Supplementary Material (ESI) for Chemical Communications

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β-sheet recognition in the non-interpenetrated and interpenetrated two-dimensional coordination networks containing cavities

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Supplementary Information

ORTEP drawings and crystallographic tables for **2**, **3** and **4**,
TGA plot for complex **2** and syntheses of **2** and **3** (19 pages)

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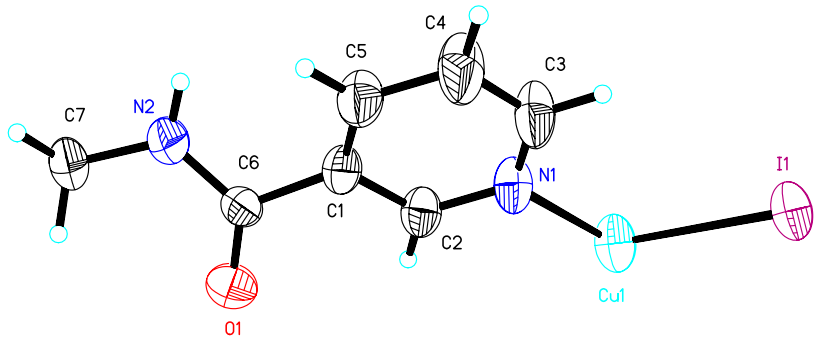


Fig. S1. Ortep drawing of complex **2**

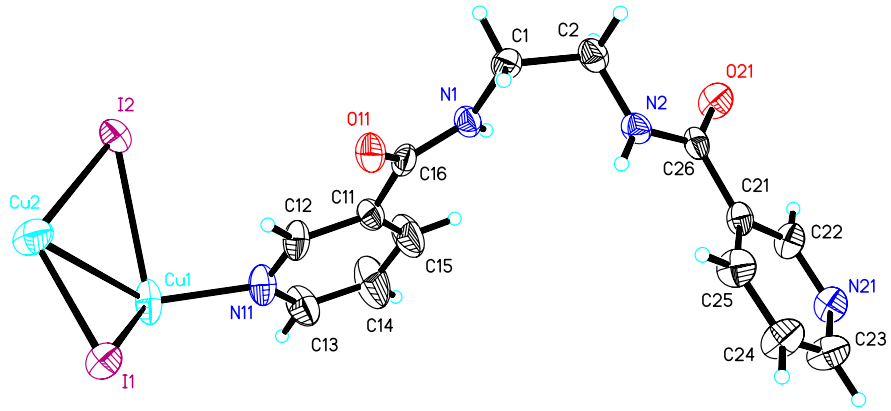


Fig. S2. Ortep drawing of complex **3**

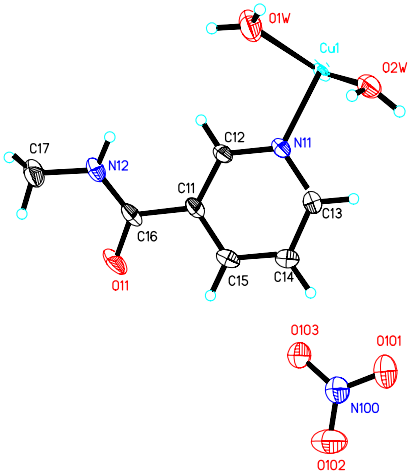


Fig. S3. Ortep drawing of complex **4**

Supplementary Material (ESI) for Chemical Communications

Table 1.1. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C31 H31 Cl9 Cu2 I2 N8 O4	
Formula weight	1279.57	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/m	
Unit cell dimensions	a = 9.6490(19) Å	α= 90°.
	b = 15.559(3) Å	β= 91.96(3)°.
	c = 15.163(3) Å	γ = 90°.
Volume	2275.1(8) $Å^3$	
Z	2	
Density (calculated)	1.868 Mg/m^3	
Absorption coefficient	2.864 mm^{-1}	
F(000)	1244	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.34 to 24.97°.	
Index ranges	0<=h<=11, 0<=k<=18, -18<=l<=18	
Reflections collected	2064	
Independent reflections	1933 [R(int) = 0.0353]	
Completeness to theta = 24.97°	92.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1933 / 0 / 103	
Goodness-of-fit on F^2	0.848	
Final R indices [I>2sigma(I)]	R1 = 0.0485, wR2 = 0.1277	
R indices (all data)	R1 = 0.0666, wR2 = 0.1467	
Largest diff. peak and hole	0.793 and -0.747 $e.Å^{-3}$	

