Supplementary Material

Synthesis and Characterization of chloridobis(dimethylglyoxamato)4-(2-ferrocenylvinyl)pyridinecobalt(III). A New Heterobinuclear Cobaloxime.

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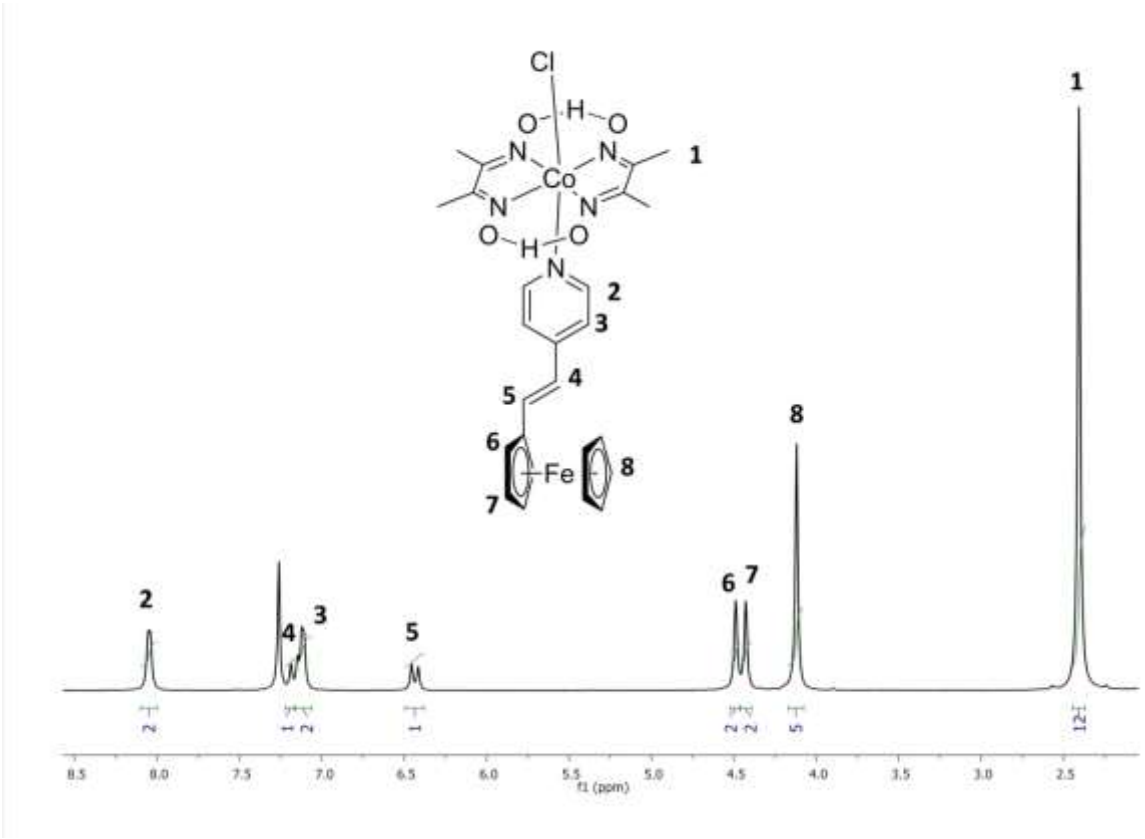


Figure S 1: ^{1}H-NMR of the complex [CoCl(dmgH)2(fcvpy)] recorded on $CDCl_3$

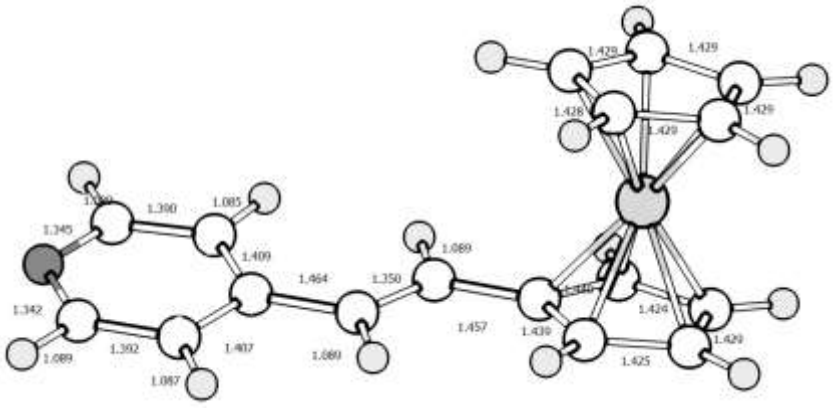


Figure S 2: Optimized geometry of the ligand fcvpy showing selected bond distances in Angstroms.

