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Pargyline-phosphine Copper(I) Clusters with Tunable Emission for Light-Emitting Devices

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Characterizations

Additional IR Analysis



Fig. S1 FTIR spectra of (a) 1, (b) 2, and (c) 3.

Characterizations ¹H NMR Analysis



Fig. S2 ¹H NMR spectra of 1, 2 and 3.

Characterizations

³¹P{¹H} NMR Analysis



Characterizations XPS Analysis



Fig. S4 XPS full-scan spectra of (a) 1, (c) 2, (e) 3 and Cu 2p spectra of (b) 1, (d) 2, (f) 3.

Characterizations



Crystal Structural Determination

The crystals 1, 2 and 3 coated with epoxy resin was measured on D8 Venture under a cold nitrogen stream. The structure was solved by direct methods using the *SHELXS97* program and was refined by full matrix least–squares on F^2 using the program *SHELXL97*¹. The positions of the nonhydrogen atoms were refined with anisotropic displacement factors. The crystallographic parameters and details for data collections and refinements are summarized in Table S1, and the selected bond lengths and angles are listed in Tables S2-S3. Full crystallographic data are also provided there as CIF files.

Table S1. Crystallographic data for clusters 1, $2 \cdot 1/2CH_2Cl_2$ and $3 \cdot CH_2Cl_2$.

Cluster	1	2·1/2CH ₂ Cl ₂	3·CH ₂ Cl ₂
Empirical formula	$C_{105}H_{96}Cu_4F_6N_3P_5$	$C_{112.5}H_{105}ClCu_6F_{12}N_8P_6$	$C_{113}H_{106}Cl_4Cu_6N_8O_8P_4$
Formula weight	1922.85	2399.55	2350.97
Temperature(K)	296.15	100.15	296.15
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Triclinic	Triclinic
space group	P21/c	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Á)	14.6739(10)	14.51350(10)	14.4931(11)
b (Á)	21.6181(12)	14.80280(10)	14.8552(10)
<i>c</i> (Á)	29.0977(16)	26.8559(2)	26.891(2)
α(°)	90	74.6580(10)	75.823(3)
β(°)	91.273(2)	78.7900(10)	79.117(3)
γ (°)	90	72.0250(10)	69.750(4)
Volume (Å ³)	9228.1(10)	5252.41(8)	5231.7(7)
Ζ	4	2	2
$\rho_{calcd}, g/cm^3$	1.384	1.517	1.492
μ , mm ⁻¹	1.058	1.384	1.423
F(000)	3968.0	2450.0	2412.0
2θ (°)	3.9 to 50.108	3.482 to 55	3.888 to 50.262
	-17<=h<=17,	-18<=h<=18,	-17<=h<=17,
Limiting indices	-25<=k<=25,	-19<=k<=19,	17<=h<=17,
Deflections	-34<=1<=34	-34<=1<=34	-32<=1<=32
collected/unique	198701 / 16338	113448 / 24051	187095 / 18642
R (int)	0.0449	0.0402	0.0588
Goodness-of-fit on F ²	1.029	1.055	1.048
R1 (F _o)	0.0642	0.0563	0.0571
$wR2(F_o^2)$	0.1783	0.1551	0.1217
Largest diff. peak and hole	2.10 / -0.70	1.66 / -1.25	1.72/-2.42

1				
Bond distance [Å]				
Cu-Cu	Cu1-Cu2 2.4908(7)	Cu1-Cu3 2.5121(8)	Cu4-Cu1 2.4860(7)	
Cu-P	Cu1-P1 2.2247(13) Cu2-P2 2.2441(12)	Cu3-P3 2.2400(15)	Cu4-P4 2.2301(13)	
Cu-C _o	Cu1-C1 2.165(5)	Cu1-C21 2.129(4)	Cu1-C11 2.109(5)	
	Cu2-C1 1.983(5)	Cu4-C21 2.015(4)	Cu3-C11 2.012(5)	
Cu-C _π	Cu2-C21 2.131(4)	Cu3-C1 2.149(5)	Cu4-C11 2.108(5)	
	Cu2-C22 2.118(4)	Cu3-C2 2.154(11)	Cu4-C12 2.231(5)	
Bond angles[°]				
P-Cu-Cu1	P2-Cu2-Cu1 166.71(4)	P3-Cu3-Cu1 159.67(5)	P4-Cu4-Cu1 169.80(4)	
P1-Cu1-Cu	P1-Cu1-Cu2 116.91(4)	P1-Cu1-Cu3 134.26(4)	P1-Cu1-Cu4 124.84(4)	
Cu1-C-Cu	Cu1-C1-Cu2 73.67(15)	Cu1-C11-Cu3 75.08(16)	Cu1-C21-Cu2 71.56(2)	
	Cu1-C1-Cu3 71.24(14)	Cu1-C11-Cu4 72.25(14)	Cu1-C21-Cu4 73.68(14)	

 Table S2. Bond lengths and bond angles for 1.