Table 1.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	8427(1)	-5000	-1133(1)	63(1)
Cu(1)	8938(1)	-5000	568(1)	61(1)
O(1)	9502(4)	-2973(4)	3531(3)	68(1)
N(1)	8065(6)	-3910(3)	1118(3)	57(1)
N(2)	7437(5)	-2383(4)	3780(3)	58(1)
C(1)	7832(6)	-2961(4)	2345(4)	48(1)
C(2)	8443(7)	-3659(4)	1927(4)	52(1)
C(3)	7083(8)	-3437(5)	681(4)	71(2)
C(4)	6476(9)	-2738(6)	1054(4)	88(3)
C(5)	6870(7)	-2482(5)	1888(4)	64(2)
C(6)	8354(5)	-2767(4)	3282(3)	45(1)
C(7)	7765(7)	-2167(5)	4699(4)	62(2)

Table 1.3. Bond lengths [Å] and angles [°] for **2**.

I(1)-Cu(1)	2.6085(13)	N(1)#2-Cu(1)-I(1)#1	105.47(15)
I(1)-Cu(1)#1	2.6554(15)	N(1)-Cu(1)-I(1)#1	105.47(15)
Cu(1)-N(1)#2	2.081(5)	I(1)-Cu(1)-I(1)#1	117.73(5)
Cu(1)-N(1)	2.081(5)	N(1)#2-Cu(1)-Cu(1)#1	125.29(15)
Cu(1)-I(1)#1	2.6554(15)	N(1)-Cu(1)-Cu(1)#1	125.29(15)
Cu(1)-Cu(1)#1	2.722(3)	I(1)-Cu(1)-Cu(1)#1	59.71(5)
O(1)-C(6)	1.202(7)	I(1)#1-Cu(1)-Cu(1)#1	58.02(5)
N(1)-C(2)	1.326(7)	C(2)-N(1)-C(3)	117.2(5)
N(1)-C(3)	1.355(8)	C(2)-N(1)-Cu(1)	120.6(4)
N(2)-C(6)	1.326(7)	C(3)-N(1)-Cu(1)	122.2(4)
N(2)-C(7)	1.458(8)	C(6)-N(2)-C(7)	121.4(5)
C(1)-C(5)	1.361(8)	C(5)-C(1)-C(2)	119.0(6)
C(1)-C(2)	1.399(8)	C(5)-C(1)-C(6)	124.5(5)
C(1)-C(6)	1.521(8)	C(2)-C(1)-C(6)	116.5(5)
C(3)-C(4)	1.367(10)	N(1)-C(2)-C(1)	122.8(6)
C(4)-C(5)	1.367(9)	N(1)-C(3)-C(4)	122.2(6)
C(7)-C(7)#3	1.483(15)	C(3)-C(4)-C(5)	120.3(6)
		C(1)-C(5)-C(4)	118.4(6)
Cu(1)-I(1)-Cu(1)#1	62.27(5)	O(1)-C(6)-N(2)	124.6(5)
N(1)#2-Cu(1)-N(1)	109.2(3)	O(1)-C(6)-C(1)	120.9(5)
N(1)#2-Cu(1)-I(1)	109.36(14)	N(2)-C(6)-C(1)	114.5(5)
N(1)-Cu(1)-I(1)	109.36(14)	N(2)-C(7)-C(7)#3	111.0(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y-1,-z #2 x,-y-1,z #3 -x+3/2,-y-1/2,-z+1

Table 1.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	87(1)	58(1)	43(1)	0	-10(1)	0
Cu(1)	92(1)	45(1)	46(1)	0	-2(1)	0
O(1)	50(2)	88(4)	66(3)	-9(3)	-14(2)	7(2)
N(1)	80(4)	48(3)	44(3)	-10(2)	2(2)	2(3)
N(2)	54(3)	73(4)	46(3)	-12(2)	-7(2)	9(3)
C(1)	55(3)	46(3)	42(3)	-2(2)	9(2)	1(3)
C(2)	67(4)	49(3)	40(3)	5(3)	3(3)	4(3)
C(3)	112(6)	61(4)	38(3)	-4(3)	-12(3)	31(4)
C(4)	122(7)	96(6)	45(4)	-6(4)	-18(4)	60(5)
C(5)	77(4)	65(4)	49(3)	-5(3)	-7(3)	28(4)
C(6)	38(3)	57(3)	41(3)	0(3)	1(2)	-7(3)
C(7)	68(4)	66(4)	51(4)	-20(3)	-5(3)	-3(3)

