Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Synthesis, Structural Characterization and Luminescent Properties of A Series of Cu(I) Complexes Based on Polyphosphine Ligands

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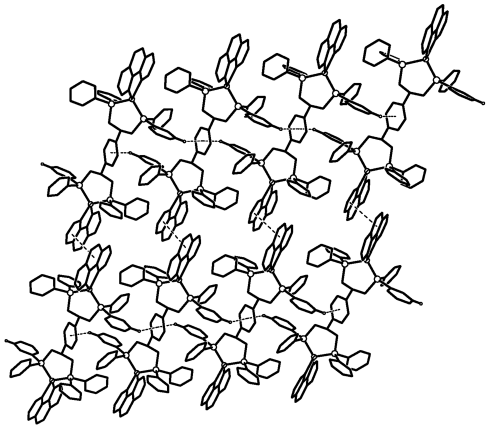

Fig. S1 showing 2-D supramolecular structure of **2a** constructed by intermolecular π···π interactions between phen planes and C-H···π interactions between arene amine rings and phenyl H atoms.

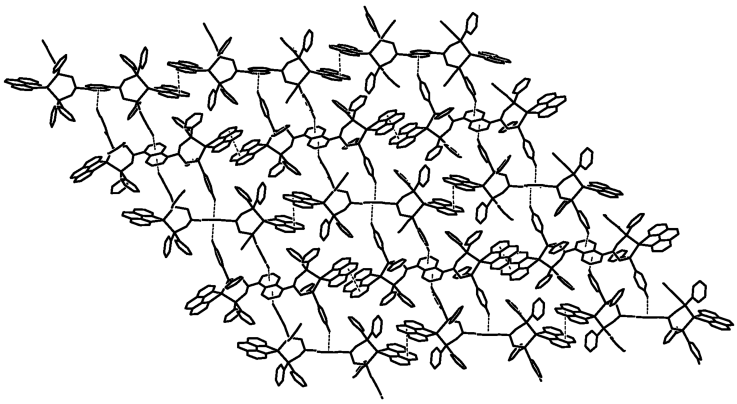

Fig. S2 showing 2-D supramolecular structure of **3a** constructed by intermolecular C-H···π interactions between arene amine rings and phenyl H atoms.

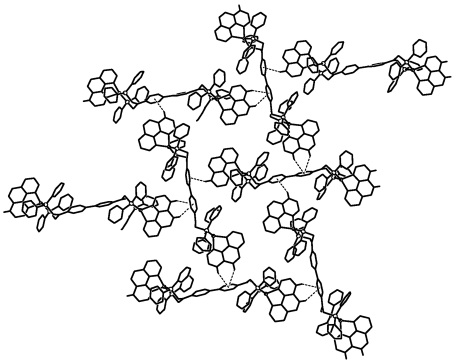

Fig. S3 showing 2-D supramolecular structure of **4a** constructed by intermolecular T-shaped C-H···π interactions between arene amine rings and H atoms on phen.

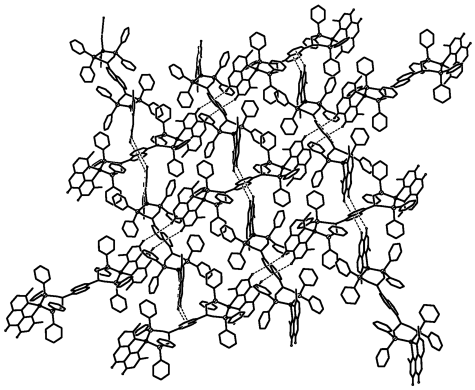

Fig. S4 showing 2-D supramolecular structure of **3b** constructed by intermolecular T-shaped C-H···π interactions between arene amine rings and H atoms on dmp.