$ \begin{array}{c} \mbox{Cu-Cu} & \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$		2·1/2CH2Cl2		3·CH ₂ Cl ₂		
$ \begin{array}{c c} Cu+Cu}{Cu+Cu} & 2.5795(6) & Cu3-Cu5 2.630(6) & Cu1-Cu4 2.391(3) & Cu3-Cu4 2.812(3) \\ Cu2-Cu3 2.845(13) & Cu4-Cu5 2.4653(6) & Cu2-Cu4 2.391(3) & Cu3-Cu4 2.812(3) \\ Cu2-Cu5 2.2333(6) & Cu4-Cu5 2.818(6) & Cu2-Cu5 2.318(4) & Cu3-Cu5 2.415(3) \\ Cu2-Cu5 2.7397(6) & Cu2-Cu5 2.7391(8) & Cu4-Cu5 2.415(3) \\ Cu2-Cu5 2.7397(6) & Cu4-Cu5 2.2380(1) & Cu4-Cu5 2.415(3) \\ Cu2-Cu5 2.7397(6) & Cu4-Cu5 2.2380(1) & Cu4-Cu5 2.7391(8) & Cu5-Cu6 2.6855(8) \\ Cu2-Cu4 2.2132(10) & Cu4-P2 2.2020(10) & Cu2-P3 2.2356(12) & Cu4-P2 2.203(13) \\ Cu-P & Cu1-N1 2.127(3) & Cu6-N3 2.021(3) & Cu1-N1 2.085(4) & Cu6-N4 2.027(3) \\ Cu1-N2 2.115(3) & Cu6-N4 2.137(3) & Cu1-N2 2.018(4) & Cu6-N4 2.027(3) \\ Cu2-C1 2.089(3) & Cu4-C23 2.162(4) & Cu2-C1 2.019(5) & Cu4-C33 2.131(4) \\ Cu2-C1 2.089(3) & Cu4-C23 2.162(4) & Cu2-C1 2.2019(5) & Cu4-C34 2.110(5) \\ Cu2-C2 & 2.370(8) & Cu5-C13 2.2038(4) & Cu3-C1 2.320(6) & Cu5-C32 2.099(4) \\ Cu3-C2 & 2.370(8) & Cu5-C3 2.2038(4) & Cu3-C1 2.320(6) & Cu5-C32 2.099(4) \\ Cu4-C2 & 2.381(3) & Cu6-C12 1.996(3) & Cu4-C1 2.291(6) & Cu6-C12 1.999(3) \\ Cu4-C1 & 2.881(3) & Cu5-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.350(9) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.350(9) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.350(9) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.350(9) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.350(9) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.259(5) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.259(5) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.098(5) & Cu1-C2 2.111(5) & Cu1-C24 2.259(5) \\ Cu1-C2 & 2.378(6) & Cu3-C12 2.074(7) & Cu3-C11 2.252(16) \\ P3-Cu2-C1 & 104.56(9) & P3-Cu2-C1 & 118.80(13) \\ P1-Cu3-C1 & 100.1(5) & P1-Cu3-C12 & 119.84(10) \\ P3-Cu2-C2 & 114.39(10) & P2-Cu4-C3 & 112.84(10) \\ P2-Cu4-C3 & 114.39(10) & P2-Cu4-C2 & 112.84(18) \\ P2-Cu4-C3 & 114.39(10) & P2-Cu4-C2 & 112.84(18) \\ P2-Cu4-C2 & 118.39(10) & C1-Cu2-C3 & 117.87(16) \\ C1-Cu3-C1 & 100.3(6) & C$		Cu1-Cu3 2 777(6)	$C_{12}-C_{11}6 = 2.6738(6)$	Cu1-Cu3 2.654(2)	$C_{12}-C_{11}6 = 2.5555(9)$	
$ \begin{array}{c} {\rm Cu-Cu} & {\rm Cu}_2-{\rm Cu}_3 & {\rm 2.845(13)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_5 & {\rm 2.4653(6)}{\rm Cu} & {\rm Cu}_2-{\rm Cu}_4 & {\rm 2.336(3)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_5 & {\rm 2.503(2)}{\rm Cu} & {\rm Cu}_2-{\rm Cu}_4 & {\rm 2.336(3)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_5 & {\rm 2.503(2)}{\rm Cu} & {\rm Cu}_2-{\rm Cu}_4 & {\rm 2.336(3)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_5 & {\rm 2.503(2)}{\rm Cu} & {\rm Cu}_2-{\rm Cu}_5 & {\rm 2.336(3)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_2 & {\rm 2.318(3)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_2 & {\rm 2.318(3)}{\rm Cu} & {\rm Cu}_5-{\rm Cu}_2 & {\rm 2.303(3)}{\rm Cu} & {\rm Cu}_4-{\rm Cu}_2 & {\rm 2.318(3)}{\rm Cu} & {\rm Cu}_5-{\rm Cu}_2 & {\rm 2.303(3)}{\rm Cu} & {\rm Cu}_2-{\rm Cu}_2 & {\rm 2.307(5)}{\rm Cu} & {\rm cu}_2-{\rm Cu}_2 & {\rm 2.306(3)}{\rm Cu} & {\rm cu}_2-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_5-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_5-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_2-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_5-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_2-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_3-{\rm Cu}_2 & {\rm 2.330(3)}{\rm Cu} & {\rm cu}_2-{\rm 2.311(3)}{\rm Cu} & {\rm cu}_2-{\rm 2.231(3)}{\rm Cu}$		Cu1-Cu4 = 2.5795(6)	$Cu_2 - Cu_5 - 2.630(6)$	Cu1-Cu4 = 2.391(3)	$Cu_2 Cu_3 - Cu_4 = 2.812(3)$	
$ \begin{array}{c} \mbox{Cu2-Cu4} & 2.5233(6) & Cu5-Cu6} & 2.5818(6) & Cu2-Cu4} & 2.386(3) & Cu4-Cu5} & 2.415(5) \\ \mbox{Cu2-Cu3} & 2.7397(6) & Cu4-P2 & 2.200(10) & Cu2-P3 & 2.2356(12) & Cu4-P2 & 2.2371(3) \\ \mbox{Cu3-P1} & 2.2132(10) & Cu4-P2 & 2.234(10) & Cu3-P1 & 2.334(02) & Cu5-P4 & 2.2233(13) \\ \mbox{Cu1-N1} & 2.112(3) & Cu6-N3 & 2.021(3) & Cu1-N1 & 2.085(4) & Cu6-N3 & 2.131(4) \\ \mbox{Cu1-N2} & 2.115(3) & Cu6-N3 & 2.021(3) & Cu1-N1 & 2.085(4) & Cu6-N3 & 2.131(4) \\ \mbox{Cu1-N2} & 2.115(3) & Cu6-N3 & 2.021(3) & Cu1-N2 & 2.103(4) & Cu6-N4 & 2.027(3) \\ \mbox{Cu2-C1} & 2.089(3) & Cu4-C23 & 2.162(4) & Cu2-C1 & 2.019(5) & Cu4-C23 & 2.139(5) \\ \mbox{Cu2-C1} & 2.038(3) & Cu4-C23 & 2.036(4) & Cu2-C1 & 2.019(5) & Cu4-C23 & 2.139(5) \\ \mbox{Cu2-C2} & 2.330(3) & Cu5-C12 & 2.125(3) & Cu2-C23 & 2.009(4) \\ \mbox{Cu3-C23} & 2.370(8) & Cu5-C23 & 2.038(3) & Cu3-C23 & 2.007(5) & Cu5-C23 & 2.099(4) \\ \mbox{Cu3-C23} & 2.370(8) & Cu5-C23 & 2.038(3) & Cu3-C23 & 2.007(5) & Cu5-C23 & 2.099(4) \\ \mbox{Cu3-C2} & 2.378(6) & Cu3-C12 & 2.0385(6) & Cu1-C2 & 2.138(5) & Cu1-C2 & 2.338(6) \\ \mbox{Cu1-C2} & 2.378(6) & Cu3-C12 & 2.098(5) & Cu1-C2 & 2.511(5) & Cu3-C12 & 1.2350(9) \\ \mbox{Cu1-C2} & 2.378(6) & Cu3-C12 & 2.098(5) & Cu1-C2 & 2.511(5) & Cu3-C12 & 2.206(5) \\ \mbox{Cu1-C2} & 112463(9) & P3-Cu2-C12 & 111.26(12) & P3-Cu2-C12 & 111.26(12) & P3-Cu2-C12 & 111.26(12) & P3-Cu2-C12 & 112.463(9) & P3-Cu2-C12 & 111.26(12) & P3-Cu2-C12 & 112.463(9) & P1-Cu3-C13 & 99.54(15) & P1-Cu3-C13 & 108.1(2) & P1-Cu3-C13 & 99.54(15) & P1-Cu3-C13 & 110.80(14) & P2-Cu4-C23 & 112.47(18) & P2-Cu4-C3 & 114.42(3) & P1-Cu3-C13 & 199.54(15) & P2-Cu4-C23 & 114.42(3) & P1-Cu3-C13 & 199.54(15) & P2-Cu4-C23 & 114.42(3) & P1-Cu3-C12 & 113.83(15) & P2-Cu4-C23 & 114.42(3) & P1-Cu3-C12 & 113.84(15) & P2-Cu4-C23 & 114.42(3) & P1-Cu3-C12 & 113.84(15) & P2-Cu4-C23 & 114.42(3) & P1-Cu3-C12 & 113.84(15) & P2-Cu4-C23 & 114.42(3) & P1-Cu3-C12 & 113.84(16) & P2-Cu4-C23 & 115.68(19) & P2-Cu4-C23 & 116.68(19) & P2-Cu4-C23 & 116.68(19) & P2-Cu4-C23 & 116.68(19) & P2-Cu4-C23 & 116.68(19) & P2$	Cu-Cu	Cu2-Cu3 = 2.845(13)	Cu4-Cu5 2.4653(6)	Cu2-Cu3 = 2.814(2)	Cu3-Cu5 2.503(2)	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		Cu2-Cu4 = 2.5233(6)	Cu5-Cu6 2.5818(6)	Cu2-Cu4 = 2.386(3)	Cu3 Cu3 2.305(2) Cu4-Cu5 2.415(3)	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		Cu2-Cu5 2.7397(6)		Cu2-Cu5 = 2.7931(8)	Cu5-Cu6 2.6855(8)	