Table 1.5. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **2**.

	x	y	z	U(eq)
H(2)	6631	-2259	3557	69
H(2A)	9145	-3960	2228	62
H(3)	6814	-3592	109	85
H(4)	5792	-2434	739	106
H(5)	6490	-1994	2137	76
H(7A)	7354	-1616	4837	74
H(7B)	8762	-2116	4788	74

Table 2.1. Crystal data and structure refinement for **3**.

Identification code	**3**	
Empirical formula	C14 H14 Cu2 I2 N4 O2	
Formula weight	651.17	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2/c	
Unit cell dimensions	a = 11.312(2) Å	α= 90°.
	b = 10.012(2) Å	β= 97.25(3)°.
	c = 16.597(3) Å	γ = 90°.
Volume	1864.7(6) Å^3	
Z	4	
Density (calculated)	2.320 Mg/m^3	
Absorption coefficient	5.606 mm^{-1}	
F(000)	1224	
Crystal size	0.10 x 0.08 x 0.08 mm^3	
Theta range for data collection	2.03 to 24.97°.	
Index ranges	0<=h<=13, 0<=k<=11, -19<=l<=19	
Reflections collected	3247	
Independent reflections	3078 [R(int) = 0.0632]	
Completeness to theta = 24.97°	93.9 %	
Absorption correction	None	
Max. and min. transmission	0.6041 and 0.4868	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3078 / 0 / 217	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.1003	
R indices (all data)	R1 = 0.0524, wR2 = 0.1101	
Largest diff. peak and hole	1.115 and -1.075 e.Å^{-3}	

Table 2.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	-2178(1)	8797(1)	-2319(1)	43(1)
I(2)	532(1)	6040(1)	-1053(1)	42(1)
Cu(1)	-1204(1)	6487(1)	-2542(1)	52(1)
Cu(2)	-20(1)	8321(1)	-1680(1)	56(1)
N(1)	-3827(4)	3041(5)	37(3)	35(1)
N(2)	-6023(4)	1941(5)	486(3)	35(1)
C(1)	-4122(6)	3085(6)	855(4)	39(1)
C(2)	-4917(6)	1908(6)	1014(4)	39(1)
O(11)	-3497(4)	5242(4)	-31(3)	42(1)
C(11)	-3207(6)	3955(6)	-1201(4)	39(1)
C(12)	-2634(6)	5008(6)	-1517(4)	43(2)
N(11)	-2290(5)	5001(6)	-2261(4)	49(1)
C(13)	-2555(9)	3926(7)	-2726(5)	60(2)
C(14)	-3113(10)	2845(9)	-2443(6)	85(3)
C(15)	-3433(8)	2832(8)	-1664(5)	68(2)
C(16)	-3529(5)	4129(6)	-338(4)	35(1)
O(21)	-6303(4)	-271(4)	512(3)	45(1)
C(21)	-7827(5)	1017(5)	-219(4)	33(1)
C(22)	-8394(6)	-111(6)	-557(4)	40(1)
N(21)	-9436(5)	-94(5)	-1020(3)	40(1)
C(23)	-9978(7)	1079(6)	-1137(5)	51(2)
C(24)	-9518(6)	2250(7)	-816(5)	54(2)
C(25)	-8422(6)	2217(6)	-346(4)	48(2)
C(26)	-6646(5)	846(6)	297(4)	33(1)

Table 2.3. Bond lengths [Å] and angles [°] for **3**.

