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Supporting Information

Pyridine–Triazole Ligands for Copper–Catalyzed Aerobic Alcohol Oxidation

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Crystallographic Data and Structures

Table S1. Crystallographic data

	1•2H_2O	**3**	**4**
empirical formula	$C_{28}H_{20}CuF_6N_8O_6S_2$•2($H_2O$)	$C_{26}H_{18}CuF_6N_{10}O_6S_2$	$C_{22}H_{16}CuF_6N_4O_6S_2$
formula weight	842.22	808.16	674.05
T (K)	293	293	293
crystal system	orthorhombic	triclinic	monoclinic
space group	*P*cba	*P*-1	*C*2/c
a (Å)	17.9015(3)	8.6034(3)	10.0099(3)
b (Å)	9.3530(2)	9.2137(4)	13.9540(5)
c (Å)	19.7128(4)	11.0129(5)	18.8133(8)
α (deg)	90	111.653(2)	90
β (deg)	90	92.753(2)	100.1196(14)
γ (deg)	90	102.528(2)	90
V (Å^3)	3300.57(11)	784.13(6)	2586.93
Z	4	1	4
ρ_{calc} (mg m^{-3})	1.695	1.711	1.731
μ (mm^{-1})	0.885	0.925	1.096
crystal size (mm)	0.28x0.20x0.10	0.15x0.12x0.10	0.20x0.18x0.15
color, habit	green, plate	blue, block	blue, block
reflections collected	14453	8677	4368
independent reflections (R_{int})	3375 (0.055)	2708 (0.062)	1871 (0.050)
data/restraints/parameters	3373/3/248	2708/0/233	1868/0/187
goodness of fit	1.05	1.14	1.05
final R indices [I > 2σ(I)]	R_1 = 0.0574	R_1 = 0.0393	R_1 = 0.0543
	wR_2 = 0.1429	wR_2 = 0.1289	wR_2 = 0.1427
final R indices (all data)	R_1 = 0.0722	R_1 = 0.0422	R_1 = 0.0631
	wR_2 = 0.1510	wR_2 = 0.1342	wR_2 = 0.1553
largest diff. peak/hole	0.607, –0.606	0.388, –0.378	0.423, –0.742