$ \begin{array}{c cu-P} \hline Cu3-P1 & 2.249(4) & Cu5-P4 & 2.2341(9) & Cu3-P1 & 2.340(2) & Cu5-P4 & 2.2203(13) \\ \hline Cu-N & Cu1+N1 & 2.127(3) & Cu6-N3 & 2.021(3) & Cu1-N2 & 2.038(4) & Cu6-N3 & 2.131(4) \\ \hline Cu1-N2 & Cu12(4) & Cu1-N1 & 2.173(3) & Cu1-N2 & 2.103(4) & Cu6-N3 & 2.131(4) \\ \hline Cu1-C2 & 2.115(3) & Cu4-C3 & 2.157(3) & Cu1-N2 & 2.103(4) & Cu6-N3 & 2.131(5) \\ \hline Cu2-C1 & 2.089(3) & Cu4-C3 & 2.122(3) & Cu2-C1 & 2.119(5) & Cu4-C3 & 2.139(5) \\ \hline Cu2-C1 & 2.380(3) & Cu4-C3 & 2.122(3) & Cu2-C3 & 2.272(4) & Cu5-C1 & 2.427(5) \\ \hline Cu2-C1 & 2.381(3) & Cu5-C1 & 2.122(3) & Cu3-C1 & 2.392(6) & Cu5-C3 & 2.099(4) \\ \hline Cu3-C2 & 2.370(8) & Cu5-C3 & 2.303(3) & Cu3-C2 & 2.007(5) & Cu5-C3 & 2.099(4) \\ \hline Cu-C_{\pi} & Cu1-C2 & 2.381(3) & Cu1-C2 & 2.385(4) & Cu1-C1 & 2.413(5) & Cu1-C2 & 2.530(9) \\ \hline Cu1-C2 & 2.381(3) & Cu1-C2 & 2.385(4) & Cu1-C2 & 2.11(5) & Cu3-C12 & 2.206(5) \\ \hline Cu1-C2 & 2.337(6) & Cu3-C1 & 2.098(5) & Cu1-C2 & 2.11(5) & Cu3-C12 & 2.206(5) \\ \hline Cu1-C2 & 2.337(6) & Cu3-C1 & 2.098(5) & Cu1-C2 & 2.148(4) & Cu3-C1 & 2.259(5) \\ \hline \hline P-Cu-C & P1-Cu3-C1 & 104.50(8) & P3-Cu2-C1 & 118.60(14) \\ P3-Cu2-C1 & 124.63(9) & P3-Cu2-C1 & 118.60(14) \\ P3-Cu2-C3 & 110.31(15) & P1-Cu3-C1 & 129.25(16) \\ P1-Cu3-C1 & 100.1(5) & P1-Cu3-C1 & 129.25(16) \\ P1-Cu3-C1 & 100.1(5) & P1-Cu3-C1 & 129.25(16) \\ P1-Cu3-C1 & 100.1(5) & P1-Cu3-C1 & 129.25(16) \\ P1-Cu3-C1 & 11.40(9) & P2-Cu4-C23 & 112.34(18) \\ P2-Cu4-C23 & 114.39(10) & P2-Cu4-C23 & 112.34(18) \\$		Cu2-P3 = 2.2132(10)	Cu4-P2 2 2020(10)	Cu2-P3 = 2.2356(12)	Cu4-P2 = 2.371(3)	
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Cu-P	$Cu_2 P_1 = 2.249(4)$	Cu5-P4 = 2.2341(9)	Cu3-P1 = 2.340(2)	Cu5-P4 $2.2203(13)$	
$ \begin{array}{c cu-N} \hline Cu-N & Cu-N & 2.115(3) & Cu-N & 2.137(3) & Cu-N & 2.103(4) & Cu-N & 2.027(3) \\ \hline Cu-Cu & Cu-C1 & 2.089(3) & Cu-4.C3 & 2.162(4) & Cu-C1 & 2.109(5) & Cu+C23 & 2.139(5) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.138(3) & Cu-C3 & 2.016(3) & Cu-C21 & 2.119(5) & Cu+C3 & 2.110(5) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.380(3) & Cu-C3 & 2.038(4) & Cu-C21 & 2.129(5) & Cu+C3 & 2.110(5) \\ \hline Cu-Cu-Cu & Cu-C1 & 2.468(16) & Cu-5.C3 & 2.038(4) & Cu-C2 & 2.22(4) & Cu-5.C3 & 2.099(4) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.370(8) & Cu-C24 & 2.385(4) & Cu-C2 & 2.017(5) & Cu-5.C3 & 2.099(4) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.378(6) & Cu-C2 & 2.385(4) & Cu-C2 & 2.11(5) & Cu-C2 & 2.130(7) \\ \hline Cu-Cu & Cu-C2 & 2.337(6) & Cu-C1 & 2.385(6) & Cu-C2 & 2.11(5) & Cu-C2 & 2.130(9) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.337(6) & Cu-3-C1 & 2.098(5) & Cu-C2 & 2.11(5) & Cu-C2 & 2.206(5) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.337(6) & Cu-3-C1 & 2.098(5) & Cu-C2 & 2.118(6) & Cu-C2 & 2.51(6) \\ \hline Cu-Cu-Cu & Cu-C2 & 2.337(6) & Cu-3-C1 & 2.098(5) & Cu-C2 & 2.112(5) & Cu-C3 & 2.259(5) \\ \hline \hline P-Cu-C & P-Cu-Cc & P-Cu-Cc & P-Cu-Cu & P-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu-Cu & P-Cu-Cu-Cu & P-C$		Cu1-N1 $2.127(3)$	$\frac{\text{Cu6-N3}}{\text{Cu6-N3}} = 2.021(3)$	Cu1-N1 2.085(4)	Cu6-N3 $2.131(4)$	
$ \begin{array}{c} \label{eq:cu-c} \\ Cu-C_{\pi} & \begin{array}{c} Cu^2-Cl & 2.089(3) \\ Cu^2-Cl^2 & 2.380(3) \\ Cu^4-Cl^2 & 2.162(4) \\ Cu^2-Cl^2 & 2.19(5) \\ Cu^2-Cl^2 & 2.139(5) \\ Cu^2-Cl^2 & 2.138(3) \\ Cu^2-Cl^2 & 2.123(3) \\ Cu^2-Cl^2 & 2.123(3) \\ Cu^2-Cl^2 & 2.2427(5) \\ Cu^2-Cl^2 & 2.370(8) \\ Cu^2-Cl^2 & 2.381(3) \\ Cu^2-Cl^2 & 2.338(4) \\ Cu^2-Cl^2 & 104.50(8) \\ P^2-Cu^2-Cl & 124.63(9) \\ P^2-Cu^2-Cl & 111.26(12) \\ P^2-Cu^2-Cl & 104.50(8) \\ P^2-Cu^2-Cl & 104.63(9) \\ P^2-Cu^2-Cl & 111.26(12) \\ P^2-Cu^2-Cl & 108.1(2) \\ P^1-Cu^3-Cl & 100.1(5) \\ P^2-Cu^2-Cl & 108.1(2) \\ P^1-Cu^3-Cl & 100.1(5) \\ P^2-Cu^4-Cl & 111.40(9) \\ P^2-Cu^4-Cl & 111.80(14) \\ P^2-Cu^4-Cl & 111.40(9) \\ P^2-Cu^4-Cl & 111.80(15) \\ P^2-Cu^4-Cl & 111.87(12) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 102.31(13) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 103.31(16) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 102.41(15.42(2) \\ P^2-Cu^2-Cl & 103.5(12) \\ P^2-Cu^2-Cl & 102.41(12.41(15.42(2) \\ P^2-Cu^2-Cl & 102.41(12$	Cu-N	Cu1-N2 $2.115(3)$	Cu6-N4 $2.137(3)$	Cu1-N2 $2.103(4)$	Cu6-N4 $2.027(3)$	
$\begin{array}{c c} Cu-C_{\sigma} & Cu^2-Ci2 & 2.380(3) \\ Cu^2-Ci2 & 2.380(3) \\ Cu^2-Ci2 & 2.380(3) \\ Cu^2-Ci2 & 2.134(3) \\ Cu^2-Ci2 & 2.125(3) \\ Cu^2-Ci2 & 2.272(4) \\ Cu^2-Ci2 & 2.487(6) \\ Cu^2-Ci2 & 2.370(8) \\ Cu^2-Ci2 & 2.381(4) \\ Cu^2-Ci2 & 2.385(4) \\ Cu^2-Ci2 & 2.385(4) \\ Cu^2-Ci2 & 2.378(6) \\ Cu^2-Ci2 & 2.390(4) \\ Cu^2-Ci2 & 2.298(5) \\ Cu^2-Ci2 & 2.48(4) \\ Cu^2-Ci2 & 2.390(4) \\ Cu^2-Ci2 & 2.299(5) \\ \hline \end{array} $		Cu2-C1 = 2.089(3)	Cu4-C23 = 2.162(4)	Cu2-C1 = 2.019(5)	Cu4-C23 = 2.139(5)	
$\begin{array}{c} Cu+C_{\sigma} & \begin{array}{c} Cu+C_{\sigma} \\ Cu+C_{\sigma} \\$		Cu2-C12 2.380(3)	Cu4-C34 = 2.016(3)	Cu2-C12 2.119(5)	Cu4-C34 2.110(5)	
$\begin{array}{c c} Cu-C_{0} & Cu3-C1 & 2.468(16) \\ Cu3-C23 & 2.370(8) & Cu5-C23 & 2.038(4) \\ Cu3-C23 & 2.370(8) & Cu5-C34 & 2.303(3) \\ Cu3-C23 & 2.007(5) & Cu5-C34 & 2.134(5) \\ Cu4-C1 & 2.381(3) & Cu6-C12 & 1.996(3) & Cu4-C1 & 2.061(6) & Cu5-C12 & 1.999(4) \\ Cu1-C2 & 2.378(6) & Cu3-C12 & 2.098(5) & Cu1-C2 & 2.511(5) & Cu1-C2 & 2.530(9) \\ Cu1-C2 & 2.330(4) & Cu3-C12 & 2.098(5) & Cu1-C2 & 2.511(5) & Cu3-C12 & 2.206(5) \\ Cu1-C2 & 2.330(4) & Cu3-C13 & 2.085(5) & Cu1-C2 & 2.511(5) & Cu3-C12 & 2.206(5) \\ Cu1-C2 & 2.330(4) & Cu3-C13 & 2.085(6) & Cu1-C23 & 2.148(4) & Cu3-C13 & 2.259(5) \\ \hline \\ $		Cu2-C34 2.134(3)	Cu5-C12 2.125(3)	Cu2-C34 2.272(4)	Cu5-C12 2.427(5)	
$\begin{array}{c cccc} Cu3-C23 & 2.370(8) & Cu5-C34 & 2.303(3) & Cu3-C23 & 2.007(5) & Cu5-C34 & 2.134(5) \\ \hline Cu4-C1 & 2.381(3) & Cu1-C21 & 1.996(3) & Cu4-C1 & 2.061(6) & Cu6-C12 & 1.999(4) \\ \hline Cu-C_n & Cu1-C2 & 2.338(3) & Cu1-C24 & 2.385(4) & Cu1-C2 & 2.413(5) & Cu1-C24 & 2.530(9) \\ \hline Cu1-C2 & 2.338(4) & Cu3-C12 & 2.098(5) & Cu1-C2 & 2.111(5) & Cu3-C12 & 2.206(5) \\ \hline Cu1-C23 & 2.330(4) & Cu3-C13 & 2.085(6) & Cu1-C23 & 2.148(4) & Cu3-C13 & 2.259(5) \\ \hline & & & & & & & & & & & & & & & & & &$	Cu-C _σ	Cu3-C1 2.468(16)	Cu5-C23 2.038(4)	Cu3A-C1 2.392(6)	Cu5-C23 2.099(4)	