I(1)-Cu(2)	2.5802(12)	C(24)-C(25)	1.379(10)
I(1)-Cu(1)	2.6090(11)		
I(2)-Cu(2)	2.5542(11)	Cu(2)-I(1)-Cu(1)	60.00(3)
I(2)-Cu(1)#1	2.5814(11)	Cu(2)-I(2)-Cu(1)#1	64.01(3)
I(2)-Cu(1)	2.9904(15)	Cu(2)-I(2)-Cu(1)	55.13(3)
Cu(1)-N(11)	2.020(6)	Cu(1)#1-I(2)-Cu(1)	57.63(4)
Cu(1)-I(2)#1	2.5814(11)	N(11)-Cu(1)-I(2)#1	109.74(17)
Cu(1)-Cu(2)	2.5947(13)	N(11)-Cu(1)-Cu(2)	132.86(18)
Cu(1)-Cu(1)#1	2.7092(19)	I(2)#1-Cu(1)-Cu(2)	115.52(4)
Cu(1)-Cu(2)#1	2.7220(14)	N(11)-Cu(1)-I(1)	109.86(17)
Cu(2)-N(21)#2	1.992(5)	I(2)#1-Cu(1)-I(1)	117.38(4)
Cu(2)-Cu(1)#1	2.7220(14)	Cu(2)-Cu(1)-I(1)	59.45(3)
Cu(2)-Cu(2)#1	2.729(2)	N(11)-Cu(1)-Cu(1)#1	128.65(18)
N(1)-C(16)	1.320(8)	I(2)#1-Cu(1)-Cu(1)#1	68.79(4)
N(1)-C(1)	1.439(8)	Cu(2)-Cu(1)-Cu(1)#1	61.71(4)
N(2)-C(26)	1.319(7)	I(1)-Cu(1)-Cu(1)#1	115.63(2)
N(2)-C(2)	1.435(8)	N(11)-Cu(1)-Cu(2)#1	165.13(18)
C(1)-C(2)	1.526(8)	I(2)#1-Cu(1)-Cu(2)#1	57.51(3)
O(11)-C(16)	1.224(7)	Cu(2)-Cu(1)-Cu(2)#1	61.72(5)
C(11)-C(15)	1.367(10)	I(1)-Cu(1)-Cu(2)#1	73.65(4)
C(11)-C(12)	1.376(9)	Cu(1)#1-Cu(1)-Cu(2)#1	57.08(3)
C(11)-C(16)	1.531(10)	N(11)-Cu(1)-I(2)	93.11(18)
C(12)-N(11)	1.341(9)	I(2)#1-Cu(1)-I(2)	118.92(4)
N(11)-C(13)	1.336(9)	Cu(2)-Cu(1)-I(2)	53.86(3)
C(13)-C(14)	1.366(11)	I(1)-Cu(1)-I(2)	105.07(3)
C(14)-C(15)	1.386(12)	Cu(1)#1-Cu(1)-I(2)	53.58(4)
O(21)-C(26)	1.222(7)	Cu(2)#1-Cu(1)-I(2)	99.96(4)
C(21)-C(22)	1.381(8)	N(21)#2-Cu(2)-I(2)	116.18(16)
C(21)-C(25)	1.380(9)	N(21)#2-Cu(2)-I(1)	108.04(16)
C(21)-C(26)	1.503(9)	I(2)-Cu(2)-I(1)	120.17(4)
C(22)-N(21)	1.324(8)	N(21)#2-Cu(2)-Cu(1)	168.27(16)
N(21)-C(23)	1.328(8)	I(2)-Cu(2)-Cu(1)	71.01(4)
N(21)-Cu(2)#3	1.992(5)	I(1)-Cu(2)-Cu(1)	60.55(4)
C(23)-C(24)	1.364(9)	N(21)#2-Cu(2)-Cu(1)#1	130.15(16)