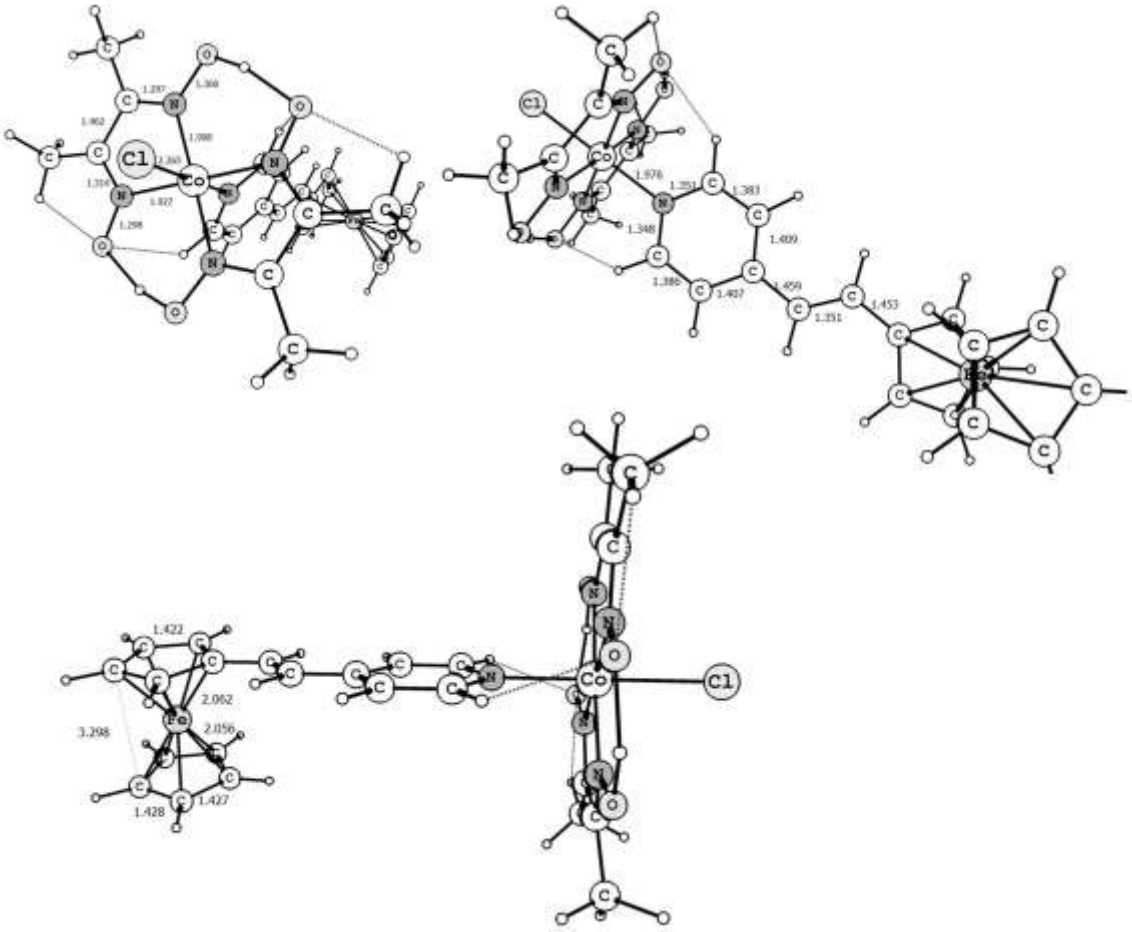


Figure S 3: Optimized geometry of the complex [CoCl(dmgH)$_2$(fcvpy)] showing selected bond distances in Angstroms.

