Table S1. Crystal data and structure refinement for [Cu2Cl2(4,4,-bpy)] (**I**).

Sample Code	bc3-13a
Formula:	$Cu_2C_{10}H_8N_2Cl_2$
Formula weight:	354.16
Crystal class:	monoclinic
Space group:	$P2_1/c$ (#14)
Z	2
Cell constants:	
a	3.79610(10)Å
b	12.7478(6)Å
c	11.5244(5)Å
β	94.910(4)°
V	555.64(4)Å^3
μ	42.74 cm^{-1}
crystal size, mm	0.32 x 0.20 x 0.03
D_{calc}	2.117 g/cm^3
F(000)	348
Radiation:	Mo -K_α (λ=0.71069Å)
2θ range	6.4 – 50.68 °
hkl collected:	$-4 \le h \le 4$; $-15 \le k \le 15$; $-13 \le l \le 13$
No. reflections measured:	4499
No. unique reflections:	1000 (R_{int}=0.0451)
No. observed reflections	917 (F>4σ)
No. reflections used in refinement	1000
No. parameters	77
R indices (F>4σ)	R_1=0.0469
	wR_2=0.1155
R indices (all data)	R_1=0.0523
	wR_2=0.1189
GOF:	1.146
Final Difference Peaks, e/Å^3	+0.449, -0.707

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (angs^2) for [Cu2Cl2(C10H8N2)](**I**).

Atom	x	y	z	U_{eq}, Å^2
Cu	0.2371(2)	0.07385(6)	0.94662(7)	0.0615(3)
Cl	0.6912(3)	0.00137(10)	0.85298(10)	0.0426(4)
N1	0.1502(11)	0.2265(3)	0.9675(4)	0.0413(10)
C2	0.2542(14)	0.2773(4)	1.0668(4)	0.0468(13)
H2	0.3688(14)	0.2394(4)	1.1277(4)	0.07(2)
C3	0.1991(14)	0.3829(4)	1.0826(4)	0.0447(12)
H3	0.2755(14)	0.4143(4)	1.1531(4)	0.05(2)
C4	0.0292(12)	0.4429(4)	0.9934(4)	0.0344(10)
C5	-0.0763(14)	0.3895(4)	0.8913(4)	0.0412(11)
H5	-0.1892(14)	0.4255(4)	0.8285(4)	0.05(2)
C6	-0.0149(14)	0.2840(4)	0.8828(4)	0.0463(12)
H6	-0.0931(14)	0.2504(4)	0.8137(4)	0.05(2)

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*c$

Table S3. Bond lengths [A] and angles [deg] for [Cu2Cl2(C10H8N2)](**I**).

Cu-N1	1.991(4)	Cu-Cl	2.3039(14)	Cu-Cl#1	2.4351(14)
Cu-Cl#2	2.4939(14)	Cu-Cu#2	2.9364(14)	Cu-Cu#3	2.946(2)
Cl-Cu#4	2.4351(14)	Cl-Cu#2	2.4939(14)	N1-C6	1.334(6)
N1-C2	1.345(6)	C2-C3	1.376(8)	C3-C4	1.395(7)
C4-C5	1.388(6)	C4-C4#5	1.483(9)	C5-C6	1.371(7)

N1-Cu-Cl	125.92(13)	N1-Cu-Cl#1	106.31(12)	Cl-Cu-Cl#1	106.42(5)
N1-Cu-Cl#2	105.65(12)	Cl-Cu-Cl#2	104.64(4)	Cl#1-Cu-Cl#2	106.61(4)
N1-Cu-Cu#2	133.59(12)	Cl-Cu-Cu#2	55.26(4)	Cl#1-Cu-Cu#2	117.68(5)
Cl#2-Cu-Cu#2	49.39(4)	N1-Cu-Cu#3	117.42(13)	Cl-Cu-Cu#3	116.60(5)
Cl#1-Cu-Cu#3	54.22(4)	Cl#2-Cu-Cu#3	52.39(4)	Cu#2-Cu-Cu#3	80.38(4)
Cu-Cl-Cu#4	106.43(5)	Cu-Cl-Cu#2	75.36(4)	Cu#4-Cl-Cu#2	73.39(4)
C6-N1-C2	116.3(4)	C6-N1-Cu	121.4(3)	C2-N1-Cu	122.3(3)
N1-C2-C3	123.2(5)	C2-C3-C4	120.3(5)	C5-C4-C3	116.0(4)
C5-C4-C4#5	122.2(5)	C3-C4-C4#5	121.8(5)	C6-C5-C4	120.2(5)
N1-C6-C5	124.0(5)				