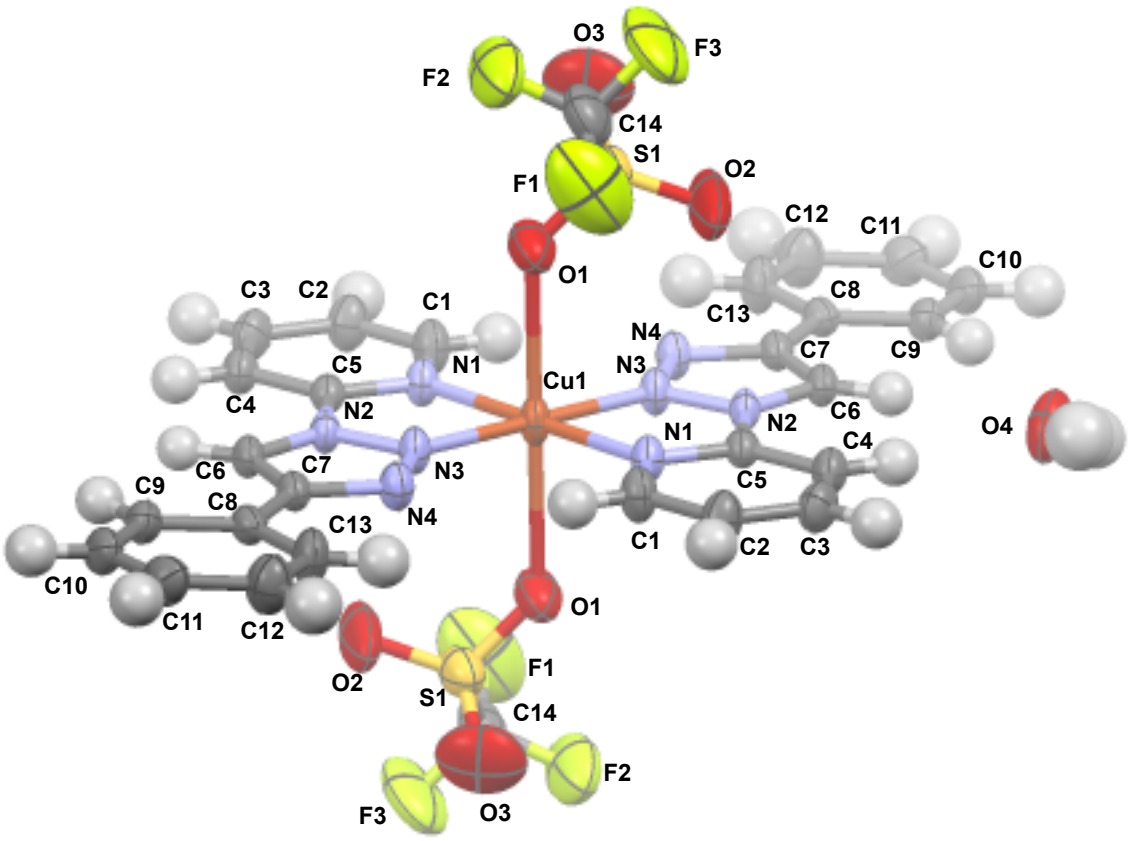


Figure S1. ORTEP diagram of **1**•2H_2O. Solvent molecules were omitted for clarity. The thermal ellipsoids were shown at the 50% probability level.