$\begin{array}{c c} Cu4-Cl & 2.381(3) & Cu5-Cl2 & 1.996(3) & Cu4-Cl & 2.061(6) & Cu5-Cl2 & 1.999(4) \\ \hline Cu-C_{\pi} & Cu1-Cl & 2.183(3) & Cu1-C24 & 2.385(4) & Cu1-Cl & 2.413(5) & Cu1-Cl2 & 2.530(9) \\ \hline Cu1-Cl2 & 2.378(6) & Cu3-Cl2 & 2.098(5) & Cu1-C2 & 2.511(5) & Cu3-Cl2 & 2.206(5) \\ \hline Cu1-Cl2 & 2.330(4) & Cu3-Cl2 & 2.098(5) & Cu1-Cl2 & 2.148(4) & Cu3-Cl1 & 2.205(5) \\ \hline Cu1-Cl2 & 2.330(4) & Cu3-Cl2 & 2.085(6) & Cu1-Cl2 & 2.148(4) & Cu3-Cl1 & 2.259(5) \\ \hline & P3-Cu2-Cl2 & 111.2(6.3(9) & P3-Cu2-Cl & 111.860(14) \\ \hline P3-Cu2-Cl3 & 111.72(9) & P3-Cu2-Cl2 & 111.26(12) \\ \hline P3-Cu2-Cl & 124.63(9) & P3-Cu2-Cl & 111.26(12) \\ \hline P1-Cu3-Cl1 & 108.1(2) & P1-Cu3-Cl2 & 113.77(15) \\ \hline P1-Cu3-Cl1 & 100.1(5) & P1-Cu3-Cl2 & 113.77(15) \\ \hline P1-Cu3-Cl & 100.1(5) & P1-Cu3-Cl2 & 113.83(15) \\ \hline P2-Cu4-Cl & 111.40(9) & P2-Cu4-Cl3 & 113.83(15) \\ \hline P2-Cu4-Cl & 111.40(9) & P2-Cu4-Cl & 113.83(15) \\ \hline P2-Cu4-Cl & 111.39(10) & P2-Cu4-Cl & 112.5(2) \\ \hline P4-Cu5-Cl2 & 110.33(9) & P4-Cu5-Cl2 & 103.31(11) \\ \hline P4-Cu5-Cl2 & 110.53(9) & P4-Cu5-Cl2 & 103.31(11) \\ \hline P4-Cu5-Cl2 & 110.53(9) & P4-Cu5-Cl2 & 103.31(1) \\ \hline P4-Cu5-Cl2 & 118.79(12) & Cl-Cu1-Cl2 & 90.33(16) \\ \hline C1-Cu1-Cl2 & 118.79(12) & Cl-Cu1-Cl2 & 115.4(2) \\ \hline C2-Cu1-Cl2 & 118.31(18) & Cl-Cu2-Cl2 & 115.8(19) \\ \hline C1-Cu2-Cl2 & 113.30(8) & Cl-Cu2-Cl2 & 110.37(19) \\ \hline C1-Cu2-Cl2 & 103.5(12) & Cl-Cu2-Cl2 & 110.37(19) \\ \hline C1-Cu2-Cl2 & 105.35(12) & Cl-Cu2-Cl2 & 110.37(19) \\ \hline C1-Cu2-Cl2 & 105.35(12) & Cl-Cu2-Cl2 & 110.37(19) \\ \hline C1-Cu2-Cl2 & 105.35(12) & Cl-Cu2-Cl2 & 115.68(19) \\ \hline C1-Cu2-Cl2 & 105.5(5) & Cl-Cu3-Cl2 & 137.78(19) \\ \hline C1-Cu3-Cl2 & 90.6(3) & Cl2-Cu3-Cl2 & 134.48(17) \\ \hline C1-Cu2-Cl2 & 105.5(5) & Cl-Cu3-Cl2 & 137.7(19) \\ \hline C1-Cu3-Cl2 & 106.5(5) & Cl-Cu3-Cl2 & 137.78(19) \\ \hline C1-Cu3-Cl2 & 106.5(5) & Cl-Cu3-Cl2 & 134.48(17) \\ \hline C12-Cu5-Cl2 & 106.3(13) & Cl2-Cu2-Cl2 & 100.9(2) \\ \hline C1-Cu4-Cl2 & 106.5(5) & Cl-Cu3-Cl2 & 134.48(17) \\ \hline C12-Cu5-Cl2 & 106.3(13) & Cl2-Cu2-Cl2 & 106.9(2) \\ \hline C1-Cu4-Cl3 & 106.9(2) & Cl-Cu3-Cl2 & 106.9(2) \\ \hline C1-Cu4-Cl3 & 106.9(2) & Cl-Cu3-Cl2 & 106.9(2) \\ \hline C1-Cu4-Cl3 & 106.9(2) & Cl-Cu3$		Cu3-C23 2.370(8)	Cu5-C34 2.303(3)	Cu3-C23 2.007(5)	Cu5-C34 2.134(5)	
$\begin{array}{c c} Cu-C_{\pi} & \begin{array}{c} Cu1-C1 & 2.183(3) \\ Cu1-C2 & 2.378(6) \\ Cu1-C2 & 2.378(6) \\ Cu3-C12 & 2.098(5) \\ Cu1-C2 & 2.511(5) \\ Cu1-C2 & 2.511(5) \\ Cu3-C12 & 2.206(5) \\ Cu3-C12 & 2.098(5) \\ Cu1-C2 & 2.511(5) \\ Cu3-C12 & 2.205(5) \\ Cu3-C12 & 2.205(6) \\ Cu3-C12 & 112.20(1) \\ P3-Cu2-C1 & 114.63(9) \\ P3-Cu2-C1 & 114.63(9) \\ P1-Cu3-C12 & 108.1(2) \\ P1-Cu3-C1 & 100.1(5) \\ P2-Cu4-C2 & 114.2(3) \\ P2-Cu4-C2 & 114.39(10) \\ P2-Cu4-C3 & 112.34(18) \\ P2-Cu4-C3 & 119.94(10) \\ P4-Cu5-C12 & 110.53(9) \\ P4-Cu5-C3 & 119.94(10) \\ P4-Cu5-C12 & 110.53(9) \\ P4-Cu5-C3 & 119.94(10) \\ P4-Cu5-C12 & 110.53(9) \\ P4-Cu5-C23 & 117.45(16) \\ C1-Cu1-C24 & 118.79(12) \\ C1-Cu1-C24 & 117.45(16) \\ C1-Cu1-C24 & 117.45(16) \\ C1-Cu1-C24 & 117.45(16) \\ C1-Cu2-C12 & 100.5(5) \\ C1-Cu3-C12 & 100.5(5) \\ C1-Cu3-C23 & 83.0(3) \\ C12-Cu3-C23 & 83.0(3) \\ C12-Cu3-C23 & 83.0(3) \\ C12-Cu3-C23 & 100.8(14) \\ C12-Cu3-C23 & 90.6(1) \\ C12-Cu3-C23 & 90.6(1) \\ C12-Cu5-C23 & 100.3(13) \\ C12-Cu5-C2$		Cu4-C1 2.381(3)	Cu6-C12 1.996(3)	Cu4-C1 2.061(6)	Cu6-C12 1.999(4)	
$\begin{array}{c c} Cu-C_{\pi} & Cu1-C2 & 2.378(6) \\ Cu1-C23 & 2.330(4) \\ Cu3-C13 & 2.085(6) \\ Cu1-C23 & 2.148(4) \\ Cu3-C13 & 2.259(5) \\ \hline \\ Bond angles["1] \\ \hline \\ Back angles["2] \\ \hline \\ Back$		Cu1-C1 2.183(3)	Cu1-C24 2.385(4)	Cu1-C1 2.413(5)	Cu1-C24 2.530(9)	
$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	Cu-C _π	Cu1-C2 2.378(6)	Cu3-C12 2.098(5)	Cu1-C2 2.511(5)	Cu3-C12 2.206(5)	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		Cu1-C23 2.330(4)	Cu3-C13 2.085(6)	Cu1-C23 2.148(4)	Cu3-C13 2.259(5)	
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $			Bond angles[°	2		
$C-Cu-C = C-Cu-C = \begin{array}{c c c c c c c c c c c c c c c c c c c $		P3-Cu2-C12 104.50	(8)	P3-Cu2-C1 118.	60(14)	
C-Cu-C = Cu-Cu = C = C = C = C = C = C = C = C = C =		P3-Cu2-C34 111.72	$\tilde{2}(9)$	P3-Cu2-C12 111.	26(12)	
$C-Cu-C = C-Cu-C = C-Cu-C = \begin{array}{ccccccccccccccccccccccccccccccccccc$		P3-Cu2-C1 124.63(9)		P3-Cu2-C34 108.	35(13)	
$C-Cu-C = C-Cu-C = \begin{array}{c c c c c c c c c c c c c c c c c c c $		P1-Cu3-C13 108.1(2)		P1-Cu3-C12 129.	25(16)	
$\begin{array}{c c} P-Cu-C & P1-Cu3-C1 & 100.1(5) & P1-Cu3-C13 & 99.54(15) \\ P-Cu-C & P1-Cu3-C23 & 114.2(3) & P1 & Cu3A & C1 & 113.83(15) \\ P2-Cu4-C23 & 114.39(10) & P2-Cu4-C23 & 112.34(18) \\ P2-Cu4-C23 & 114.39(10) & P2-Cu4-C23 & 110.46(15) \\ P2-Cu4-C34 & 120.00(10) & P2-Cu4-C3 & 109.46(15) \\ P2-Cu4-C34 & 120.00(10) & P2-Cu4-C3 & 112.5(2) \\ P4-Cu5-C23 & 119.94(10) & P4-Cu5-C12 & 103.31(11) \\ P4-Cu5-C12 & 110.53(9) & P4-Cu5-C34 & 112.61(12) \\ P4-Cu5-C34 & 108.60(9) & P4-Cu5-C23 & 127.28(12) \\ \hline \\ C1-Cu1-C23 & 90.49(12) & C1-Cu1-C23 & 90.33(16) \\ C1-Cu1-C23 & 90.49(12) & C2-Cu1-C23 & 117.45(16) \\ C2-Cu1-C23 & 118.13(18) & C1-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 117.45(18) & C2-Cu1-C24 & 1143.8(2) \\ C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C12 & 100.5(5) & C1-Cu3A-C23 & 82.84(18) \\ C13-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 90.6(12) & C1-Cu3-C12 & 100.9(2) \\ C1-Cu4-C23 & 104.37(13) & C1-Cu4-C23 & 100.9(2) \\ C1-Cu4-C23 & 104.37(13) & C1-Cu4-C23 & 100.9(2) \\ C1-Cu4-C23 & 104.37(13) & C1-Cu3-C23 & 133.82(15) \\ C23-Cu4-C34 & 105.98(14) & C23-Cu5-C34 & 109.70(16) \\ C12-Cu5-C23 & 99.3(412) & C34-Cu5-C12 & 93.75(16) \\ \hline \end{array}$		P1-Cu3-C12 142.2(2)		P1-Cu3-C23 113.77(15)		
