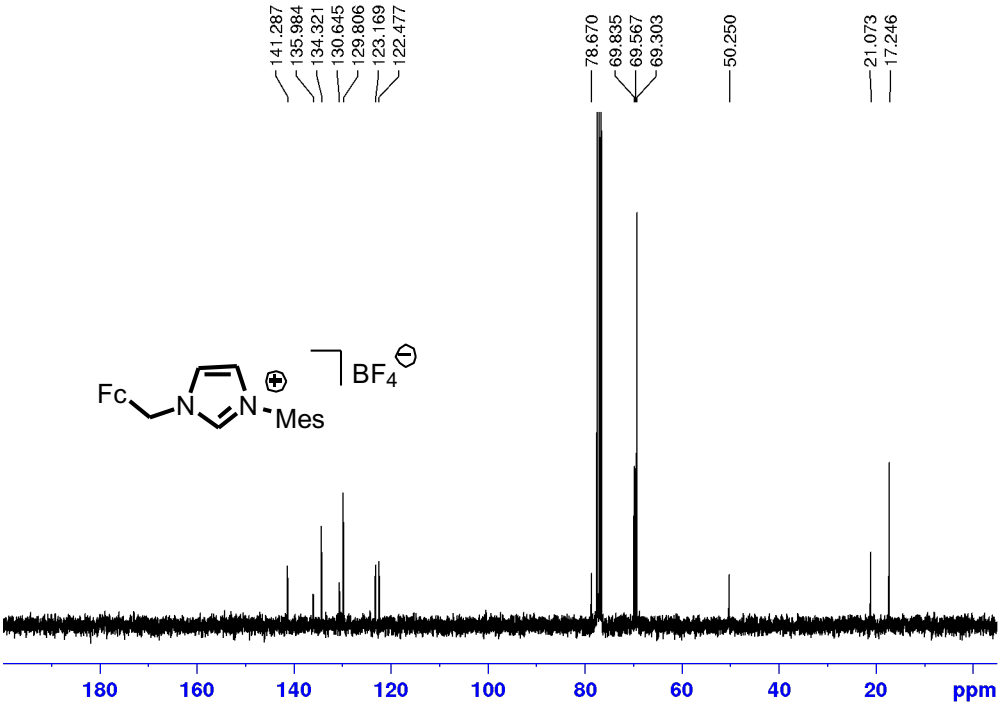

Figure S2. ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

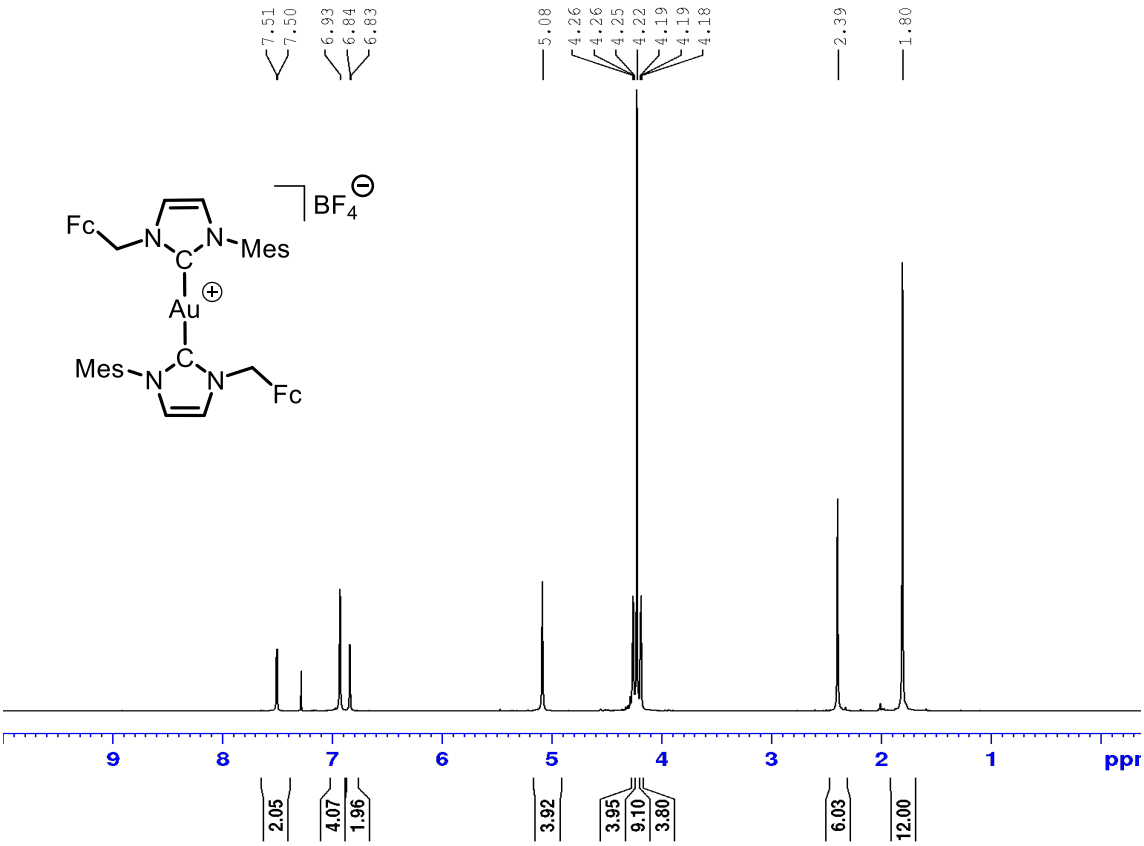