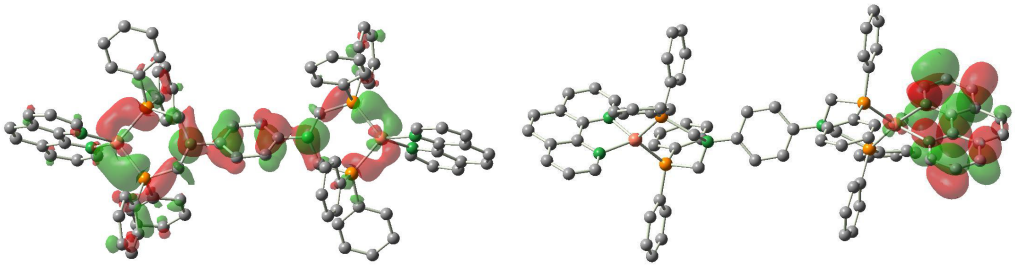

Fig. S5 Contour plots of the HOMO (the left) and LUMO (the right) of **2a**

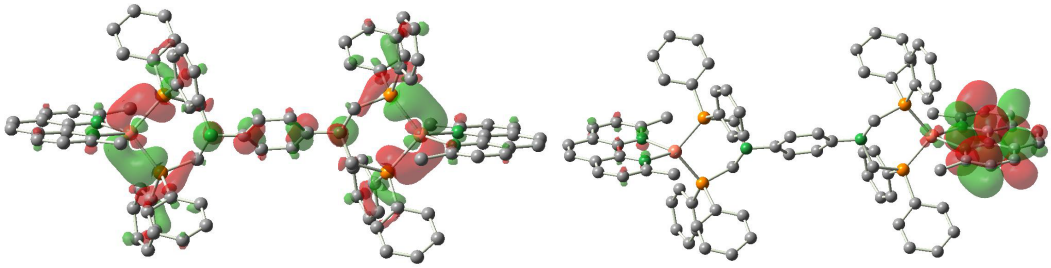

Fig. S6 Contour plots of the HOMO (the left) and LUMO (the right) of **2b**

Table S1. Selected bond Lengths (Å) and angles (°) for complexes 1a, 1b, 2a, 2b, 3a, 3b, 4a and 4b

		1a	
Cu(1)-N(2)	2.060(3)	Cu(1)-N(3)	2.077(3)
Cu(1)-P(1)	2.2404(11)	Cu(1)-P(2)	2.2474(10
N(2)-Cu(1)-N(3)	80.95(11)	N(2)-Cu(1)-P(1)	118.03(8)
N(3)-Cu(1)-P(1)	109.91(8)	N(2)-Cu(1)-P(2)	125.85(8)
N(3)-Cu(1)-P(2)	114.03(8)	P(1)-Cu(1)-P(2)	105.36(3)
		1b	
Cu(1)-N(3)	2.046(3)	Cu(1)-N(2)	2.076(3)
Cu(1)-P(1)	2.2368(9)	Cu(1)-P(2)	2.2382(9
N(3)-Cu(1)-N(2)	81.68(12)	N(3)-Cu(1)-P(1)	121.65(8)
N(2)-Cu(1)-P(1)	121.30(8)	N(3)-Cu(1)-P(2)	115.61(8)
N(2)-Cu(1)-P(2)	117.16(8)	P(1)-Cu(1)-P(2)	100.39(4)
		2a	
Cu(1)-N(4)	2.055(2)	Cu(1)-N(3)	2.068(2)
Cu(1)-P(2)	2.2273(8)	Cu(1)-P(1)	2.2482(7)
Cu(2)-N(5)	2.034(2)	Cu(2)-N(6)	2.047(2)
Cu(2)-P(4)	2.2235(8)	Cu(2)-P(3)	2.2306(7)
N(4)-Cu(1)-N(3)	81.47(9)	N(4)-Cu(1)-P(2)	124.06(7)
N(3)-Cu(1)-P(2)	119.84(7)	N(4)-Cu(1)-P(1)	109.12(6)
N(3)-Cu(1)-P(1)	120.82(7)	P(2)-Cu(1)-P(1)	101.89(3)
N(5)-Cu(2)-N(6)	82.48(10)	N(5)-Cu(2)-P(4)	127.08(7)
N(6)-Cu(2)-P(4)	113.41(7)	N(5)-Cu(2)-P(3)	113.76(7)
N(6)-Cu(2)-P(3)	117.39(7)	P(4)-Cu(2)-P(3)	102.85(3)
		2b	
Cu(1)-N(3)	2.046(5)	Cu(1)-N(2)	2.080(5)
Cu(1)-P(1)	2.2435(18)	Cu(1)-P(2)	2.2440(17)
N(3)-Cu(1)-N(2)	81.6(2)	N(3)-Cu(1)-P(1)	120.12(15)
N(2)-Cu(1)-P(1)	112.39(14)	N(3)-Cu(1)-P(2)	122.55(14)
N(2)-Cu(1)-P(2)	118.14(14)	P(1)-Cu(1)-P(2)	101.90(6
		3a	
Cu(1)-N(2)	2.054(4)	Cu(1)-N(3)	2.071(4)
Cu(1)-P(2)	2.2266(13)	Cu(1)-P(1)	2.2512(13)
N(2)-Cu(1)-N(3)	81.66(16)	N(2)-Cu(1)-P(2)	118.27(11)
N(3)-Cu(1)-P(2)	125.41(12)	N(2)-Cu(1)-P(1)	110.67(11)
N(3)-Cu(1)-P(1)	119.22(12)	P(2)-Cu(1)-P(1)	101.16(5

3b

Cu(1)-N(3)	2.057(5)	Cu(1)-N(2)	2.071(6)
Cu(1)-P(2)	2.2257(17)	Cu(1)-P(1)	2.2472(18)
N(3)-Cu(1)-N(2)	81.9(2)	N(3)-Cu(1)-P(2)	120.71(16)
N(2)-Cu(1)-P(2)	119.89(15)	N(3)-Cu(1)-P(1)	107.71(14)
N(2)-Cu(1)-P(1)	121.33(15)	P(2)-Cu(1)-P(1)	104.41(7)