Table S4. Anisotropic displacement parameters (angs^2) for [Cu2Cl2(C10H8N2)](**I**).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu	0.0708(6)	0.0451(5)	0.0674(6)	-0.0087(3)	-0.0025(4)	0.0124(3)
Cl	0.0382(6)	0.0523(8)	0.0364(6)	-0.0036(5)	-0.0024(5)	0.0029(5)
N1	0.042(2)	0.037(2)	0.044(2)	0.001(2)	0.000(2)	0.002(2)
C2	0.052(3)	0.043(3)	0.043(3)	0.004(2)	-0.010(2)	0.006(2)
C3	0.055(3)	0.038(3)	0.038(2)	-0.001(2)	-0.009(2)	0.002(2)
C4	0.035(2)	0.034(3)	0.035(2)	-0.002(2)	0.003(2)	-0.001(2)
C5	0.051(3)	0.037(3)	0.034(2)	-0.001(2)	-0.003(2)	0.006(2)
C6	0.054(3)	0.047(3)	0.038(3)	-0.005(2)	-0.001(2)	0.004(2)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table S5. Crystal data and structure refinement for [Cu2Br2(4,4,-bpy)] (**II**).

Sample Code	j-121a
Empirical formula	C10 H8 Br2 Cu2 N2
Formula weight	443.08
Temperature	293(2) K
Wavelength	0.71073 Angs
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 3.9090(8) Angs alpha = 90 deg. b = 12.752(3) Angs beta = 94.05(3) deg. c = 11.905(2) Angs gamma = 90 deg.
Volume	592.0(2) Angs^3
Z, Calculated density	2, 2.486 g/cm^3
Absorption coefficient	10.311 mm^-1
F(000)	420
Crystal size	0.05 x 0.1 x 0.5 mm
Theta range for data collection	3.20 to 24.96 deg.
Index ranges	-1<=h<=4, -2<=k<=15, -14<=l<=14
Reflections collected / unique	1206 / 1041 [R(int) = 0.0159]
Completeness to 2theta = 24.96	95.2%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1041 / 0 / 74
Goodness-of-fit on F^2	1.772
Final R indices [I>4sigma(I)]	R1 = 0.0297, wR2 = 0.0481
R indices (all data)	R1 = 0.0422, wR2 = 0.0496
Extinction coefficient	0.0005(4)
Largest diff. peak and hole	0.373 and -0.593 e.A^-3

Table S6. Atomic coordinates and equivalent isotropic displacement parameters (angs^2) for [Cu2Br2(C10H8N2)](**II**).

atom	x	y	z	U(eq)	s.o.f.
Br(1)	0.19469(12)	0.50444(4)	0.34746(4)	0.03784(16)	1
Cu(1)	0.26651(19)	0.42729(5)	0.54390(5)	0.0523(2)	1
N(1)	0.3426(10)	0.2726(3)	0.5272(3)	0.0369(10)	1
C(1)	0.4678(12)	0.0574(3)	0.5057(4)	0.0299(10)	1
C(2)	0.5044(13)	0.2168(4)	0.6104(4)	0.0419(13)	1
C(3)	0.5691(12)	0.1117(4)	0.6027(4)	0.0368(13)	1
C(4)	0.3022(13)	0.1157(4)	0.4198(4)	0.0437(14)	1
C(5)	0.2494(13)	0.2205(4)	0.4341(4)	0.0434(13)	1

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S7. Bond lengths [A] and angles [deg] for [Cu2Br2(C10H8N2)](**II**).

Br(1)-Cu(1)#1	2.4516(10)
Br(1)-Cu(1)	2.5344(9)
Br(1)-Cu(1)#2	2.5460(11)
Cu(1)-N(1)	2.007(4)
Cu(1)-Br(1)#1	2.4516(10)
Cu(1)-Br(1)#2	2.5460(11)
Cu(1)-Cu(1)#2	2.8518(15)
Cu(1)-Cu(1)#1	2.9266(14)
N(1)-C(5)	1.322(5)
N(1)-C(2)	1.341(5)
C(1)-C(3)	1.380(6)
C(1)-C(4)	1.386(6)
C(1)-C(1)#3	1.494(8)
C(2)-C(3)	1.368(6)
C(4)-C(5)	1.364(6)