$\begin{array}{c c} P-Cu-C & P1-Cu3-C23 & 114.2(3) & P1 Cu3A C1 & 113.83(15) \\ P2-Cu4-C1 & 111.40(9) & P2-Cu4-C23 & 112.34(18) \\ P2-Cu4-C23 & 112.39(10) & P2-Cu4-C23 & 112.34(18) \\ P2-Cu4-C34 & 120.00(10) & P2-Cu4-C1 & 112.5(2) \\ P4-Cu5-C23 & 119.94(10) & P4-Cu5-C12 & 103.31(11) \\ P4-Cu5-C12 & 110.53(9) & P4-Cu5-C34 & 112.61(12) \\ P4-Cu5-C34 & 108.60(9) & P4-Cu5-C23 & 127.28(12) \\ \hline \\ C1-Cu1-C23 & 90.49(12) & C1-Cu1-C23 & 90.33(16) \\ C1-Cu1-C23 & 90.49(12) & C2-Cu1-C23 & 117.45(16) \\ C2-Cu1-C24 & 118.79(12) & C2-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 118.79(12) & C2-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 118.79(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C13 & 120.0(6) & C13-Cu3-C23 & 115.68(19) \\ C1-Cu3-C12 & 100.5(5) & C1-Cu3A-C23 & 82.84(18) \\ C13-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3-C13 & 124.2(2) \\ C1-Cu4-C34 & 104.37(13) & C1-Cu4-C23 & 100.9(2) \\ C1-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 109.1(2) \\ C23-Cu4-C34 & 105.98(14) & C23-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) & C12-Cu5-C12 & 93.75(16) \\ \hline \end{array}$		P1-Cu3-C1 100.1(5)	P1-Cu3-C13 99.54(15)		
$C-Cu-C \begin{bmatrix} P2-Cu4-C1 & 111.40(9) & P2-Cu4-C23 & 112.34(18) \\ P2-Cu4-C23 & 114.39(10) & P2-Cu4-C34 & 109.46(15) \\ P2-Cu4-C34 & 120.00(10) & P2-Cu4-C1 & 112.5(2) \\ P4-Cu5-C23 & 119.94(10) & P4-Cu5-C12 & 103.31(11) \\ P4-Cu5-C12 & 110.53(9) & P4-Cu5-C23 & 112.61(12) \\ P4-Cu5-C34 & 108.60(9) & P4-Cu5-C23 & 127.28(12) \\ \hline C1-Cu1-C23 & 90.49(12) & C1-Cu1-C23 & 90.33(16) \\ C1-Cu1-C24 & 118.79(12) & C2-Cu1-C23 & 117.45(16) \\ C2-Cu1-C24 & 118.79(12) & C2-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 147.86(18) & C2-Cu1-C24 & 143.8(2) \\ C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C1-Cu2-C34 & 96.74(12) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 137.87(19) \\ C1-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.64(12) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 100.5(5) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 100.3(13) & C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) & C12-Cu5-C23 & 103.82(15) \\ C23-Cu5-C34 & 99.34(12) & C34-Cu5-C12 & 93.75(16) \\ \hline \\ $	P-Cu-C	P1-Cu3-C23 114.2(3)		P1 Cu3A C1 113.83(15)		
C-Cu-C $P2-Cu4-C23 114.39(10) P2-Cu4-C34 109.46(15) P2-Cu4-C34 120.00(10) P2-Cu4-C1 112.5(2) P4-Cu5-C23 119.94(10) P4-Cu5-C12 103.31(11) P4-Cu5-C12 110.53(9) P4-Cu5-C34 112.61(12) P4-Cu5-C34 108.60(9) P4-Cu5-C23 127.28(12) P4-Cu5-C34 108.60(9) P4-Cu5-C23 127.28(12) C1-Cu1-C23 90.33(16) C1-Cu1-C24 118.79(12) C1-Cu1-C23 90.33(16) C1-Cu1-C24 118.79(12) C2-Cu1-C23 117.45(16) C2-Cu1-C24 118.13(18) C1-Cu1-C24 115.4(2) C2-Cu1-C24 147.86(18) C2-Cu1-C24 143.8(2) C1-Cu2-C12 103.65(12) C1-Cu2-C12 110.37(19) C1-Cu2-C34 111.05(13) C1-Cu2-C34 107.5(2) C1-Cu2-C34 96.74(12) C12-Cu2-C34 98.77(17) C1-Cu3-C23 83.0(3) C12-Cu3-C23 115.68(19 C1-Cu3-C13 120.0(6) C13-Cu3-C23 137.87(19) C1-Cu3-C23 126.8(5) C1-Cu3-C12 134.48(17) C12-Cu3-C23 99.6(3) C1-Cu3-C13 124.2(2) C1-Cu4-C23 100.9(2) C1-Cu4-C23 100.9(2) C1-Cu4-C23 100.9(2) C1-Cu4-C23 100.9(2) C1-Cu4-C34 112.3(13) C12-Cu3-C23 103.82(15) C23-Cu4-C34 105.98(14) C23-Cu3-C12 93.75(16) C12-Cu3-C34 99.34(12) C13-Cu3-C23 100.9(2) C12-Cu5-C34 105.98(14) C23-Cu4-C34 109.70(16) C12-Cu5-C34 99.34(12) C3+Cu5-C12 93.75(16) C1-Cu3-C12 93.75(16) C12-Cu5-C34 99.34(12) C3+Cu5-C12 93.75(16) C12-Cu5-C34 99.34(12) C3+Cu5-C12 93.75(16) C12-Cu5-C34 99.34(12) C3+Cu5-C12 93.75(16) C13-Cu3-C12 100.75(15) C3+Cu3-C13 120.0(16) C12-Cu5-C34 99.34(12) C3+Cu5-C12 93.75(16) C12-Cu5-C34 99.34(12) C3+Cu5-C12 93.75(16) C13-Cu3-C12 93.75(16) C13-Cu3-C13 103-C12-Cu5-C33 103.22(15) C13-Cu3-C13 103.22(15) C13-Cu3-Cu3-Cu3-Cu3-Cu3-Cu3-Cu3-Cu3-Cu3-Cu$		P2-Cu4-C1 111.40	0(9)	P2-Cu4-C23 112.34(18)		
$C-Cu-C \begin{pmatrix} P2-Cu4-C34 & 120.00(10) \\ P4-Cu5-C23 & 119.94(10) \\ P4-Cu5-C12 & 103.31(11) \\ P4-Cu5-C12 & 110.53(9) \\ P4-Cu5-C34 & 112.61(12) \\ P4-Cu5-C34 & 108.60(9) \\ P4-Cu5-C23 & 127.28(12) \\ P4-Cu5-C23 & 108.60(9) \\ P4-Cu5-C23 & 127.28(12) \\ C1-Cu1-C23 & 90.49(12) \\ C1-Cu1-C23 & 90.49(12) \\ C1-Cu1-C23 & 90.33(16) \\ C1-Cu1-C24 & 118.79(12) \\ C2-Cu1-C23 & 118.13(18) \\ C1-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 147.86(18) \\ C2-Cu1-C24 & 147.86(18) \\ C2-Cu1-C24 & 143.8(2) \\ C1-Cu2-C12 & 103.65(12) \\ C1-Cu2-C34 & 111.05(13) \\ C1-Cu2-C34 & 107.5(2) \\ C1-Cu2-C34 & 96.74(12) \\ C1-Cu3-C13 & 120.0(6) \\ C13-Cu3-C23 & 83.0(3) \\ C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C12 & 100.5(5) \\ C1-Cu3-C12 & 100.5(1) \\ C1-Cu3-C13 & 120.0(6) \\ C1-Cu3-C13 & 124.8(17) \\ C12-Cu3-C23 & 99.6(3) \\ C1-Cu3-C13 & 124.2(2) \\ C1-Cu4-C34 & 104.37(13) \\ C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 112.26(14) \\ C23-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) \\ C12-Cu5-C23 & 103.82(15) \\ C23-Cu5-C34 & 105.98(14) \\ C23-Cu5-C12 & 93.75(16) \\ \end{pmatrix}$		P2-Cu4-C23 114.39	9(10)	P2-Cu4-C34 109.46(15)		
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		P2-Cu4-C34 120.00	0(10)	P2-Cu4-C1 112.5(2)		
$C-Cu-C \begin{bmatrix} C-Cu-C \\ C-Cu-CU \\ C-Cu-C \\ C-Cu-CU \\ C-CU-CU \\ C-CU-CU \\ C-CU-CU \\ C-CU-$		P4-Cu5-C23 119.94	(10)	P4-Cu5-C12 103.	31(11)	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		P4-Cu5-C12 110.53	6(9)	P4-Cu5-C34 112.61(12)		
$C-Cu-C = \begin{pmatrix} C1-Cu1-C23 & 90.49(12) & C1-Cu1-C23 & 90.33(16) \\ C1-Cu1-C24 & 118.79(12) & C2-Cu1-C23 & 117.45(16) \\ C2-Cu1-C23 & 118.13(18) & C1-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 147.86(18) & C2-Cu1-C24 & 143.8(2) \\ C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C12-Cu2-C34 & 96.74(12) & C12-Cu2-C34 & 98.77(17) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C13 & 120.0(6) & C13-Cu3-C23 & 137.87(19) \\ C1-Cu3-C12 & 100.5(5) & C1-Cu3A-C23 & 82.84(18) \\ C13-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 89.64(12) & C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 112.26(14) & C23-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) & C12-Cu5-C23 & 103.82(15) \\ C23-Cu5-C34 & 105.98(14) & C23-Cu5-C12 & 93.75(16) \\ \hline \end{pmatrix}$		P4-Cu5-C34 108.60	0(9)	P4-Cu5-C23 127.28(12)		