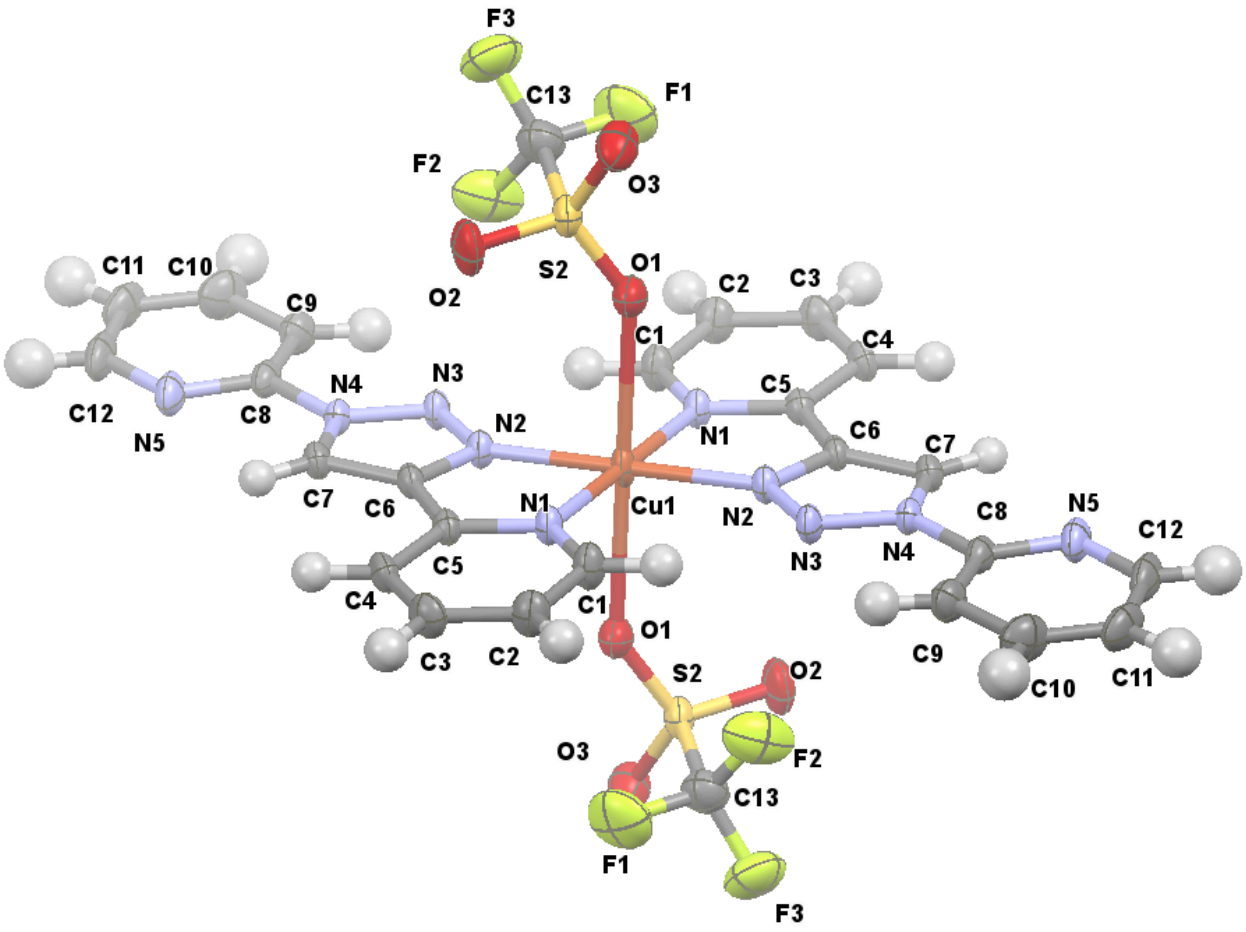


Figure S2. ORTEP diagram of **3**. The thermal ellipsoids were shown at the 50% probability level.

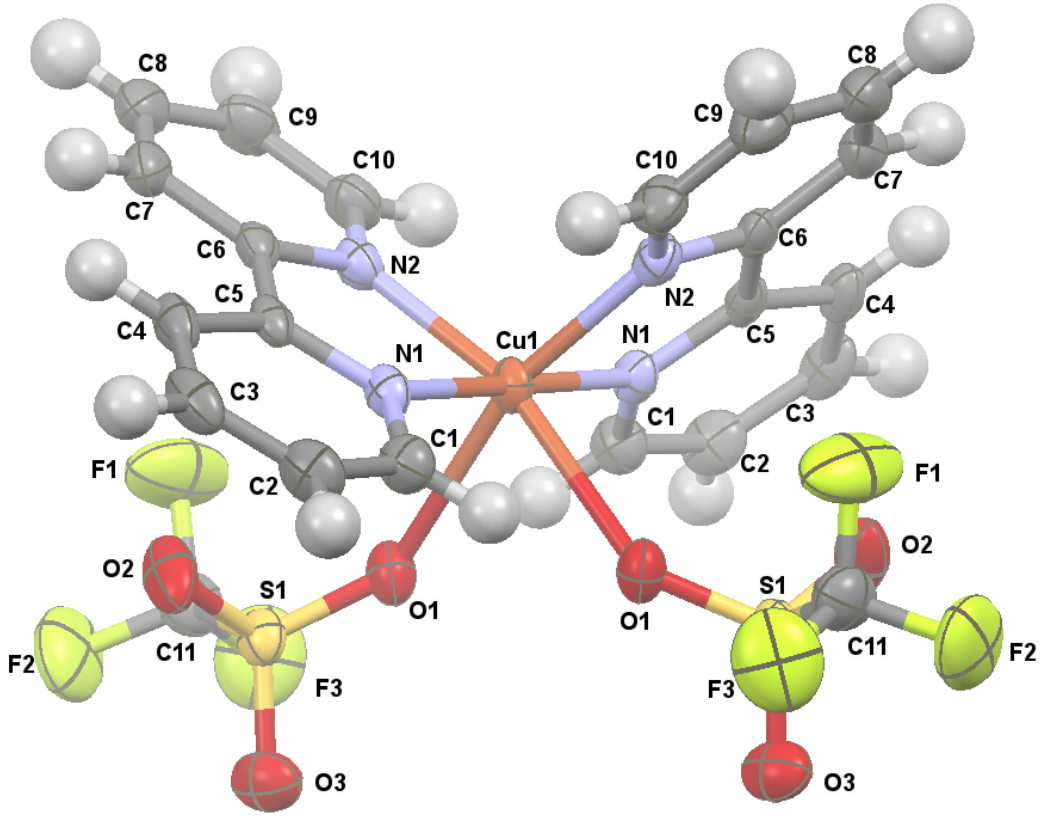
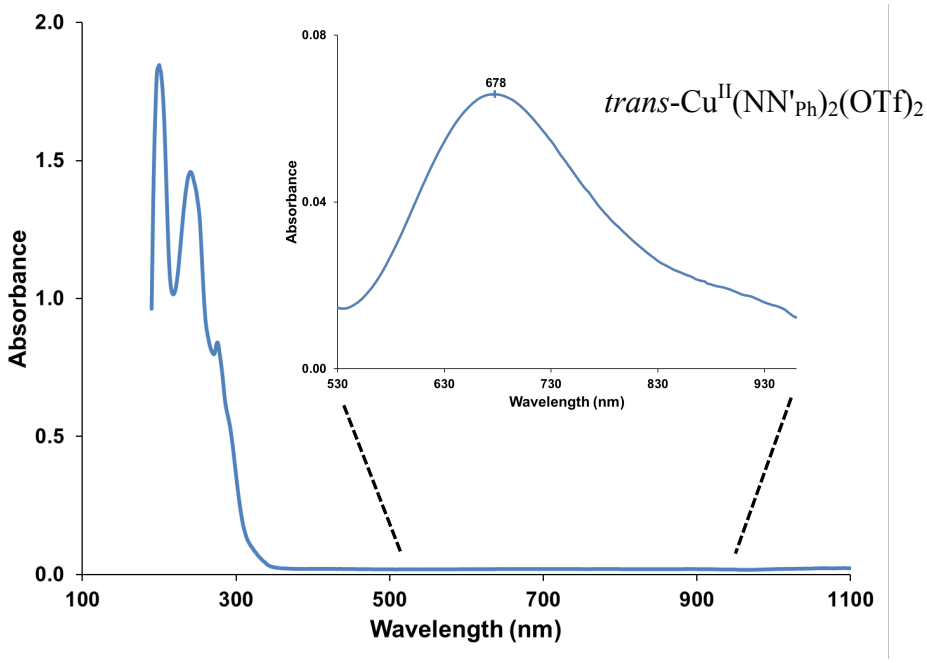