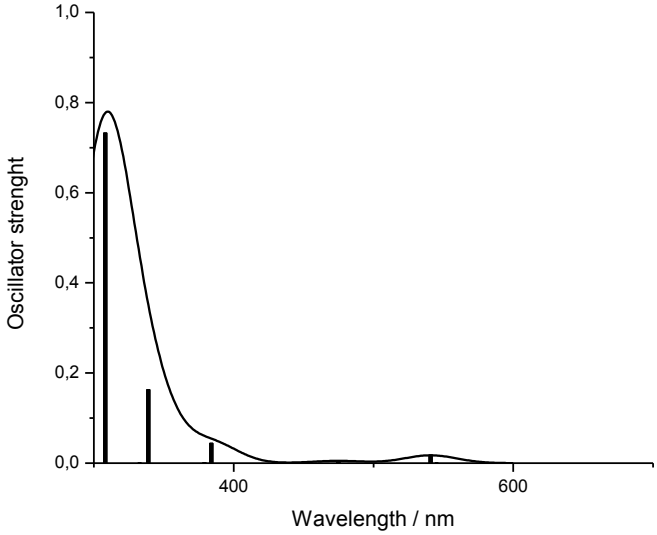


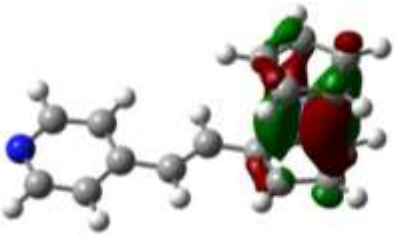
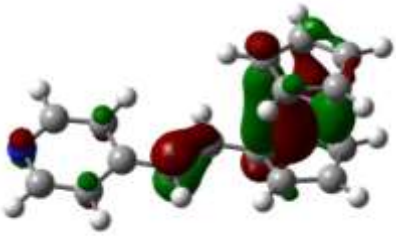
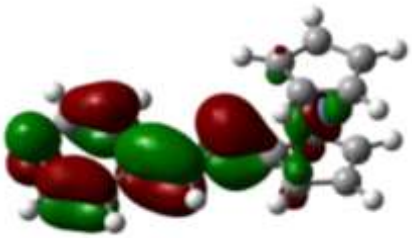
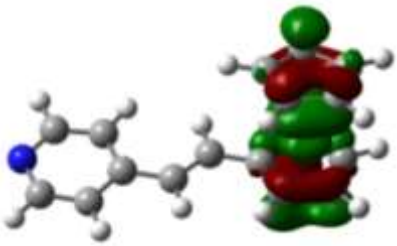
Figure S 4: Calculated UV-Vis spectra of 4-ferrocenylvinylpyridine. Band width on ½ height 42 nm

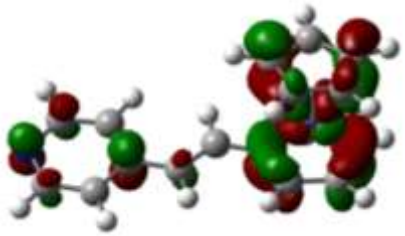
Table S1. TD-DFT Calculated Data fcvpy

λ_{calc} (nm)	E_{calc} (eV)	f_{os}	Major contributions (weight, %)
546	2.271	0.0004	H-1→L (33); H-1→L+3 (35); H→L+2 (20)
542	2.288	0.0162	H-1→L+3 (22); H→L (29); H→L+3 (36)
475	2.609	0.0047	H-3→L (17); H-3→L+3 (35); H-1→L+2 (35)
462	2.683	0.0001	H-3→L+2 (31); H→L+2 (40)
383	3.230	0.0431	H-3→L (13); H-3→L+3 (13); H-1→L+2(25); H→L (42)
378	3.275	0.0012	H-3→L+2 (28); H-1→L (51)
338	3.660	0.1535	H→L (27); H→L+3 (44)

All calculations used the 6-31G(d) basis set with the B3LYP functional. Only contributions greater than 12 % are shown. H = HOMO, L = LUMO

Table S2. Energies (hartree) and surfaces of the molecular orbitals involved in electronic transitions.

