Synchronized Motion and Electron Transfer of a Redox-active Rotor

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Electronic Supplementary Information

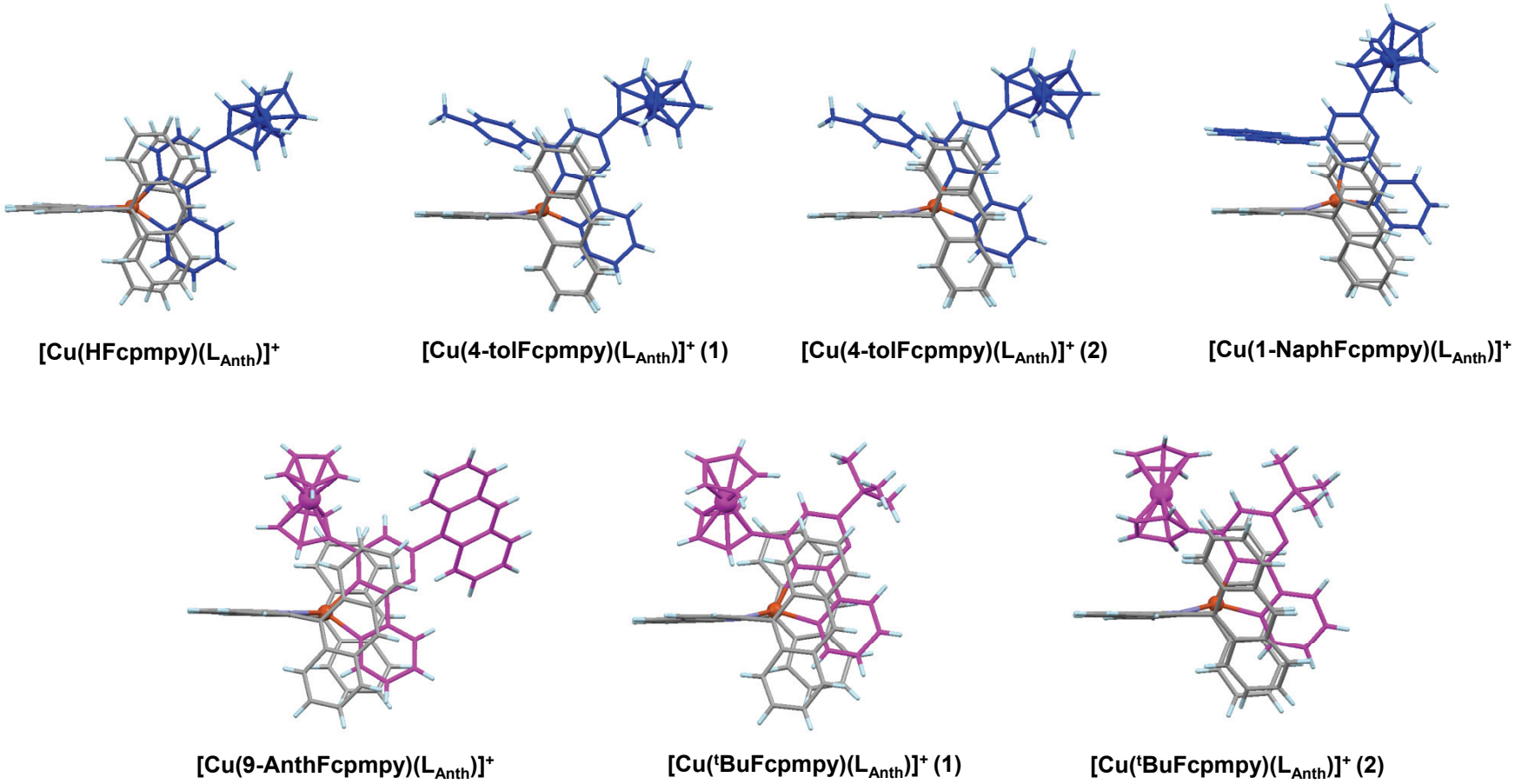

Fig. S1 Crystal structures of the [Cu(RFcpmpy)(L$_{Anth}$)]$^+$ families. Anions and solvent molecules are omitted for clarity.

Table S1 Crystallographic data for the Cu complexes.

