Supporting Information

Copper(I) Heteroleptic bis(NHC) and NHC/ Phosphine Complexes: Syntheses and Catalytic Activities in the One-Pot Sequential CuAAC Reaction of Aromatic Amines

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Table SI-1. Selected X-ray Crystallographic Data for Complexes **2**, **3**, **4**·$CHCl_3$, **5**, **6**, and **7**·$0.75CHCl_3$·$0.25C_4H_{10}O$.

Comp.	**2**	**3**	**4**·$CHCl_3$	**5**	**6**	**7**·$0.75CHCl_3$·$0.25C_4H_{10}$
Formula	$C_{44}H_{52}CuF_6N_4P$	$C_{40}H_{54}CuF_6N_4P$	$C_{39}H_{49}Cl_3CuF_6N_4$	$C_{45}H_{51}CuF_6N_2P_2$	$C_{53}H_{60}CuF_6N_2P_3$	$C_{62.75}H_{67.25}Cl_{2.25}CuF_6FeP$
Formula weight	845.41	799.38	888.68	859.36	995.48	1259.50
Crystal size [mm]	0.28 × 0.26 × 0.13	0.24 × 0.22 × 0.02	0.56 × 0.21 × 0.20	0.19 × 0.15 × 0.13	0.56 × 0.26 × 0.10	0.28 × 0.14 × 0.08
Temperature [K]	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Crystal system	Tetragonal	Monoclinic	Monoclinic	Tetragonal	Monoclinic	Monoclinic
Space group	P4(3)2(1)2	Pc	P2(1)/c	P4(3)	P2(1)/n	P2(1)/n
a [Å]	11.7715(6)	9.566(10)	9.2075(12)	11.8195(17)	25.5858(11)	12.517(2)
b [Å]	11.7715(6)	13.125(14)	24.347(3)	11.8195(17)	15.3973(7)	23.360(4)
c [Å]	29.608(3)	16.287(17)	18.989(2)	30.481(9)	25.8328(12)	20.715(4)
α [°]	90	90	90	90	90	90
β [°]	90	96.61(4)	98.763(3)	90	94.3970(10)	91.851(6)
γ [°]	90	90	90	90	90	90
V [$Å^3$]	4102.8(5)	2031(4)	4207.1(9)	4258.3(15)	10146.9(8)	6054.0(19)
Z	4	2	4	4	8	4
D_c [$g·cm^{-3}$]	1.369	1.307	1.403	1.340	1.303	1.382
μ [mm^{-1}]	0.635	0.637	0.807	0.648	0.548	0.829
θ range [°]	1.86□27.50	2.00□27.46	1.37□25.00	1.72□24.99	1.08□25.00	1.74□27.50
no. of unique data	29535	14103	25288	23346	58256	43113
max, min	0.9220, 0.8422	0.5629, 0.4416	0.7456, 0.6294	0.9205, 0.8868	0.9439, 0.7357	0.8621, 0.6691
Final R indices	R_1 = 0.0413,	R_1 = 0.0750,	R_1 = 0.0780,	R_1 = 0.0975,	R_1 = 0.0618,	R_1 = 0.0589,
(I > 2σ(I))	wR_2 = 0.1097	wR_2 = 0.1666	wR_2 = 0.2092	wR_2 = 0.1979	wR_2 = 0.1294	wR_2 = 0.1111
R indices	R_1 = 0.0533,	R_1 = 0.1191,	R_1 =0.0939,	R_1 = 0.1335,	R_1 = 0.0920,	R_1 = 0.1110,
(all data)	wR_2 = 0.1197	wR_2 = 0.1983	wR_2 = 0.2214	wR_2 = 0.2113	wR_2 = 0.1464	wR_2 = 0.1281
goodness of fit on	1.089	0.988	1.085	1.129	1.054	0.955
Peak/hole [$e·Å^{-3}$]	0.546 / -0.458	0.610 / -0.482	2.292/ -0.983	0.578 / -0.756	1.033 / -0.551	0.741 / -0.352