HOMO-3 -0.24690	
HOMO-1 -0.21334	
HOMO -0.20874	
LUMO -0.06746	
LUMO+2 -0.02579	

LUMO+3 -0.02012	

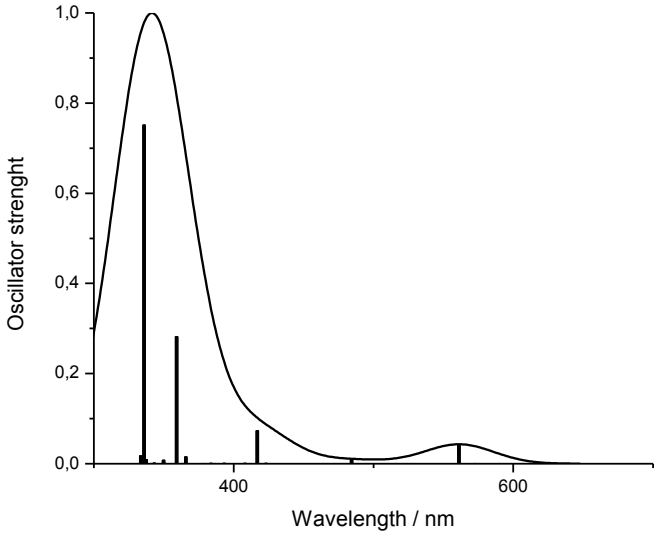


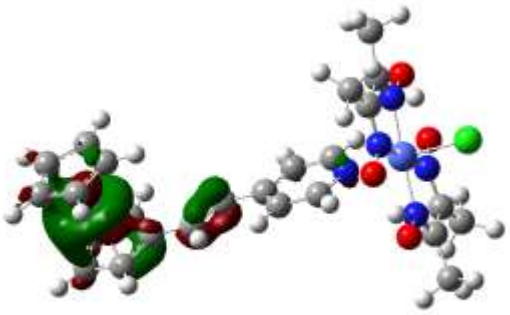
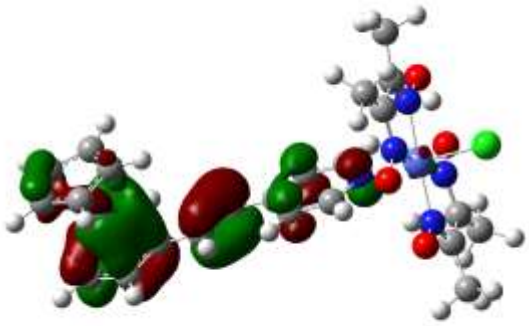
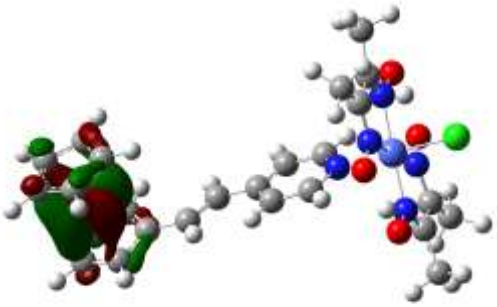
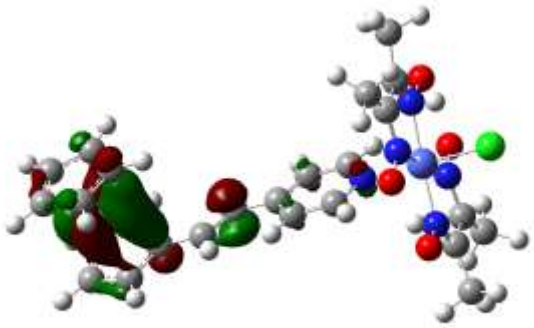
Figure S 5: Calculated UV-Vis spectra of [CoCl(dmgH)$_2$(fcvpy)].Band width on ½ height 58 nm

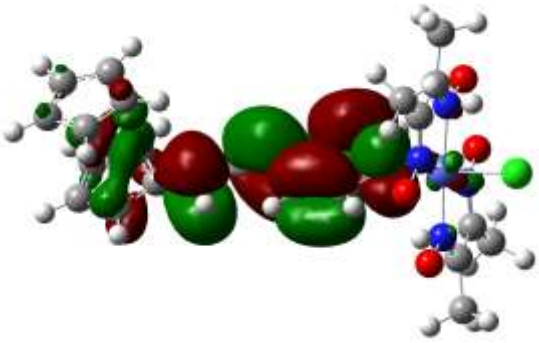
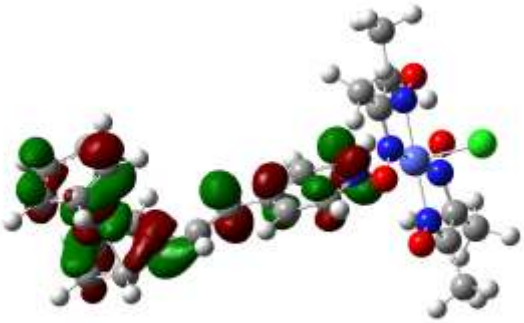
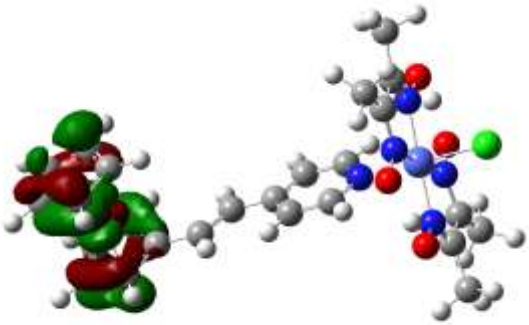
Table S3. TD-DFT Calculated Data for the cobaloxime

λ_{calc} (nm)	E_{calc} (eV)	f_{os}	Major contributions (weight, %)
561	2.210	0.0427	H-1→L+7 (21); H→L (32); H→L+6 (30)
416	2.974	0.0733	H-1→L+7 (21); H→L (45)
359	3.452	0.2819	H-4→L (23); H-1→L+7 (17); H→L (12); H→L+6 (32)
335	3.690	0.7517	H-5→L (34); H-4→L (60)

All calculations used the 6-31G(d) basis set with the B3LYP functional. Only contributions greater than 12 % are shown. H = HOMO, L = LUMO

Table S4. Energies and surfaces of the molecular orbitals involved in electronic transitions.