$C-Cu-C = \begin{pmatrix} C1-Cu1-C24 & 118.79(12) & C2-Cu1-C23 & 117.45(16) \\ C2-Cu1-C23 & 118.13(18) & C1-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 147.86(18) & C2-Cu1-C24 & 143.8(2) \\ C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu2-C34 & 98.77(17) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C13 & 120.0(6) & C13-Cu3-C23 & 137.87(19) \\ C1-Cu3-C12 & 100.5(5) & C1-Cu3A-C23 & 82.84(18) \\ C13-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 89.64(12) & C1-Cu4-C23 & 100.9(2) \\ C1-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 112.26(14) & C23-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) & C12-Cu5-C23 & 103.82(15) \\ C23-Cu5-C34 & 109.98(14) & C23-Cu5-C34 & 109.70(16) \\ C12-Cu5-C34 & 99.34(12) & C14-Cu5-C12 & 93.75(16) \\ \hline \end{pmatrix}$		C1-Cu1-C23 90.49((12)	C1-Cu1-C23 90.3	3(16)	
$C-Cu-C = \begin{pmatrix} C2-Cu1-C23 & 118.13(18) & C1-Cu1-C24 & 115.4(2) \\ C2-Cu1-C24 & 147.86(18) & C2-Cu1-C24 & 143.8(2) \\ C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C12-Cu2-C34 & 96.74(12) & C12-Cu2-C34 & 98.77(17) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C13 & 120.0(6) & C13-Cu3-C23 & 137.87(19) \\ C1-Cu3-C12 & 100.5(5) & C1-Cu3A-C23 & 82.84(18) \\ C13-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 89.64(12) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) & C12-Cu5-C23 & 103.82(15) \\ C23-Cu5-C34 & 105.98(14) & C23-Cu5-C34 & 109.70(16) \\ C12-Cu5-C34 & 99.34(12) & C34-Cu5-C12 & 93.75(16) \\ \hline \\ C12-Cu5-C34 & 99.34(12) & C34-Cu5-C12 & 97.5(16) \\ \hline \\ $		C1-Cu1-C24 118.79	9(12)	C2-Cu1-C23 117.45(16)		
$C-Cu-C = \begin{pmatrix} C2-Cu1-C24 & 147.86(18) \\ C1-Cu2-C12 & 103.65(12) \\ C1-Cu2-C34 & 111.05(13) \\ C1-Cu2-C34 & 96.74(12) \\ C1-Cu2-C34 & 96.74(12) \\ C1-Cu3-C23 & 83.0(3) \\ C12-Cu2-C34 & 98.77(17) \\ C1-Cu3-C23 & 83.0(3) \\ C12-Cu3-C23 & 115.68(19) \\ C1-Cu3-C13 & 120.0(6) \\ C13-Cu3-C23 & 137.87(19) \\ C1-Cu3-C12 & 100.5(5) \\ C1-Cu3A-C23 & 82.84(18) \\ C13-Cu3-C23 & 126.8(5) \\ C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) \\ C1-Cu4-C23 & 89.64(12) \\ C1-Cu4-C23 & 89.64(12) \\ C1-Cu4-C23 & 100.9(2) \\ C1-Cu4-C34 & 104.37(13) \\ C12-Cu5-C23 & 110.33(13) \\ C12-Cu5-C23 & 110.33(13) \\ C12-Cu5-C34 & 105.98(14) \\ C12-Cu5-C34 & 99.34(12) \\ C12-Cu5-C12 & 99.37(16) \\ C12-Cu5-C12 & 99.34(12) \\ C12-Cu5-C12 & 99.37(16) \\ C12-Cu5-C12 & 99.34(12) \\ C12-Cu5-C12 & 99.34(12) \\ C12-Cu5-C12 & 93.75(16) \\ C12-Cu5-C12 & 99.34(12) \\ C12-Cu5-C12 & 93.75(16) \\ C12-Cu5-C12 & 99.34(12) \\ C12-Cu5-C12 & 93.75(16) \\ C12-Cu5-C12 & 93.7$		C2-Cu1-C23 118.13	3(18)	C1-Cu1-C24 115.	4(2)	
$C-Cu-C = \begin{bmatrix} C1-Cu2-C12 & 103.65(12) & C1-Cu2-C12 & 110.37(19) \\ C1-Cu2-C34 & 111.05(13) & C1-Cu2-C34 & 107.5(2) \\ C1-Cu3-C23 & 83.0(3) & C12-Cu2-C34 & 98.77(17) \\ C1-Cu3-C13 & 120.0(6) & C13-Cu3-C23 & 115.68(19) \\ C1-Cu3-C12 & 100.5(5) & C1-Cu3-C23 & 137.87(19) \\ C1-Cu3-C23 & 126.8(5) & C1-Cu3-C12 & 134.48(17) \\ C12-Cu3-C23 & 126.8(5) & C1-Cu3A-C12 & 134.48(17) \\ C12-Cu3-C23 & 99.6(3) & C1-Cu3A-C13 & 124.2(2) \\ C1-Cu4-C23 & 89.64(12) & C1-Cu4-C23 & 100.9(2) \\ C1-Cu4-C34 & 104.37(13) & C1-Cu4-C34 & 112.3(2) \\ C23-Cu4-C34 & 112.26(14) & C23-Cu4-C34 & 109.1(2) \\ C12-Cu5-C23 & 110.33(13) & C12-Cu5-C23 & 103.82(15) \\ C23-Cu5-C34 & 99.34(12) & C34-Cu5-C12 & 93.75(16) \\ \hline \\ $		C2-Cu1-C24 147.86	5(18)	C2-Cu1-C24 143.8(2)		
$C-Cu-C = \begin{pmatrix} C1-Cu2-C34 & 111.05(13) \\ C12-Cu2-C34 & 96.74(12) \\ C1-Cu3-C23 & 83.0(3) \\ C1-Cu3-C13 & 120.0(6) \\ C1-Cu3-C12 & 100.5(5) \\ C1-Cu3-C23 & 126.8(5) \\ C13-Cu3-C23 & 126.8(5) \\ C12-Cu3-C23 & 99.6(3) \\ C1-Cu4-C23 & 89.64(12) \\ C1-Cu4-C23 & 89.64(12) \\ C1-Cu4-C34 & 104.37(13) \\ C23-Cu4-C34 & 112.26(14) \\ C12-Cu5-C23 & 110.33(13) \\ C12-Cu5-C34 & 105.98(14) \\ C12-Cu5-C34 & 99.34(12) \\ C12-Cu5-C12 & 100.9(2) \\ C12-Cu5-C12 & 100.34(12) \\ C12-Cu5-C12 & 90.34(12) \\ C12-Cu$		C1-Cu2-C12 103.65	5(12)	C1-Cu2-C12 110.37(19)		
$C-Cu-C \begin{bmatrix} C12-Cu2-C34 & 96.74(12) \\ C1-Cu3-C23 & 83.0(3) \\ C1-Cu3-C13 & 120.0(6) \\ C1-Cu3-C12 & 100.5(5) \\ C13-Cu3-C23 & 126.8(5) \\ C13-Cu3-C23 & 126.8(5) \\ C12-Cu3-C23 & 99.6(3) \\ C1-Cu4-C23 & 89.64(12) \\ C1-Cu4-C23 & 89.64(12) \\ C1-Cu4-C34 & 104.37(13) \\ C23-Cu4-C34 & 112.26(14) \\ C12-Cu5-C23 & 110.33(13) \\ C12-Cu5-C23 & 105.98(14) \\ C12-Cu5-C34 & 105.98(14) \\ C12-Cu5-C34 & 105.98(14) \\ C12-Cu5-C12 & 99.34(12) \\ C12-Cu5-C12 & 93.75(16) \\ C12-Cu5-C12 & 9$		C1-Cu2-C34 111.05	5(13)	C1-Cu2-C34 107.5(2)		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		C12-Cu2-C34 96.74((12)	C12-Cu2-C34 98.77(17)		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		C1-Cu3-C23 83.0(3		C12-Cu3-C23 115.68(19		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C-Cu-C	C1-Cu3-C13 120.0(<u>(5)</u>	C13-Cu3-C23 137.87(19)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C1-Cu3-C12 100.5(5)	C1-Cu3A-C23 82.84(18)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C13-Cu3-C23 126.8(5)	C1-Cu3A-C12 134.48(17)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C12-Cu3-C23 99.6(3	() (10)	C1-Cu3A-C13 124.2(2)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C1-Cu4-C23 89.64((12)	C1-Cu4-C23 = 100.9(2)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C1-Cu4-C34 = 104.3	(13)	$\begin{array}{c} C1-Cu4-C34 & I12.3(2) \\ C22-Cv4-C24 & 100.1(2) \end{array}$		
C12-Cu5-C23 110.33(13) C12-Cu5-C23 103.82(15) C23-Cu5-C34 105.98(14) C23-Cu5-C34 109.70(16) C12-Cu5-C34 99.34(12) C34-Cu5-C12 93.75(16)		C_{23} -Cu4-C34 112.20	D(14)	$\begin{bmatrix} 0.23 - 0.04 - 0.34 & 109.1(2) \\ 0.12 & 0.05 & 0.02 & 102.92(15) \end{bmatrix}$		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C12-Cu5-C25 110.53	P(13)	$\begin{array}{c} C12-Cu3-C23 & 103.82(15) \\ C22 & Cu5 & C24 & 100.70(16) \end{array}$		
C12-Cu3-C54 99.34(12) C34-Cu3-C12 95.73(10) N1 0.1 100 101		C_{23} -Cu3-C34 103.98	(14) (12)	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		
		$\frac{1012 - 003 - 034}{10070} = \frac{10070}{10070}$	12)	$\frac{100}{100} \frac{100}{100} 10$	$\frac{J(10)}{12(14)}$	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	N-Cu-N	N1-Cu1-N2 = 100.70	(11)	1N1-Cu1-IN2 101.	13(14) 72(14)	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		$\frac{107.35}{120.41}$	$\frac{r(12)}{(12)}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	73(14) 77(16)	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	C-Cu-N	C12-Cu0-IN3 = 139.01 C12-Cu6-NA = 102.2A	(13) (12)	C12 Cu0 N3 = 103.	27(10) 30(16)	