4a

Cu(1)-N(3)	2.049(2)	Cu(1)-N(4)	2.052(2)
Cu(1)-P(2)	2.2120(9)	Cu(1)-P(1)	2.2347(9)
Cu(2)-N(6)	2.042(3)	Cu(2)-N(5)	2.055(2)
Cu(2)-P(3)	2.2281(9)	Cu(2)-P(4)	2.2284(9)
N(3)-Cu(1)-N(4)	82.29(10)	N(3)-Cu(1)-P(2)	112.22(8)
N(4)-Cu(1)-P(2)	122.94(8)	N(3)-Cu(1)-P(1)	108.22(8)
N(4)-Cu(1)-P(1)	120.62(7)	P(2)-Cu(1)-P(1)	106.90(3)
N(6)-Cu(2)-N(5)	82.26(11)	N(6)-Cu(2)-P(3)	123.13(8)
N(5)-Cu(2)-P(3)	109.53(8)	N(6)-Cu(2)-P(4)	120.61(9)
N(5)-Cu(2)-P(4)	110.53(7)	P(3)-Cu(2)-P(4)	107.00(3)

4b

Cu(1)-N(3)	2.072(3)	Cu(1)-N(4)	2.089(3)
Cu(1)-P(1)	2.2445(11)	Cu(1)-P(2)	2.2647(11)
Cu(2)-N(5)	2.072(5)	Cu(2)-N(6)	2.111(5)
Cu(2)-P(3)	2.2550(14)	Cu(2)-P(4)	2.2617(14)
N(3)-Cu(1)-N(4)	80.40(12)	N(3)-Cu(1)-P(1)	126.15(10)
N(4)-Cu(1)-P(1)	121.66(10)	N(3)-Cu(1)-P(2)	119.24(10)
N(4)-Cu(1)-P(2)	104.22(9)	P(1)-Cu(1)-P(2)	102.93(4)
N(5)-Cu(2)-N(6)	81.5(3)	N(5)-Cu(2)-P(3)	122.27(15)
N(6)-Cu(2)-P(3)	112.00(15)	N(5)-Cu(2)-P(4)	122.08(15)
N(6)-Cu(2)-P(4)	111.56(15)	P(3)-Cu(2)-P(4)	104.97(5)

Table S2. Crystal and structure refinement data of complexes

	1a	**1b**	**2a**	**2b**	**3a**	**3b**	**4a**	**4b**
formula	$C_{44}H_{37}N_3BF_4P_2Cu$	$C_{46}H_{41}N_3BF_4P_2Cu$	$C_{82}H_{68}N_6B_2F_8P_4Cu_2$	$C_{86}H_{76}N_6F_8P_4B_2Cu_2$	$C_{100}H_{86}B_2N_6F_8P_4Cu_2$	$C_{104}H_{94}N_6B_2F_8P_4Cu_2$	$C_{90}H_{75}N_7B_2F_8P_4Cu_2$	$C_{92}H_{80}N_6O_2B_2F_8P_4Cu_2$
fw	820.06	848.11	1562.00	1618.11	1796.33	1852.43	1679.15	1726.20
a (Å)	11.715(3)	14.871(3)	9.4138(3)	9.469(3)	15.1247(6)	12.7492(5)	21.227(2)	26.3858(4)
b (Å)	12.682(4)	4.472(3)	18.5980(7)	20.695(5)	17.5097(6)	17.7212(6)	23.148(3)	16.0439(3)
c (Å)	13.797(3)	19.411(4)	22.5631(8)	20.233(5)	18.4113(6)	21.2195(7)A	16.976(2)	19.7920(3)
α (°)	87.688(2)	90	72.718(3)	90	68.401(3)	90	90	
β (°)	73.678(2)	99.221(3	89.843(3)	100.396(6)	76.139(3)	100.035(4)	103.134(2)	92.402(2)
γ (°)	88.855(3)	90	85.223(3)	90	87.182(3)	90	90	90
V (Å^3)	1965.6(8)	4123.5(13)	3757.9(2)	3899.6(18)	4397.3(3)	4720.8(3) A^3	8123.2(16)	8371.2(2)
Z	2	4	2	2	2	2	4	4
space group	P-1	P 2_1/n	P-1	P 2_1/c	P -1	P 2_1/n	P 2_1/c	P 2_1/c
T (K)	296(2)	296(2)	150 (2)	173(2)	150(2)	150	173(2)	150(2)
λ(Å)	0.71073	0.71073	1.54180	0.71073	1.54180	1.54184	0.71073	1.54180
D_{calcd}(g cm^{-1})	1.386	1.366	1.380	1.378	1.357	1.303	1.373	1.370
R_1 (I >2σ (I))	0.0504	0.0503	0.0408	0.0636	0.0708	0.0756	0.0473	0.0671
wR_2(I>2σ (I)	0.1464	0.1516	0.0996	0.1326	0.2128	0.2163	0.1335	0.1943