Figure S3. ORTEP diagram of **4**. The thermal ellipsoids were shown at the 50% probability level.

UV-Vis Spectra

(a)



(b)

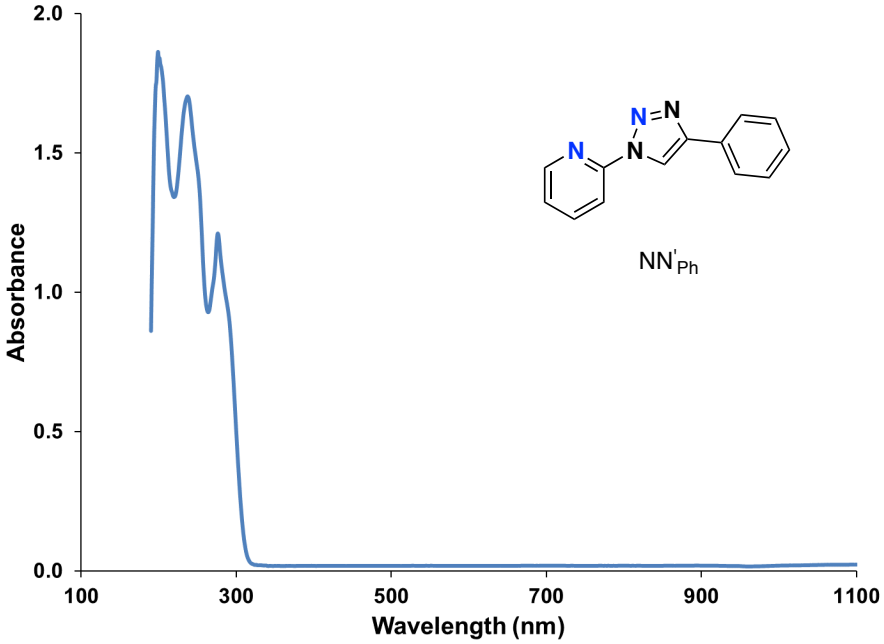
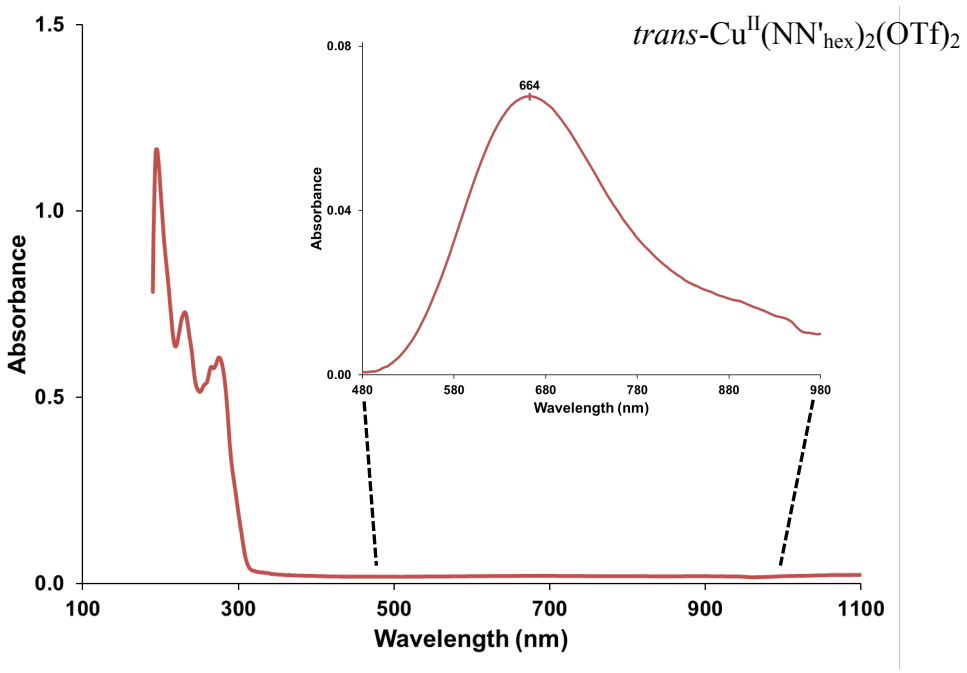