Table S3. Bond lengths and bond angles for $2 \cdot 1/2CH_2Cl_2$ and $3 \cdot CH_2Cl_2$.



Fig. S6 ORTEP drawing of **2** with atom labelling scheme. (Color labels: turquoise, Cu; purple, P; blue, N; grey, C; green, F. The hydrogen atoms are omitted for clarity.)



NCs	medium	$\begin{array}{c} \lambda_{abs} / nm \\ (\epsilon \times 10^4 / dm^3 \square mol^{-1} \square cm^{-1}) \end{array}$	$\lambda_{\rm em}$ / nm ($\tau_{\rm em}$ / μ s) (298 K)	$\lambda_{\rm em} / \rm nm$ ($\tau_{\rm em} / \mu \rm s$) (80 K)	Ф / % (298 K)
	Solid		636 (23.43)	573 (41.00)	88.5
1	CH ₂ Cl ₂	239 (4.11), 280 (3.36)	464, 614		
	DMF	226 (0.53), 277 (2.83)	438, 585		
	DMSO	226 (0.53), 274 (2.68)	460, 578		
	MeCN	229 (5.82), 258 (4.77), 284 (3.28)	437, 632		
2	Solid		611(6.68)	615 (29.21)	22.0
	CH_2Cl_2	238 (5.18), 280(3.38), 320 (2.02)	612		
	DMF	219 (0.68), 275 (2.41), 325 (1.08)	456, 615		
	DMSO	221 (0.78), 272 (3.00), 320 (1.56)	617		
	MeCN	222 (9.65), 258 (2.58), 298 (1.24)	452, 613		
	Solid		590 (6.41)	605 (27.09)	40.2
3	CH_2Cl_2	238 (4.87), 280 (3.34), 325 (2.26)	608		
	DMF	218 (0.69), 275 (2.65), 318 (1.46)	457, 613		
	DMSO	221 (0.65), 271 (2.60), 318 (1.49)	434, 615		
	MeCN	229 (9.77), 285 (3.15), 300 (2.46)	455, 612		