HOMO-5	
HOMO-4	
HOMO-1	
HOMO	

LUMO	
LUMO +6	
LUMO +7	

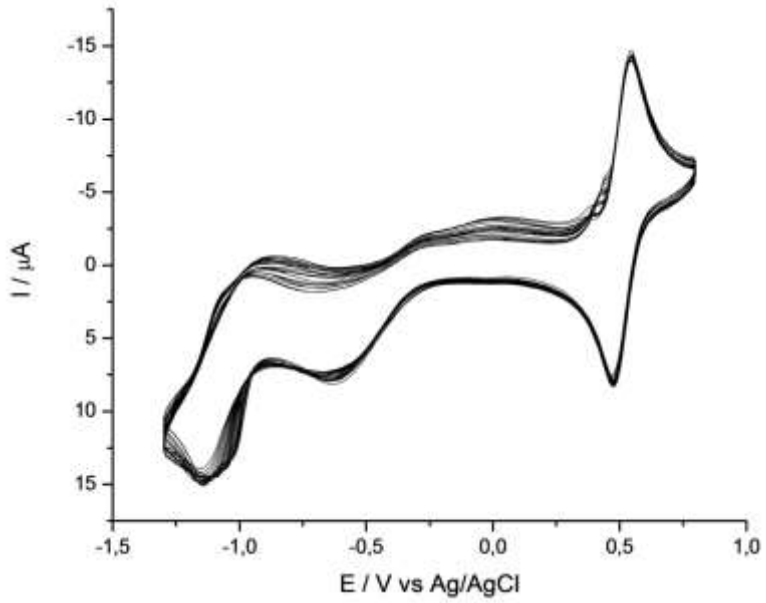


Figure S 6: Cyclic voltammogram of [CoCl(dmgH)$_2$(fcvpy)] recorded in acetonitrile solution of n-Bu4NPF6 (0.1 mol L^{-1}) on a glassy carbon electrode at 100 mVs^{-1}, 20 cycles.

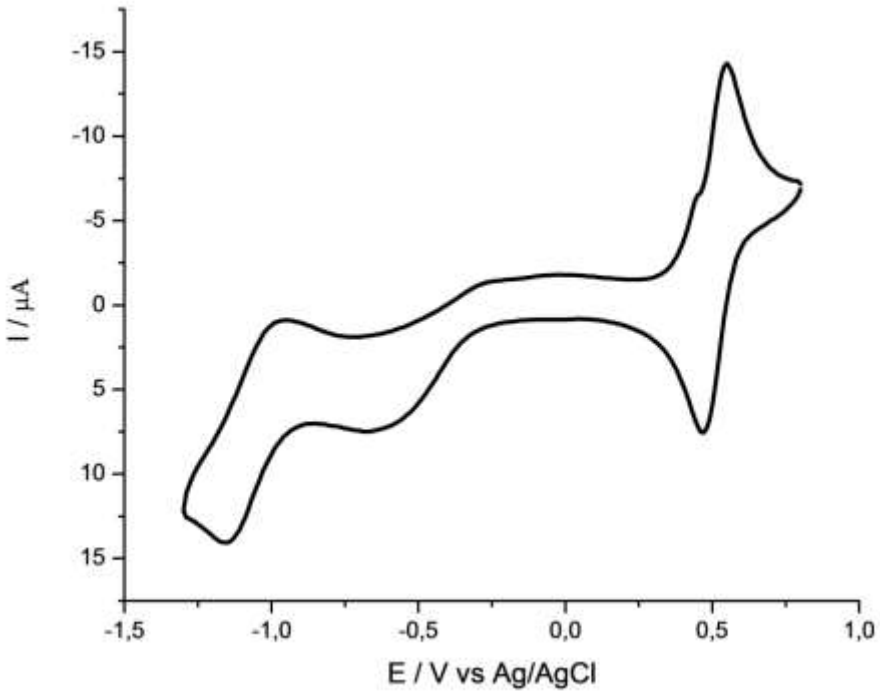


Figure S 7: Cyclic voltammogram of [CoCl(dmgH)2(fcvpy)] recorded in acetonitrile solution of n-Bu4NPF6 (0.1 mol L^{-1}) on a glassy carbon electrode at 100 mVs^{-1}. After 20 cycles.