Figure S3. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

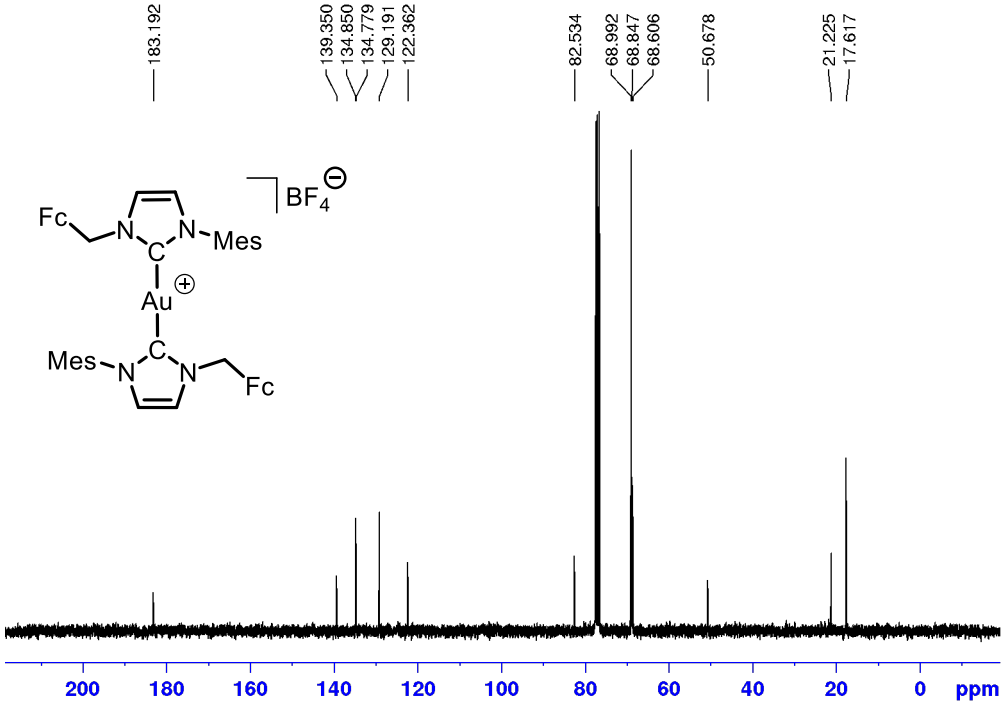

Figure S4. ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