Table S4: Photophysical data of 1, 2 and 3 in different solvents and solid states.

Photophysical Properties Absorption spectra







Fig. S9 Absorption spectra of (a) 1, (b) 2 and (c) 3 in CH₂Cl₂ with the different concentration.



Fig. S10 Solid-state UV-vis diffuse reflectance spectroscopies of (a) 1, (b) 2 and (c) 3.

Photophysical Properties Emission spectra



Fig. S11 Contour plots of the excitation-dependent emission spectra of (a) 2 and (b) 3.

Excitation and emission spectra



Fig. S12 Temperature-dependence of the emission spectra of (a) 2 and (b) 3 (λ_{ex} =470 nm) in solid state.

Photophysical Properties Time-resolved fluorescence spectra



Fig. S13 Time-resolved fluorescence spectra of (a) 1, (b) 2 and (c) 3 at 298 K (black) and 80 K (red).

Excitation and Emission spectra



Fig. S14 Excitation spectra of (a) 1, (b) 2 and (c) 3 in the solid state at 298 and 80 K.

Excitation and Emission spectra



Fig. S15 (a) Excitation spectra of 1 at $\lambda_{em} = 446$ (black line) and 614 nm (red line), emission spectra of (b) pargyline, (c) 2 and (d) 3 in various solvents (c = 1 mM).

References

1. Sheldrick, G. M. SHELXL-97, Program for the Refinement of Crystal Structures; University of Göttingen, Göttingen, Germany, 1997.