Figure S4. Electronic absorption spectra of **1** (a) and NN'_{Ph} (b).

(a)



(b)

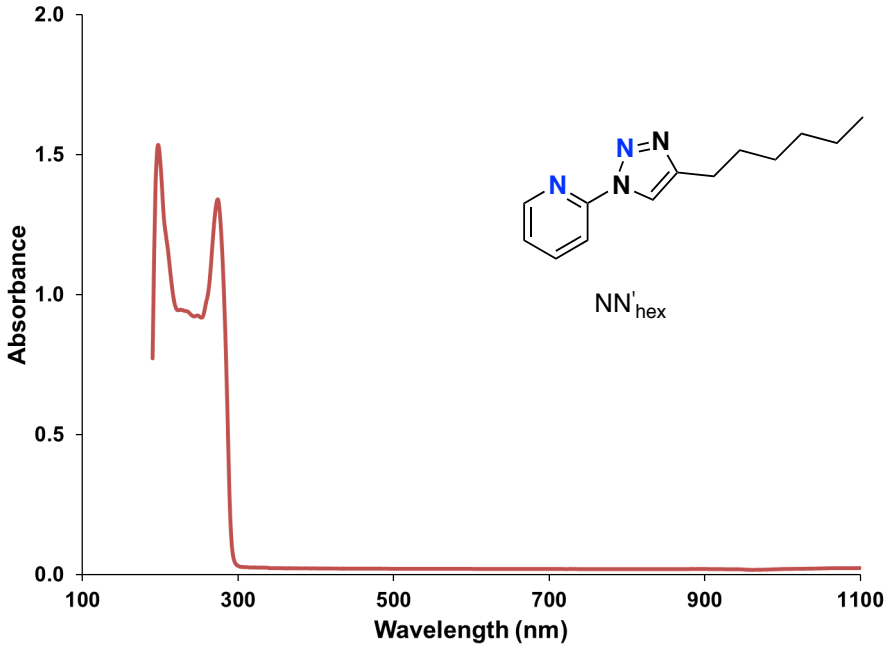
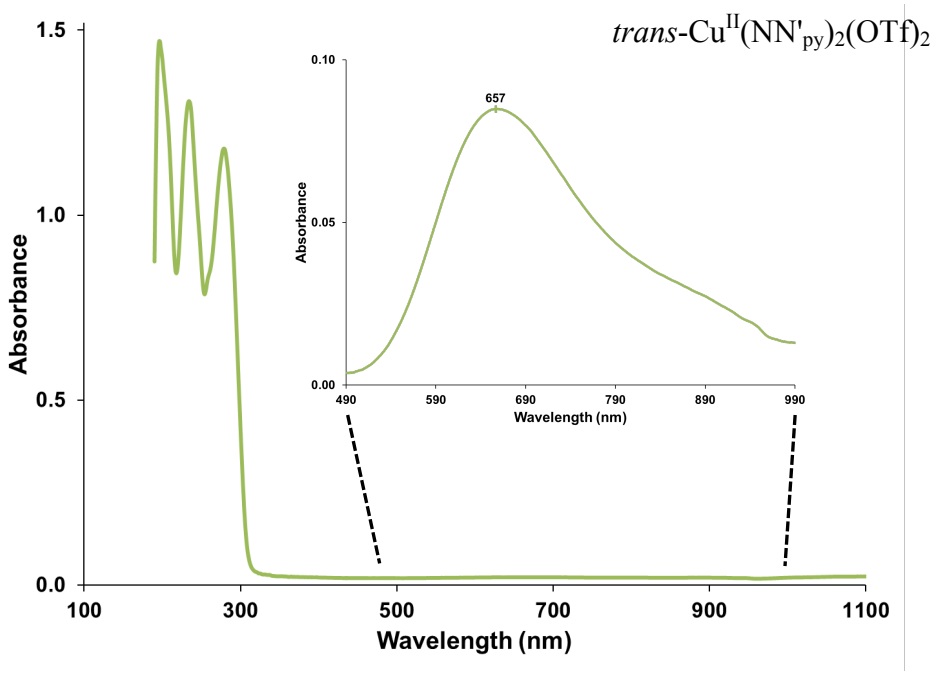