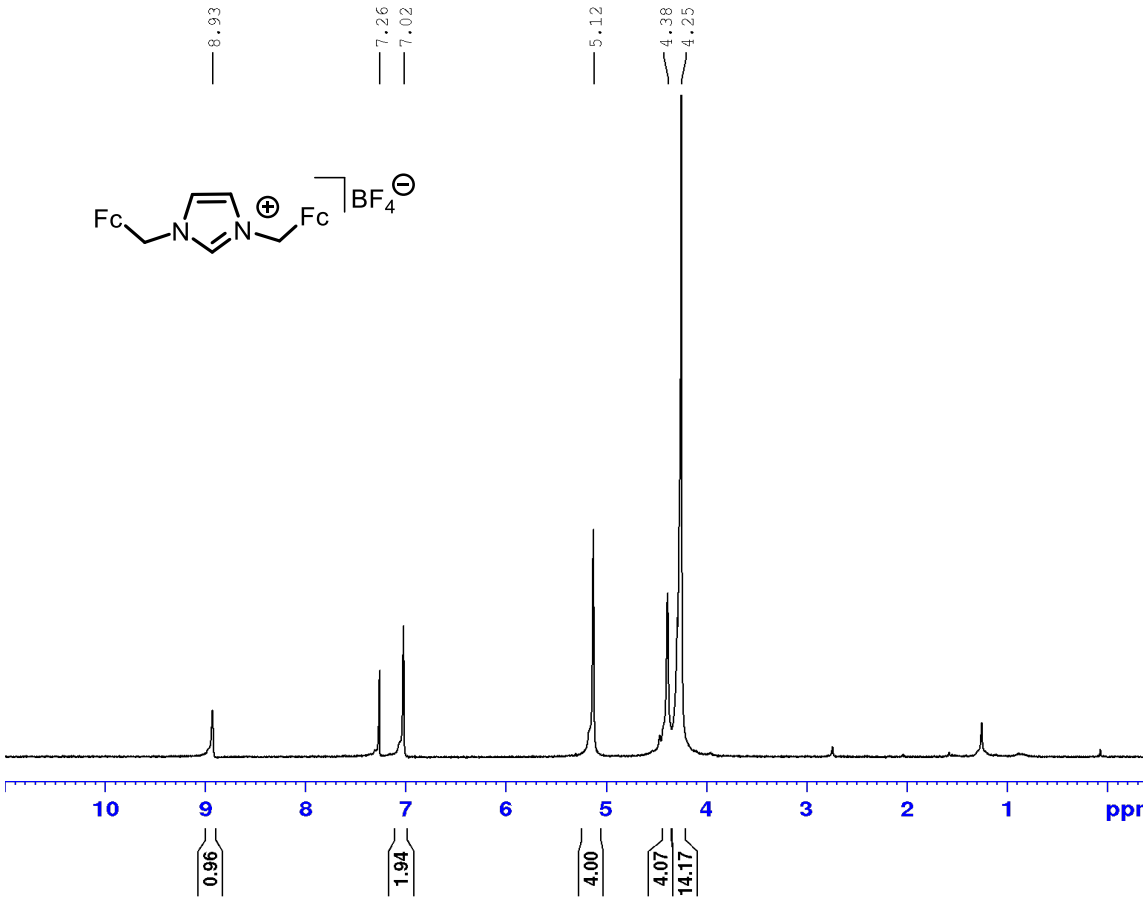

Figure S5. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