I(2)-Cu(2)-Cu(1)#1	58.48(3)	N(11)-C(13)-C(14)	121.3(7)
I(1)-Cu(2)-Cu(1)#1	116.17(4)	C(13)-C(14)-C(15)	121.0(8)
Cu(1)-Cu(2)-Cu(1)#1	61.22(5)	C(11)-C(15)-C(14)	117.7(7)
N(21)#2-Cu(2)-Cu(2)#1	120.13(17)	O(11)-C(16)-N(1)	123.4(6)
I(2)-Cu(2)-Cu(2)#1	111.87(3)	O(11)-C(16)-C(11)	119.7(5)
I(1)-Cu(2)-Cu(2)#1	73.97(5)	N(1)-C(16)-C(11)	116.9(5)
Cu(1)-Cu(2)-Cu(2)#1	61.43(4)	C(22)-C(21)-C(25)	117.2(6)
Cu(1)#1-Cu(2)-Cu(2)#1	56.85(4)	C(22)-C(21)-C(26)	118.1(5)
C(16)-N(1)-C(1)	121.6(5)	C(25)-C(21)-C(26)	124.5(5)
C(26)-N(2)-C(2)	121.7(5)	N(21)-C(22)-C(21)	124.0(6)
N(1)-C(1)-C(2)	110.6(5)	C(22)-N(21)-C(23)	117.2(5)
N(2)-C(2)-C(1)	111.4(5)	C(22)-N(21)-Cu(2)#3	121.2(4)
C(15)-C(11)-C(12)	118.6(7)	C(23)-N(21)-Cu(2)#3	120.6(4)
C(15)-C(11)-C(16)	124.7(6)	N(21)-C(23)-C(24)	123.8(7)
C(12)-C(11)-C(16)	116.6(6)	C(23)-C(24)-C(25)	118.2(6)
N(11)-C(12)-C(11)	123.6(6)	C(24)-C(25)-C(21)	119.5(6)
C(13)-N(11)-C(12)	117.7(6)	O(21)-C(26)-N(2)	123.3(6)
C(13)-N(11)-Cu(1)	124.0(5)	O(21)-C(26)-C(21)	119.8(5)
C(12)-N(11)-Cu(1)	117.7(4)	N(2)-C(26)-C(21)	116.8(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z-1/2 #2 x+1,y+1,z #3 x-1,y-1,z

Table 2.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	40(1)	42(1)	48(1)	-9(1)	3(1)	2(1)
I(2)	47(1)	36(1)	45(1)	7(1)	13(1)	4(1)
Cu(1)	58(1)	40(1)	63(1)	-13(1)	29(1)	-19(1)
Cu(2)	67(1)	31(1)	64(1)	-14(1)	-17(1)	3(1)
N(1)	35(3)	29(3)	41(3)	6(2)	7(2)	-2(2)
N(2)	42(3)	24(2)	38(3)	5(2)	4(2)	-2(2)
C(1)	40(3)	36(3)	38(3)	-1(3)	-2(3)	-8(3)
C(2)	41(3)	33(3)	45(4)	8(3)	11(3)	2(3)
O(11)	47(2)	25(2)	55(3)	-2(2)	10(2)	-6(2)
C(11)	43(3)	27(3)	47(4)	8(3)	4(3)	-4(2)
C(12)	44(3)	33(3)	55(4)	-12(3)	15(3)	-13(3)
N(11)	52(3)	35(3)	64(4)	-6(3)	17(3)	-12(3)
C(13)	88(6)	45(4)	49(4)	-4(3)	21(4)	-15(4)
C(14)	141(9)	48(5)	72(6)	-23(4)	37(6)	-45(6)
C(15)	103(7)	41(4)	62(5)	2(4)	17(5)	-30(4)
C(16)	26(3)	27(3)	50(4)	2(3)	-1(3)	-6(2)
O(21)	47(3)	25(2)	62(3)	-2(2)	0(2)	0(2)
C(21)	38(3)	22(3)	40(3)	-4(2)	9(3)	-8(2)
C(22)	38(3)	30(3)	51(4)	-10(3)	7(3)	-3(3)
N(21)	45(3)	24(3)	50(3)	-11(2)	5(3)	-2(2)
C(23)	54(4)	34(4)	61(5)	-9(3)	-13(4)	4(3)
C(24)	49(4)	25(3)	83(5)	-8(3)	-9(4)	7(3)
C(25)	58(4)	29(3)	53(4)	-11(3)	0(3)	-4(3)
C(26)	39(3)	32(3)	30(3)	-4(2)	13(2)	-9(3)

Table 2.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3**.

	x	y	z	U(eq)
H(1)	-3846	2288	-213	42
H(2)	-6287	2693	289	42
H(1A)	-4530	3915	940	46
H(1B)	-3396	3057	1235	46
H(2A)	-4505	1079	932	47
H(2B)	-5077	1933	1575	47
H(12)	-2476	5765	-1197	52
H(13)	-2356	3914	-3253	71
H(14)	-3281	2107	-2778	102
H(15)	-3789	2087	-1463	82
H(22)	-8021	-931	-451	48
H(23)	-10715	1103	-1456	62
H(24)	-9932	3049	-910	65
H(25)	-8085	2998	-117	57