Compound	**[Cu(HFcpmpy)(L_{Anth})]BF_4 ·(benzene)$_3$**	**[Cu(4-tolFcpmpy)(L_{Anth2})]BF_4 ·(CH_2Cl_2)$_{0.5}$ (p-xylene)$_{1.5}$**	**[Cu(1-NaphFcpmpy)(L_{Anth2})]BF_4 ·(CH_2Cl_2)$_2$**	**[Cu(9-AnthFcpmpy)(L_{Anth2})]BF_4 ·(CH_2Cl_2) (*p*-xylene)$_2$**	**[Cu(^{t}BuFcpmpy)(L_{Anth2})]BF_4 ·(CH_2Cl_2)$_{0.5}$ (*p*-xylene)**	**[Cu(Fcvipmpy)(L_{Anth2})]BF_4 ·(CH_2Cl_2) (*p*-xylene)$_{0.5}$**	**[Cu(tolvipmpy)(L_{Anth2})]BF_4 ·(benzene)$_2$**
Formula	$C_{77}H_{57}BCuF_4FeN_5$	$C_{157}H_{112}B_2Cl_2Cu_2F_8Fe_2N_{10}$	$C_{71}H_{49}BCl_4CuF_4FeN_5$	$C_{90}H_{69}BCl_2CuF_4FeN_5$	$C_{135.5}H_{109}B_2C_1Cu_2F_8Fe_2N_{10}$	$C_{66}H_{48}BCl_2CuF_4FeN_5$	$C_{70}H_{51}BCuF_4N_5$
FW	1258.48	2621.87	1320.15	1462.15	2361.23	1188.19	1112.52
Crystal system	triclinic	triclinic	monoclinic	triclinic	triclinic	triclinic	triclinic
a / Å	10.747(5)	13.539(5)	11.964(5)	11.548(5)	13.743(5)	11.667(5)	12.149(5)
b / Å	11.762(5)	19.954(5)	22.314(5)	15.399(5)	18.366(5)	14.676(5)	15.017(5)
c / Å	12.896(5)	24.387(5)	24.781(5)	22.187(5)	23.367(5)	16.178(5)	17.063(5)
α / °	75.128(5)	106.434(5)	90	71.587(5)	76.822(5)	83.368(5)	95.196(5)
β / °	70.329(5)	91.680(5)	117.169(12)	85.665(5)	77.796(5)	88.056(5)	110.753(5)
γ / °	86.267(5)	90.049(5)	90	68.815(5)	87.145(5)	75.878(5)	107.217(5)
V / Å^3	1483.2	6316(3)	5886	3487	5613(3)	2668.3(17)	2713.2(16)
Spacegroup	*P*1	*P*-1	$P2_1/c$	*P*-1	*P*-1	*P*-1	*P*-1
Z	1	2	4	2	2	2	2
data collected	11485	49331	46198	27757	44167	20915	21541
data unique	8896	27467	13459	15311	24500	11637	11918
data [$I>2\sigma(I)$]	7060	16162	11511	12639	20659	7127	6806
R_1[a]	0.052	0.1253	0.0562	0.0696	0.0646	0.0961	0.0985
wR_2[b]	0.1426	0.3105	0.1515	0.197	0.1851	0.2968	0.3087
GOF[c]	1.037	1.12	1.028	1.063	1.024	1.058	1.051

[a] $R1 = \Sigma||F^o|-|F^c||/\Sigma|F^o|$ $(I>2\sigma(I))$. [b] $wR2 = [\Sigma(w(F^{o2}-F^{c2})^2/\Sigma w(F^{o2})^2]^{1/2}$ $(I>2\sigma(I))$. [c] $GoF = [\Sigma(w(F^{o2}-F^{c2})^2/\Sigma(N^r-N^p)^2]$