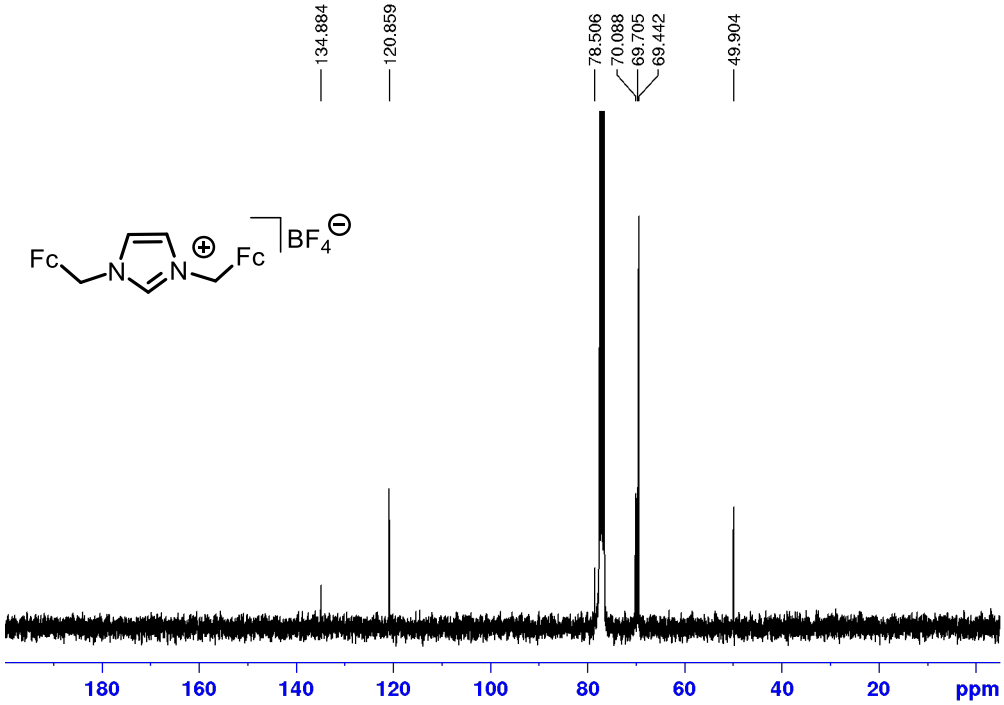

Figure S6. ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

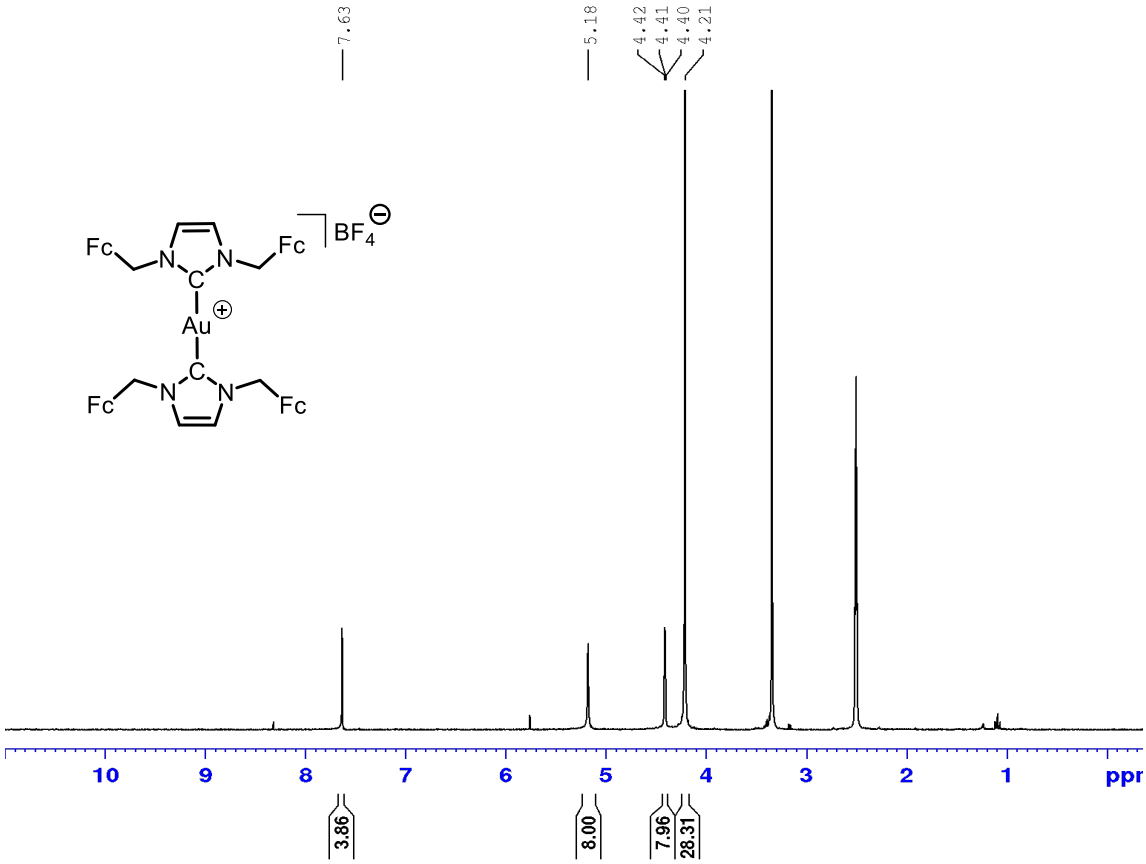