Table 3.1. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C14 H22 Cu N6 O12	
Formula weight	529.92	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 10.214(2) Å	α= 90°.
	b = 7.1250(14) Å	β= 99.98(3)°.
	c = 14.425(3) Å	γ = 90°.
Volume	1033.9(4) Å^3	
Z	2	
Density (calculated)	1.702 Mg/m^3	
Absorption coefficient	1.134 mm^{-1}	
F(000)	546	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	2.27 to 24.97°.	
Index ranges	0<=h<=12, 0<=k<=8, -17<=l<=16	
Reflections collected	1922	
Independent reflections	1815 [R(int) = 0.0213]	
Completeness to theta = 24.97°	99.9 %	
Max. and min. transmission	0.8950 and 0.8483	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1815 / 0 / 155	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.1187	
R indices (all data)	R1 = 0.0539, wR2 = 0.1333	
Largest diff. peak and hole	0.416 and -1.411 e.Å^{-3}	

Table 3.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	10000	5000	10000	22(1)
O(1W)	11279(3)	7061(4)	9388(2)	45(1)
O(2W)	9273(2)	7255(3)	10594(2)	32(1)
N(11)	8543(3)	5195(3)	8850(2)	23(1)
N(12)	9283(3)	5826(5)	6038(2)	35(1)
O(11)	7176(3)	4881(3)	5545(2)	37(1)
N(100)	2785(3)	3061(5)	7808(2)	45(1)
O(101)	2923(3)	3240(7)	8678(2)	82(1)
O(102)	1690(3)	3224(7)	7314(3)	85(1)
O(103)	3794(3)	2741(5)	7463(2)	55(1)
C(11)	7822(3)	5343(4)	7184(2)	24(1)
C(12)	8804(3)	5184(4)	7967(2)	23(1)
C(13)	7279(3)	5354(5)	8973(2)	28(1)
C(14)	6241(3)	5498(5)	8221(2)	31(1)
C(15)	6514(3)	5477(5)	7314(2)	29(1)
C(16)	8086(3)	5321(4)	6190(2)	27(1)
C(17)	9628(4)	5873(6)	5094(2)	41(1)

Table 3.3. Bond lengths [Å] and angles [°] for **4**.

Cu(1)-O(2W)	2.022(2)	O(2W)-Cu(1)-O(1W)	85.89(11)
Cu(1)-O(2W)#1	2.022(2)	O(2W)#1-Cu(1)-O(1W)	94.11(11)
Cu(1)-N(11)#1	2.032(3)	N(11)#1-Cu(1)-O(1W)	88.39(10)
Cu(1)-N(11)	2.032(3)	N(11)-Cu(1)-O(1W)	91.61(10)
Cu(1)-O(1W)	2.246(3)	O(2W)-Cu(1)-O(1W)#1	94.11(11)
Cu(1)-O(1W)#1	2.246(3)	O(2W)#1-Cu(1)-O(1W)#1	85.89(11)
N(11)-C(13)	1.338(4)	N(11)#1-Cu(1)-O(1W)#1	91.61(10)
N(11)-C(12)	1.347(4)	N(11)-Cu(1)-O(1W)#1	88.39(10)
N(12)-C(16)	1.329(5)	O(1W)-Cu(1)-O(1W)#1	180.0
N(12)-C(17)	1.463(4)	C(13)-N(11)-C(12)	118.6(3)
O(11)-C(16)	1.236(4)	C(13)-N(11)-Cu(1)	119.0(2)
N(100)-O(102)	1.223(4)	C(12)-N(11)-Cu(1)	122.4(2)
N(100)-O(103)	1.241(4)	C(16)-N(12)-C(17)	122.5(3)
N(100)-O(101)	1.244(4)	O(102)-N(100)-O(103)	121.5(3)
C(11)-C(12)	1.379(5)	O(102)-N(100)-O(101)	120.7(4)
C(11)-C(15)	1.384(5)	O(103)-N(100)-O(101)	117.8(3)
C(11)-C(16)	1.505(4)	C(12)-C(11)-C(15)	118.6(3)
C(13)-C(14)	1.382(5)	C(12)-C(11)-C(16)	123.6(3)
C(14)-C(15)	1.385(5)	C(15)-C(11)-C(16)	117.8(3)
C(17)-C(17)#2	1.508(8)	N(11)-C(12)-C(11)	122.6(3)
		N(11)-C(13)-C(14)	122.0(3)
O(2W)-Cu(1)-O(2W)#1	180.000(1)	C(15)-C(14)-C(13)	119.2(3)
O(2W)-Cu(1)-N(11)#1	88.81(9)	C(14)-C(15)-C(11)	119.0(3)
O(2W)#1-Cu(1)-N(11)#1	91.19(9)	O(11)-C(16)-N(12)	122.5(3)
O(2W)-Cu(1)-N(11)	91.19(9)	O(11)-C(16)-C(11)	119.0(3)
O(2W)#1-Cu(1)-N(11)	88.81(9)	N(12)-C(16)-C(11)	118.5(3)
N(11)#1-Cu(1)-N(11)	180.000(1)	N(12)-C(17)-C(17)#2	111.1(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+2 #2 -x+2,-y+1,-z+1