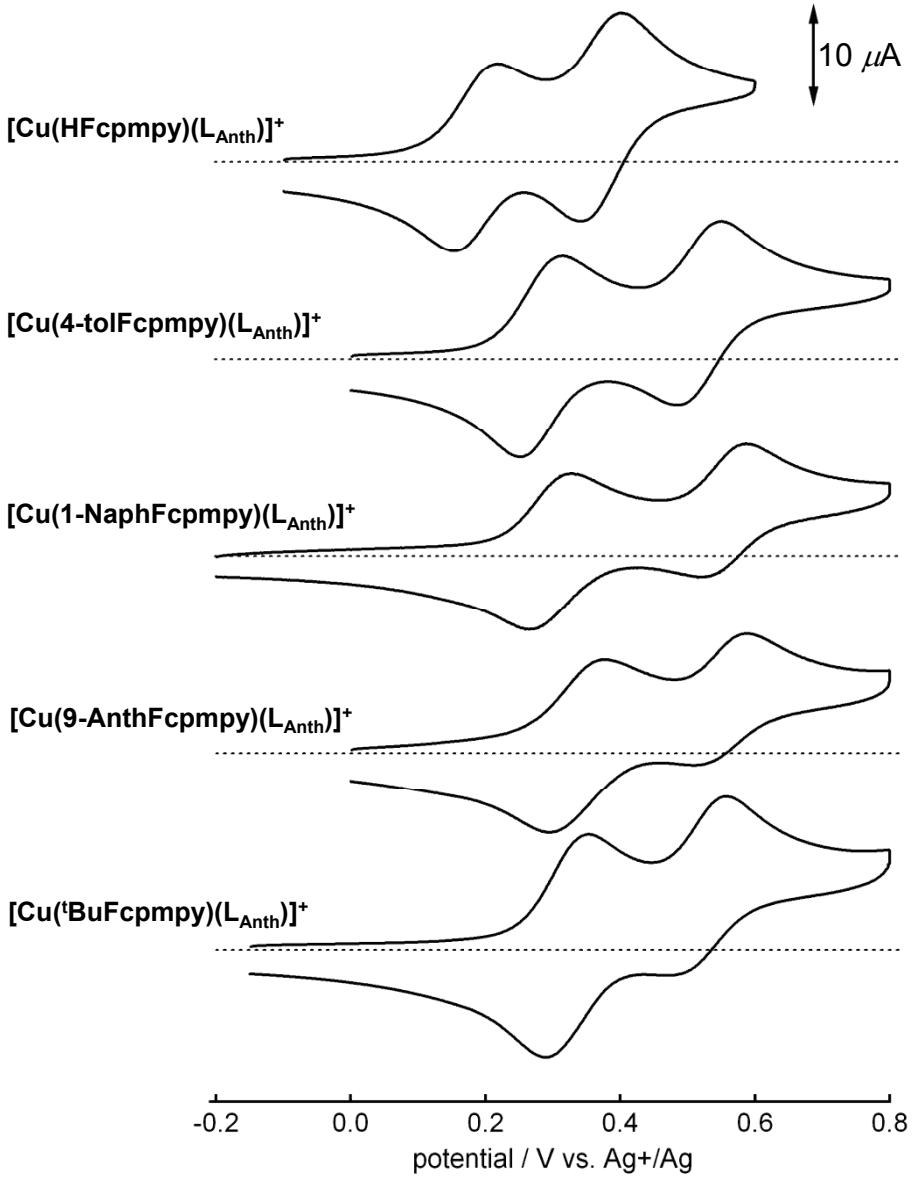

Fig. S2 Cyclic voltammograms of the [Cu(RFcpmpy)(L_{Anth})]$^+$ families recorded in 0.1 M $^nBu_4NBF_4$-acetone at room temperature. Scan rate: 25 mVs^{-1}