Figure S7. ^{1}H NMR spectrum of compound **5** in DMSO.

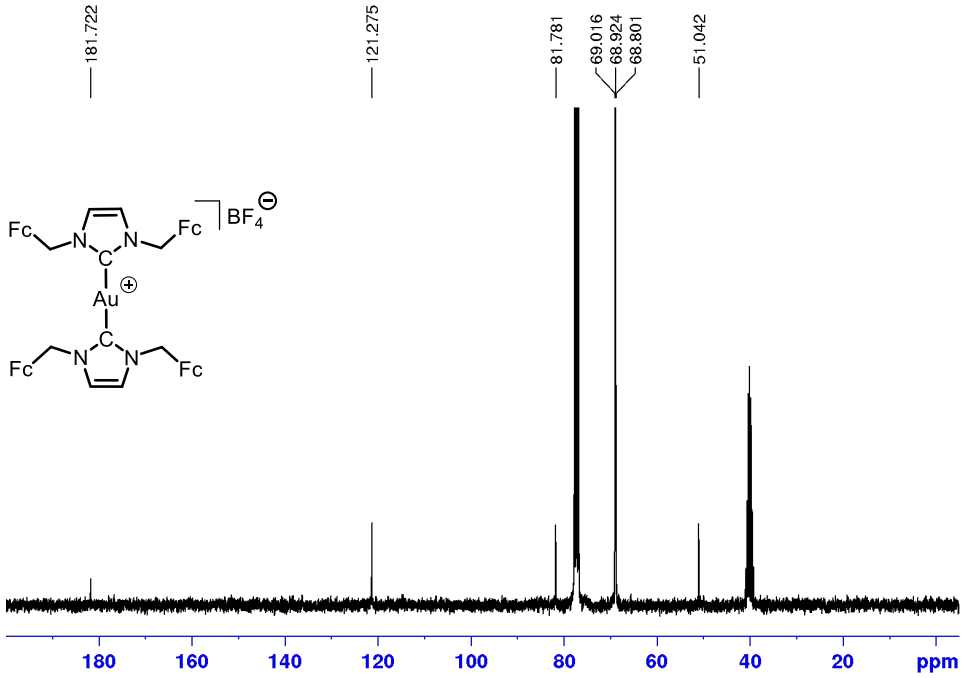

Figure S8. ^{13}C NMR spectrum of compound **5** in DMSO.

