

Rational Design of Strongly Blue-emitting Cuprous Complexes with Thermally Activated Delayed Fluorescence and Application in Solution-processed OLEDs

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SUPPORTING INFORMATION

Table S1. Crystal data and structure refinement for the cuprous complexes

Complex	(1×2)•CH ₂ Cl ₂	2•0.5CH ₂ Cl ₂	3
Empirical formula	C ₈₉ H ₇₂ B ₂ Cl ₂ Cu ₂ F ₈ N ₆ O ₂ P ₄	C _{45.5} H ₃₈ BClCuF ₄ N ₃ OP ₂	C ₄₅ H ₃₄ BCuF ₇ N ₃ OP ₂
Formula weight	1753.07	890.53	902.04
Crystal system	triclinic	triclinic	triclinic
Space group	P $\bar{1}$	P $\bar{1}$	P $\bar{1}$
a (Å)	12.8934(3)	9.8109(14)	9.846(3)
b (Å)	15.6420(4)	13.494(2)	13.394(5)
c (Å)	23.0349(5)	18.885(2)	17.194(5)
α (deg)	109.545(2)	100.677(4)	95.740(14)
β (deg)	101.1078(18)	94.954(6)	90.447(15)
γ (deg)	96.454(2)	107.203(5)	109.394(15)
V (Å ³)	4216.64(17)	2320.3(6)	2126.2(12)
Z	2	2	2
ρ_{calc} (g cm ⁻³)	1.380	1.275	1.409
μ (mm ⁻¹)	2.500	0.649	0.658
F(000)	1794	914	920
λ (Å)	1.54184	0.71073	0.71073
Reflns collected	45914	24280	18493
Unique reflns	17497	10534	9586
R _{int}	0.0392	0.0293	0.0618
Θ range (deg)	3.01-76.35	2.88-27.49	2.04-27.45
GOF on F ²	1.094	1.066	1.108
R ₁ /wR ₂ [$I \geq 2\sigma(I)$]	0.0626/0.1799	0.0709/0.2025	0.0852/0.2467

Table S2. Selected bond length (Å) and bond angles (deg) for the cuprous complexes

Complex	1	2	3
Cu-N ₁	2.074(3)	2.091(3)	2.100(5)
Cu-N ₃	2.070(3)	2.079(3)	2.141(5)
Cu-P ₁	2.2710(8)	2.2810(10)	2.2707(16)
Cu-P ₂	2.2258(8)	2.2498(11)	2.2923(16)
N ₁ -Cu-N ₃	78.73(12)	78.82(12)	78.3(2)
P ₁ -Cu-P ₂	112.20(3)	114.33(4)	115.24(6)
N ₁ -Cu-P ₁	109.92(8)	115.64(9)	114.99(13)
N ₁ -Cu-P ₂	115.83(9)	118.68(9)	115.68(13)
N ₃ -Cu-P ₁	103.77(9)	106.02(10)	119.30(14)
N ₃ -Cu-P ₂	131.47(8)	117.95(10)	108.18(14)
φ(N ₁ -Cu-N ₃ /P ₁ -Cu-P ₂)	82.3	94.5	84.8
Σmetallacycle	540.33	539.02	538.30