Cu(1)#1-Br(1)-Cu(1)	71.86(3)
Cu(1)#1-Br(1)-Cu(1)#2	102.90(3)
Cu(1)-Br(1)-Cu(1)#2	68.30(4)
N(1)-Cu(1)-Br(1)#1	121.40(12)
N(1)-Cu(1)-Br(1)	107.31(11)
Br(1)#1-Cu(1)-Br(1)	108.14(3)
N(1)-Cu(1)-Br(1)#2	105.27(12)

Br(1)#1-Cu(1)-Br(1)#2	102.90(3)
Br(1)-Cu(1)-Br(1)#2	111.70(4)
N(1)-Cu(1)-Cu(1)#2	119.97(12)
Br(1)#1-Cu(1)-Cu(1)#2	118.43(4)
Br(1)-Cu(1)-Cu(1)#2	56.04(3)
Br(1)#2-Cu(1)-Cu(1)#2	55.66(3)
N(1)-Cu(1)-Cu(1)#1	133.96(12)
Br(1)#1-Cu(1)-Cu(1)#1	55.38(3)
Br(1)-Cu(1)-Cu(1)#1	52.76(3)
Br(1)#2-Cu(1)-Cu(1)#1	120.49(4)
Cu(1)#2-Cu(1)-Cu(1)#1	85.13(4)
C(5)-N(1)-C(2)	116.1(4)
C(5)-N(1)-Cu(1)	122.9(3)
C(2)-N(1)-Cu(1)	120.9(3)
C(3)-C(1)-C(4)	116.1(4)
C(3)-C(1)-C(1)#3	121.8(5)
C(4)-C(1)-C(1)#3	122.1(5)
N(1)-C(2)-C(3)	123.4(4)
C(2)-C(3)-C(1)	120.3(4)
C(5)-C(4)-C(1)	120.0(4)
N(1)-C(5)-C(4)	124.2(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+1 #2 -x+1,-y+1,-z+1
#3 -x+1,-y,-z+1

Table S8. Anisotropic displacement parameters (angs^2) for [Cu2Br2(C10H8N2)](**II**).

atom	U11	U22	U33	U23	U13	U12
Br(1)	0.0327(3)	0.0469(3)	0.0331(3)	-0.0026(3)	-0.00372(18)	0.0030(3)
Cu(1)	0.0600(5)	0.0380(4)	0.0578(4)	-0.0061(3)	-0.0025(3)	0.0084(4)
N(1)	0.038(3)	0.031(2)	0.041(2)	-0.002(2)	-0.0012(19)	0.001(2)
C(1)	0.027(3)	0.030(2)	0.033(2)	0.000(2)	0.006(2)	-0.001(3)
C(2)	0.057(4)	0.031(3)	0.036(3)	-0.007(2)	-0.004(3)	0.004(3)
C(3)	0.047(3)	0.033(3)	0.030(3)	0.005(2)	-0.004(2)	-0.001(3)
C(4)	0.057(4)	0.030(3)	0.042(3)	-0.009(2)	-0.019(3)	0.002(3)
C(5)	0.053(4)	0.035(3)	0.040(3)	0.003(2)	-0.012(3)	0.006(3)

The anisotropic displacement factor exponent takes the form:
-2 p^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

Table S9. Crystal data and structure refinement for [(CuBr)(4,4'-bpy)](**III**).

Sample Code	j-121c
Empirical formula	C10 H8 Br Cu N2
Formula weight	299.63
Temperature	293(2) K
Wavelength	0.71073 Angs
Crystal system, space group	Tetragonal, I4(1)/acd
Unit cell dimensions	a = 14.406(2) Angs alpha = 90 deg. b = 14.406(2) Angs beta = 90 deg. c = 38.524(8) Angs gamma = 90 deg.
Volume	7995(2) Angs^3
Z, Calculated density	32, 1.991 g/cm^3
Absorption coefficient	6.140 mm^-1
F(000)	4672
Crystal size	0.2 x 0.5 x 0.5 mm
Theta range for data collection	3.02 to 24.96 deg.
Index ranges	-2<=h<=17, 0<=k<=17, -4<=l<=45
Reflections collected / unique	3411 / 1761 [R(int) = 0.0210]
Completeness to 2theta = 24.96	43.2%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1761 / 0 / 122
Goodness-of-fit on F^2	1.916
Final R indices [I>4sigma(I)]	R1 = 0.0303, wR2 = 0.0520
R indices (all data)	R1 = 0.0522, wR2 = 0.0537
Extinction coefficient	0.000339(10)
Largest diff. peak and hole	0.467 and -0.471 e.A^-3