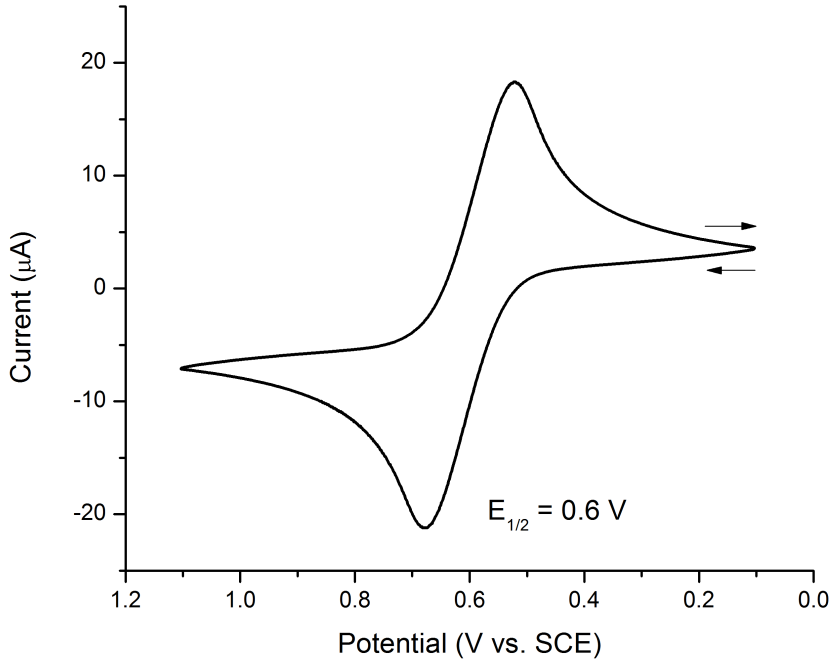

Figure S9. Cyclic Voltammogram of **2** with 0.1M $[N(nBu)_4]PF_6$ in DCM (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

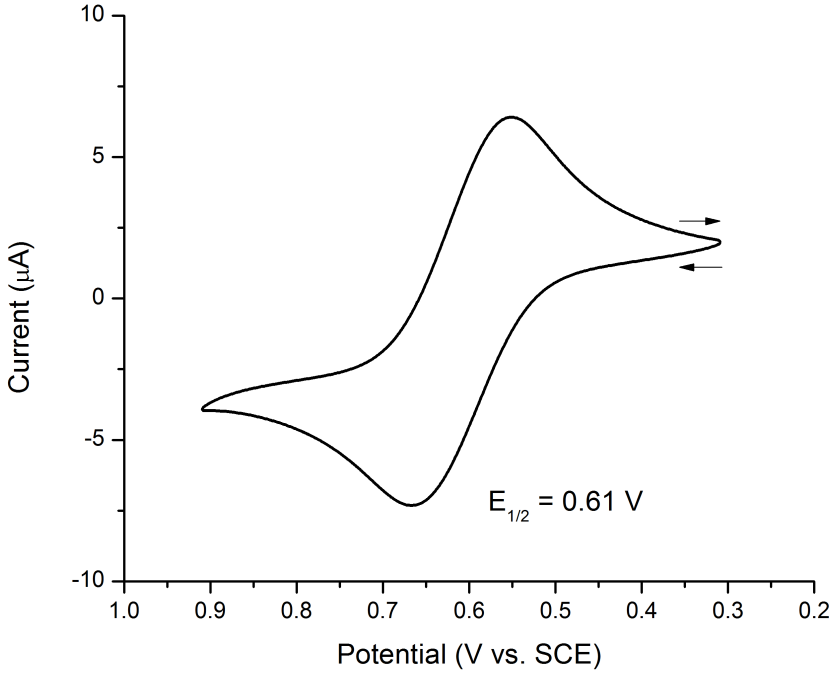

Figure S10. Cyclic Voltammogram of **5** with 0.1M $[N(nBu)_4]PF_6$ in DCM (1mM) as referenced to decamethylferrocene (internal standard, adjusted to SCE).