Figure S5. Electronic absorption spectra of **2** (a) and NN'_{hex} (b).

(a)



(b)

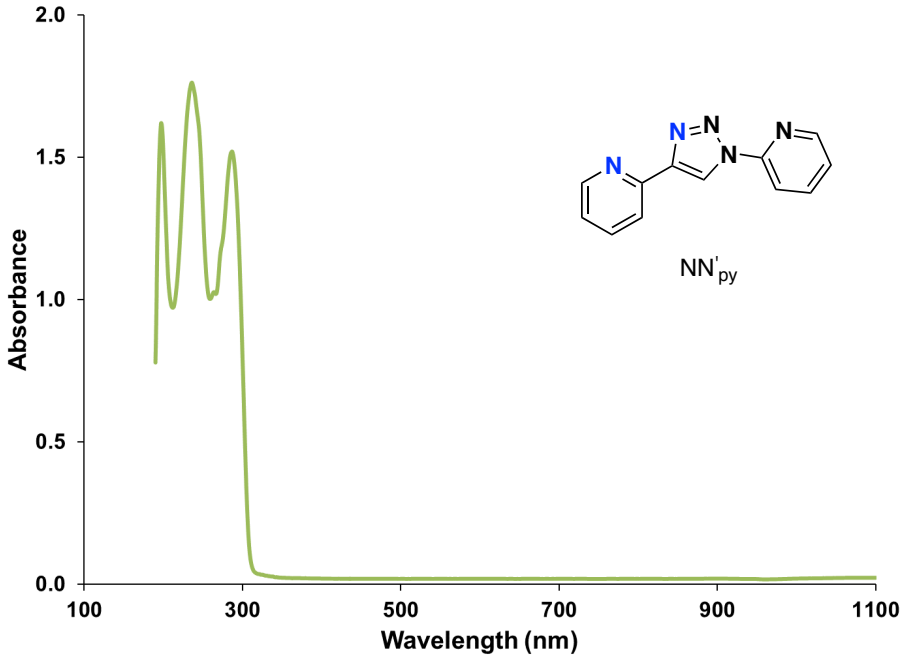
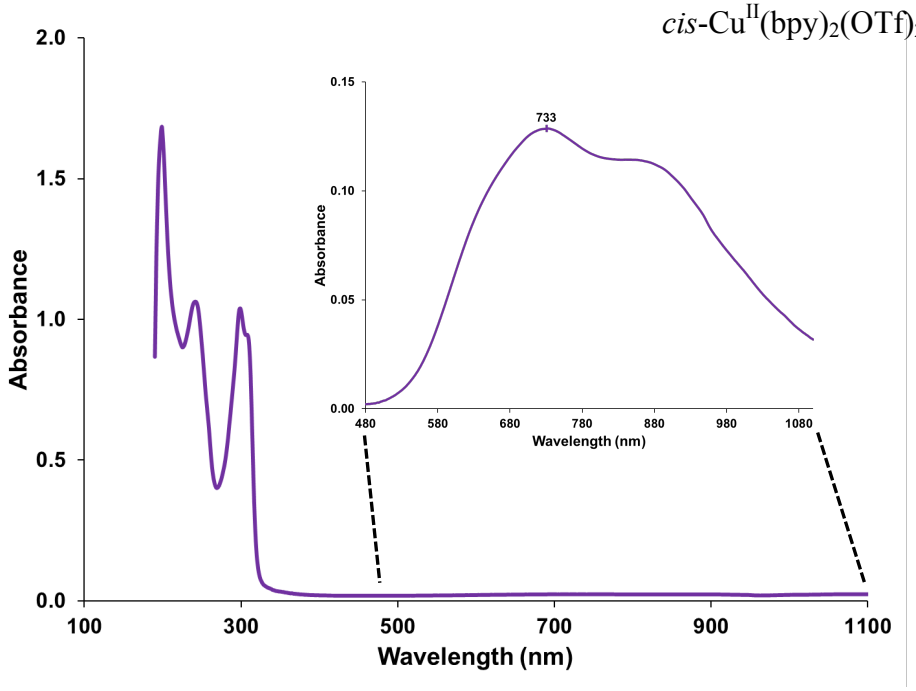