Table S10. Atomic coordinates and equivalent isotropic displacement parameters (angs^2) for [(CuBr)(C10H8N2)](**III**).

atom	x	y	z	U(eq)	s.o.f.
Br(1)	0.60405(3)	0.34706(3)	0.031306(13)	0.04675(17)	1
Cu(2)	0.43207(4)	0.32059(4)	0.017750(14)	0.04506(19)	1
N(1)	0.4111(2)	0.3376(2)	-0.03243(8)	0.0351(8)	1
N(2)	0.3738(2)	0.3939(3)	0.05607(9)	0.0375(9)	1
C(1)	0.4062(3)	0.3432(3)	-0.10579(9)	0.0296(9)	1
C(2)	0.32175(16)	0.46939(17)	0.05022(6)	0.0394(12)	1
C(3)	0.28982(16)	0.49164(17)	0.11072(6)	0.0281(10)	1
C(4)	0.34574(16)	0.41434(17)	0.11668(6)	0.0357(11)	1
C(5)	0.2798(3)	0.5182(3)	0.07684(10)	0.0355(11)	1
C(6)	0.3846(3)	0.3693(3)	0.08936(10)	0.0402(11)	1
C(7)	0.4550(3)	0.4029(3)	-0.05114(13)	0.0421(12)	1
C(8)	0.3585(4)	0.2771(3)	-0.08707(13)	0.0465(13)	1
C(9)	0.4544(3)	0.4083(3)	-0.08637(12)	0.0398(12)	1
C(10)	0.3627(4)	0.2772(3)	-0.05155(13)	0.0500(14)	1

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S11. Bond lengths [A] and angles [deg] for [(CuBr)(C10H8N2)](**III**).

Br(1)-Cu(2)#1	2.5253(9)
Br(1)-Cu(2)	2.5605(9)
Cu(2)-N(1)	1.972(3)
Cu(2)-N(2)	2.000(3)
Cu(2)-Br(1)#1	2.5252(9)
Cu(2)-Cu(2)#1	2.8227(12)
N(1)-C(10)	1.337(5)
N(1)-C(7)	1.343(5)
N(2)-C(6)	1.339(5)
N(2)-C(2)	1.340(4)
C(1)-C(8)	1.378(6)
C(1)-C(9)	1.386(6)
C(1)-C(1)#2	1.480(7)
C(2)-C(5)	1.382(4)
C(3)-C(5)	1.368(4)
C(3)-C(4)	1.3935

C(3)-C(3)#3	1.474(5)
C(4)-C(6)	1.358(4)
C(7)-C(9)	1.359(6)
C(8)-C(10)	1.370(6)