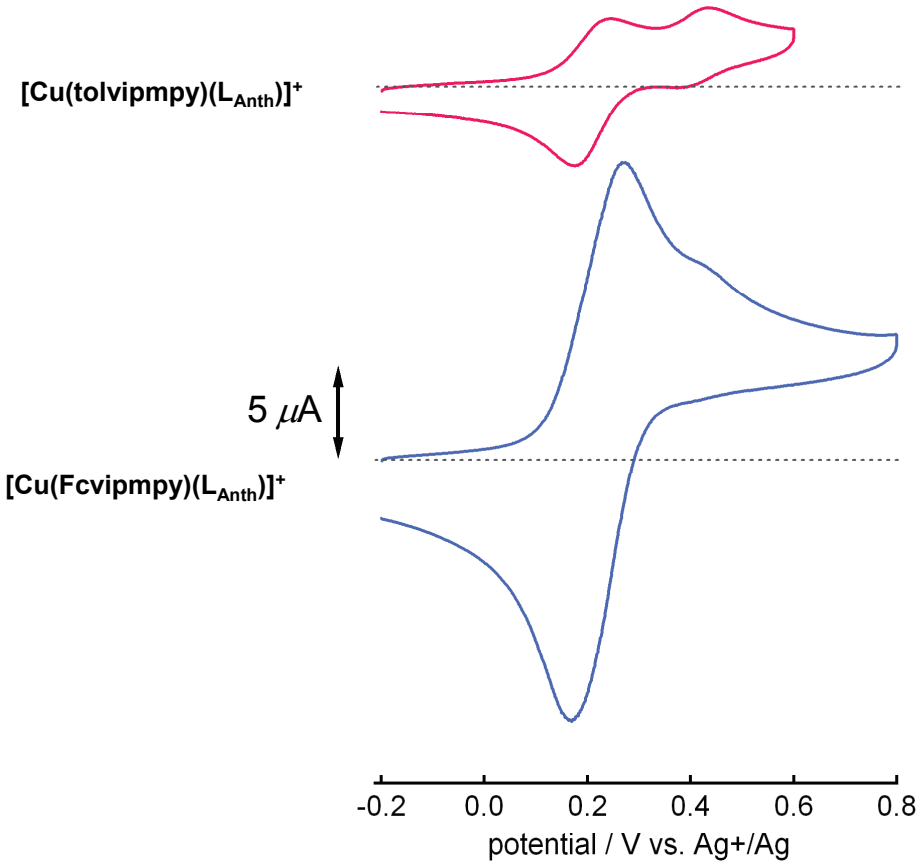

Fig. S3 Cyclic voltammograms of [Cu(Fcvipmpy)(L_{Anth})]$^+$ and [Cu(tolvipmpy)(L_{Anth})]$^+$ recorded in 0.1 M $^nBu_4NBF_4$-acetone at 298K. Scan rate: 50 mVs^{-1}

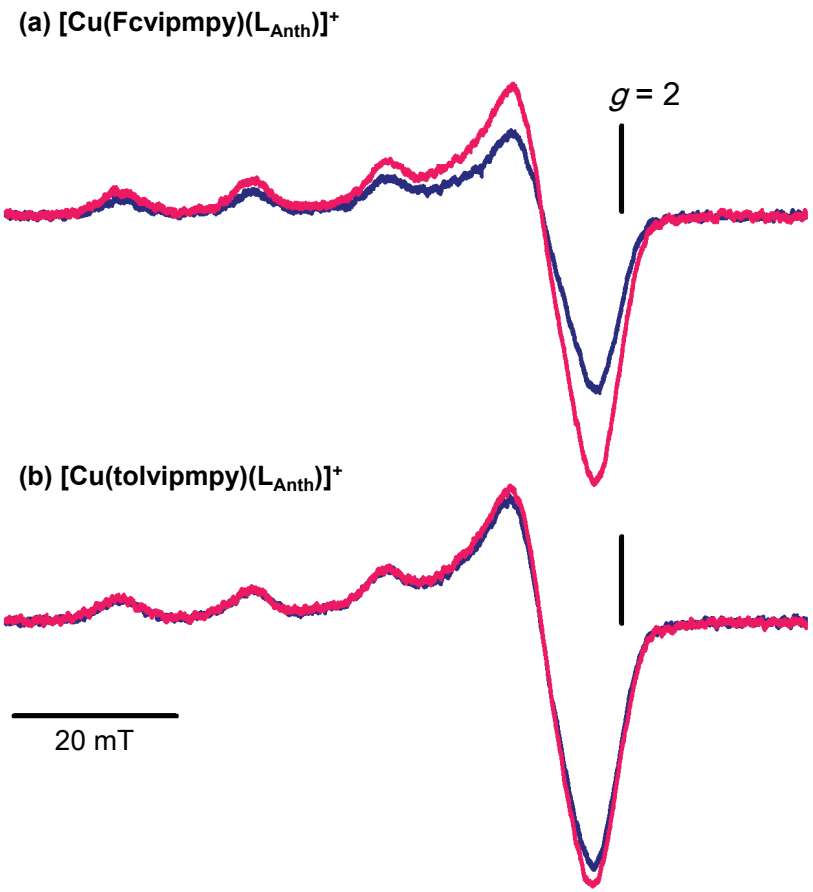

Fig.S4 EPR spectra of [Cu(Fcvipmpy)(L_{Anth})]$^+$ (a) and [Cu(tolvipmpy)(L_{Anth})]$^+$ (b) measured in acetone at 80K, after addition of 1 equiv. of $(NH_4)_2[Ce(NO_3)_6]$to a solution at 193 K (blue), and after the subsequent warming to 298K followed by cooling to 80 K(red).