Figure S6. Electronic absorption spectra of **3** (a) and NN'_{py} (b).

(a)



(b)

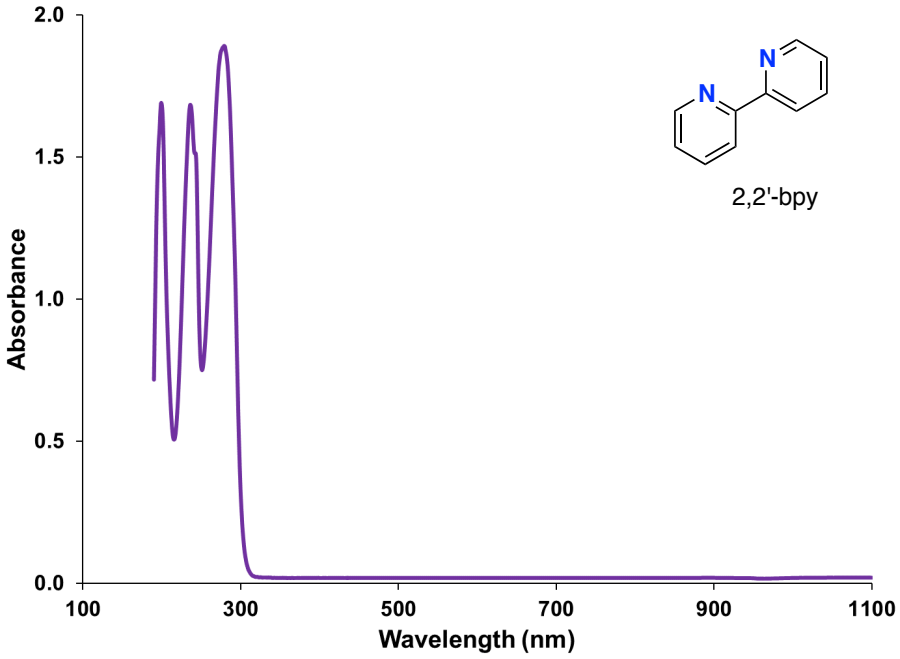


Figure S7. Electronic absorption spectra of **4** (a) and 2,2'-bpy (b).