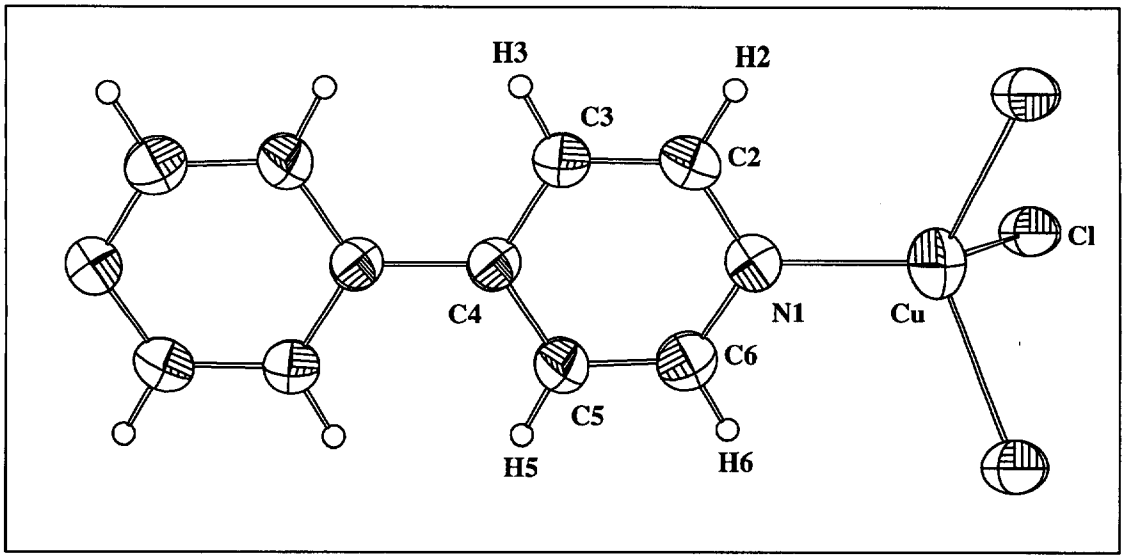
Cu(2)#1-Br(1)-Cu(2)	67.42(2)
N(1)-Cu(2)-N(2)	126.43(14)
N(1)-Cu(2)-Br(1)#1	106.87(11)
N(2)-Cu(2)-Br(1)#1	105.43(11)
N(1)-Cu(2)-Br(1)	109.24(11)
N(2)-Cu(2)-Br(1)	100.18(11)
Br(1)#1-Cu(2)-Br(1)	107.44(2)
N(1)-Cu(2)-Cu(2)#1	101.28(9)
N(2)-Cu(2)-Cu(2)#1	132.19(10)
Br(1)#1-Cu(2)-Cu(2)#1	56.89(2)
Br(1)-Cu(2)-Cu(2)#1	55.69(2)
C(10)-N(1)-C(7)	113.9(4)
C(10)-N(1)-Cu(2)	122.6(3)
C(7)-N(1)-Cu(2)	122.8(3)
C(6)-N(2)-C(2)	116.1(3)
C(6)-N(2)-Cu(2)	121.2(3)
C(2)-N(2)-Cu(2)	122.6(2)
C(8)-C(1)-C(9)	115.8(4)
C(8)-C(1)-C(1)#2	122.0(5)
C(9)-C(1)-C(1)#2	122.2(5)
N(2)-C(2)-C(5)	122.2(3)
C(5)-C(3)-C(4)	116.2(2)
C(5)-C(3)-C(3)#3	122.0(3)
C(4)-C(3)-C(3)#3	121.71(19)
C(6)-C(4)-C(3)	119.5(2)
C(3)-C(5)-C(2)	121.3(3)
N(2)-C(6)-C(4)	124.6(4)
N(1)-C(7)-C(9)	125.0(4)
C(10)-C(8)-C(1)	120.0(4)
C(7)-C(9)-C(1)	120.2(4)
N(1)-C(10)-C(8)	125.0(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1/2,z+0 #2 -y+3/4,-x+3/4,-z-1/4
#3 y-1/4,x+1/4,-z+1/4

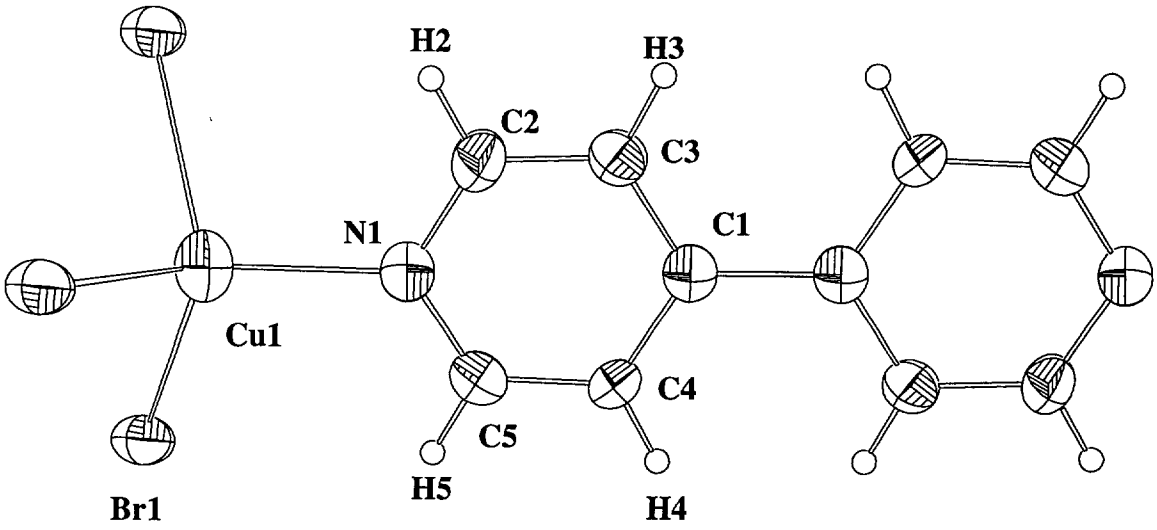
Table S12. Anisotropic displacement parameters (angs^2) for [(CuBr)(C10H8N2)](**III**).