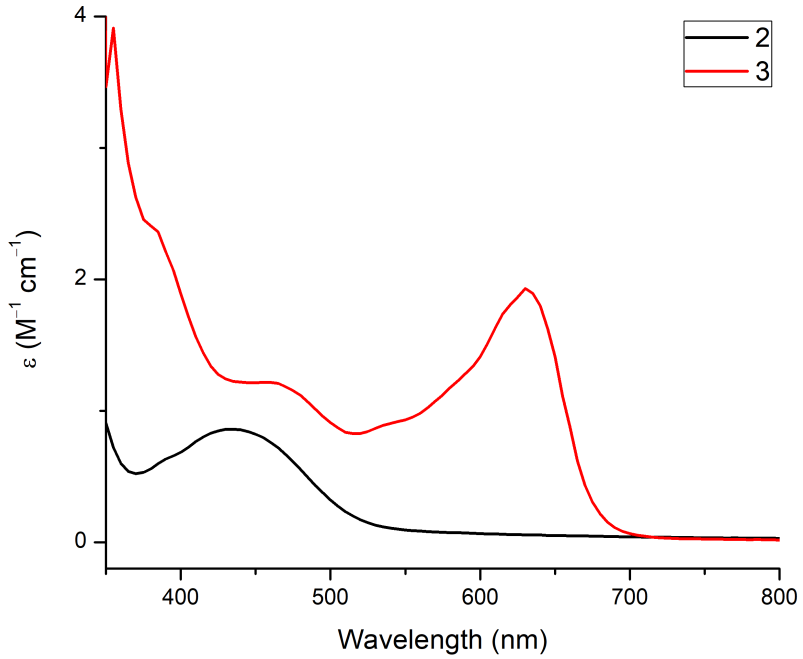

Figure S11. Electronic absorption spectra of compounds [**2**][BF_4] and [**3**][BF_4]$_3$ recorded in Acetonitrile solvent.

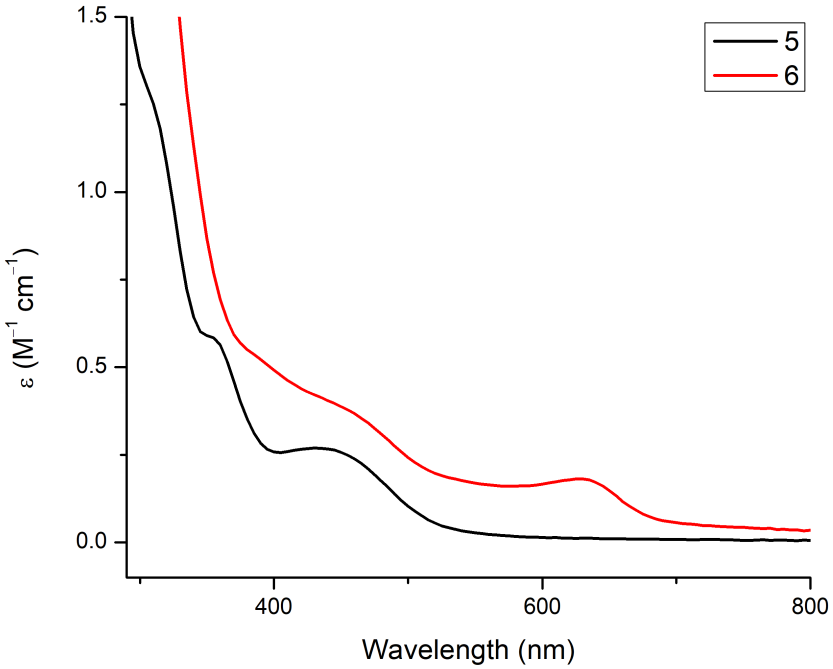

Figure S12. Electronic absorption spectra of compounds [**5**][BF_4] and [**6**][BF_4]$_5$ recorded in Acetonitrile solvent.