Powder X-ray diffraction data

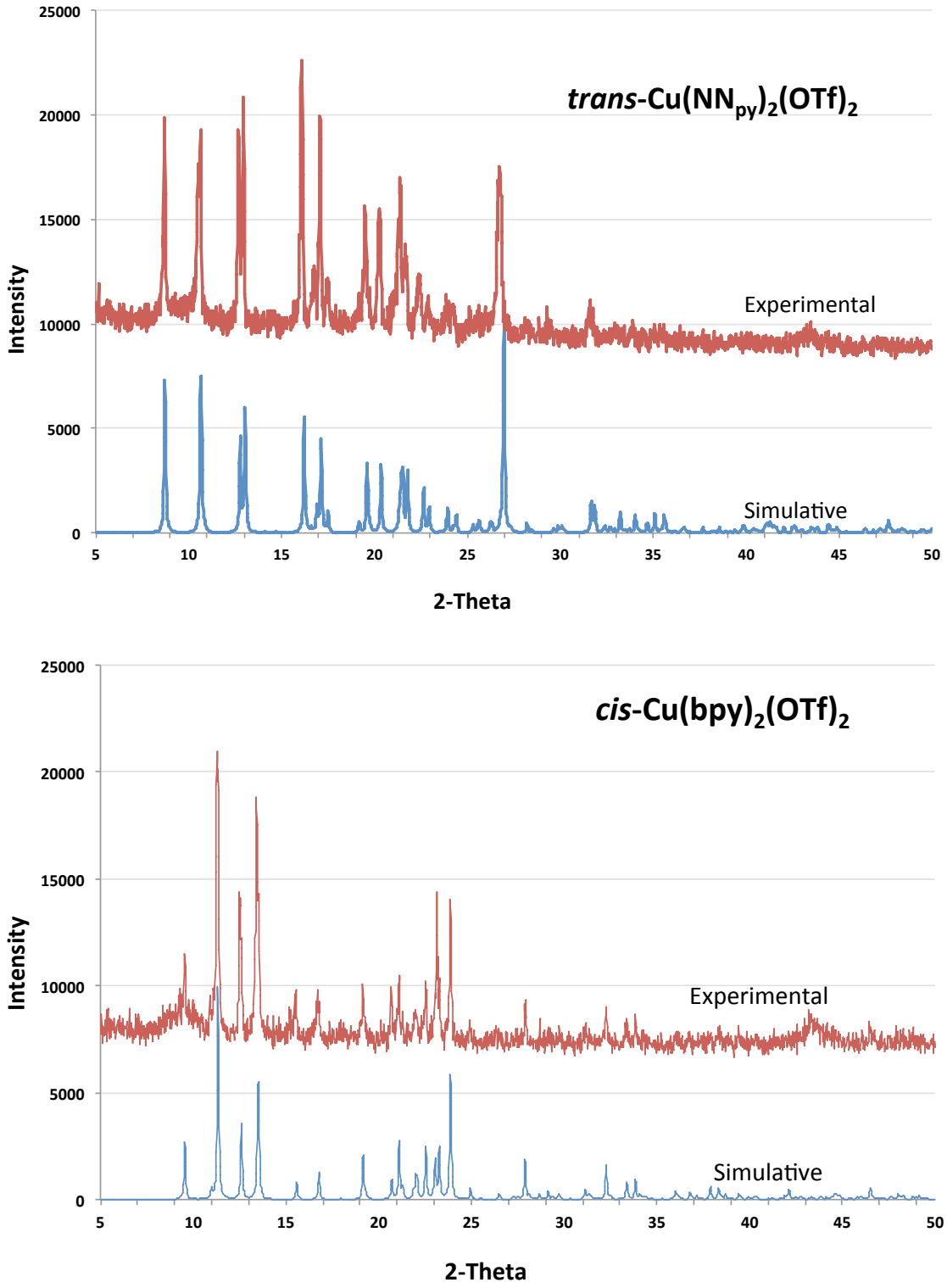
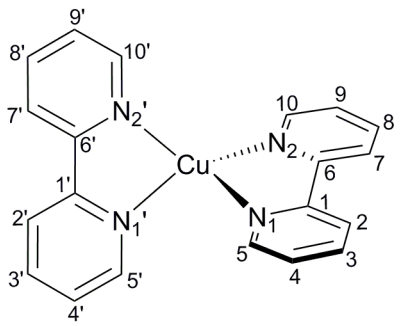


Figure S8. Powder X-ray diffraction patterns of Cu(II) complexes **3** and **4**.

DFT Calculations

Table S2. Selected geometrical parameters (bond lengths in Å and bond angles in °) of the X-ray crystal structure[a] and the calculated structure of $[Cu(bpy)_2]^+$.



$[Cu(bpy)_2]^+$

	$Cu[(bpy)_2]^+$	
	Calculation	X-ray[a]
Cu-N1	2.073	2.020(9)
Cu-N2	2.073	2.021(11)
C1-C6	1.490	1.440(15)
C1-N1	1.354	1.325(14)
C6-N2	1.354	1.385(15)
N1-Cu-N1'	125.9	127.1(4)
N1-Cu-N2	80.1	81.5(4)
N1-Cu-N2'	125.9	131.3(4)
N2-Cu-N2'	125.8	109.7(4)
C6-C1-N1	115.8	115.9(9)
C1-C6-N2	115.8	116.5(9)
Cu-N1-C1	114.2	114.2(8)
Cu-N1-C5	126.7	127.3(8)

[a]Munakata, M.; Kitagawa, S.; Asahara, A.; Masuda, H. *Bull. Chem. Soc. Jpn* **1987**, *60* , 1927-1929.

Full Gaussian 09 citation: Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, 2010.