atom	U11	U22	U33	U23	U13	U12
Br(1)	0.0426(3)	0.0452(3)	0.0525(3)	-0.0125(3)	-0.0085(3)	-0.0057(2)
Cu(2)	0.0548(4)	0.0510(4)	0.0294(3)	-0.0053(3)	0.0045(3)	0.0052(3)
N(1)	0.040(2)	0.035(2)	0.030(2)	0.0007(19)	-0.0015(19)	0.0027(16)
N(2)	0.038(2)	0.044(2)	0.030(2)	-0.0023(18)	0.0041(18)	0.0062(18)
C(1)	0.031(3)	0.033(3)	0.025(2)	-0.001(2)	-0.002(2)	0.0053(18)
C(2)	0.040(3)	0.048(3)	0.030(3)	0.003(2)	-0.001(2)	0.006(2)
C(3)	0.025(2)	0.032(2)	0.028(2)	-0.0002(18)	0.0011(17)	-0.0039(19)
C(4)	0.042(3)	0.039(3)	0.026(3)	0.004(2)	0.001(2)	0.009(2)
C(5)	0.040(3)	0.038(3)	0.029(2)	0.003(2)	0.001(2)	0.0137(19)
C(6)	0.048(3)	0.044(3)	0.028(3)	0.001(2)	0.003(2)	0.017(2)
C(7)	0.049(3)	0.037(3)	0.041(3)	-0.004(2)	-0.004(3)	-0.006(2)
C(8)	0.061(3)	0.044(3)	0.034(3)	0.002(2)	-0.007(3)	-0.019(3)
C(9)	0.050(3)	0.042(3)	0.027(3)	0.003(2)	0.000(2)	-0.009(2)
C(10)	0.059(3)	0.052(3)	0.039(4)	0.010(3)	-0.006(3)	-0.017(3)

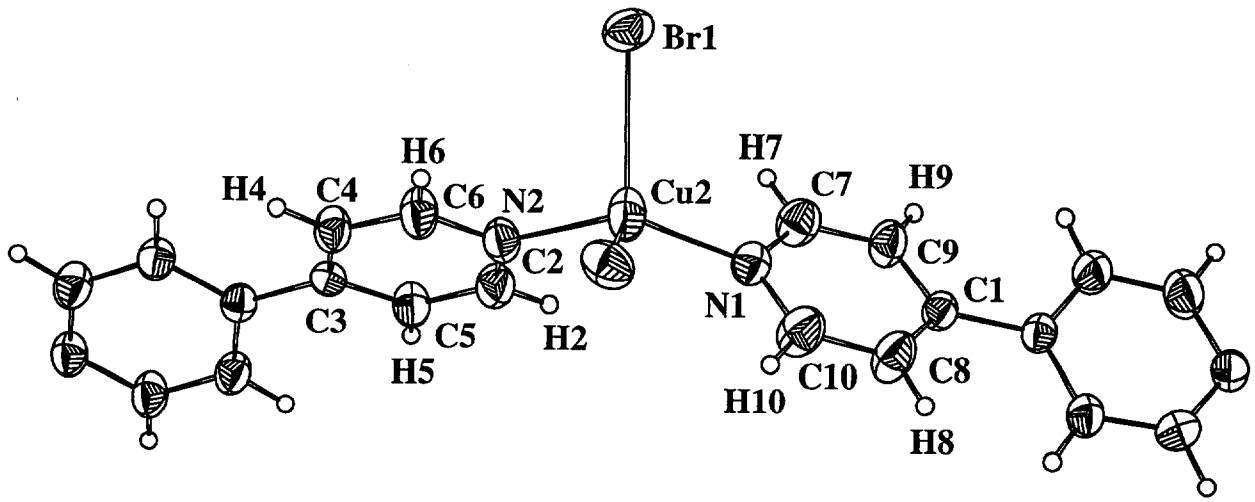
The anisotropic displacement factor exponent takes the form:
-2 p^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]



ORTEP drawing of **I** with thermal vibrational ellipsoids (50%)



ORTEP drawing of **II** with thermal vibrational ellipsoids (50%)



ORTEP drawing of **III** with thermal vibrational ellipsoids (50%)