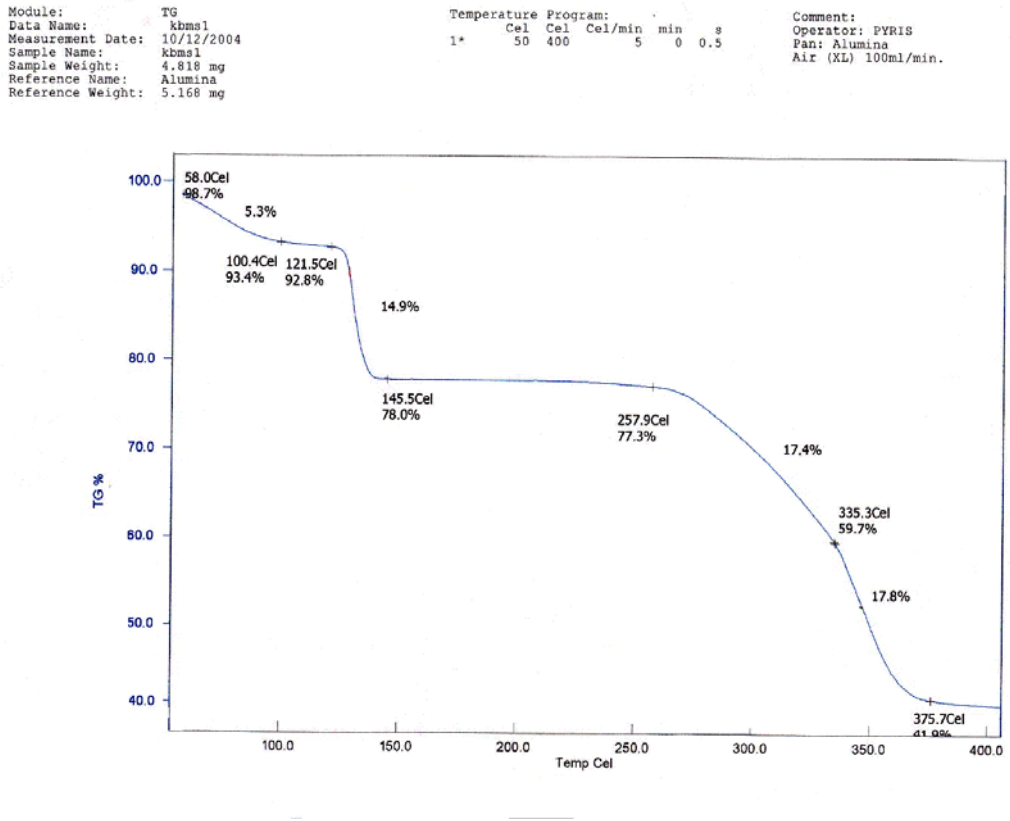
Table 3.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	20(1)	34(1)	9(1)	0(1)	-3(1)	2(1)
O(1W)	57(2)	54(2)	23(1)	-3(1)	7(1)	-21(1)
O(2W)	28(1)	42(1)	22(1)	-1(1)	-1(1)	6(1)
N(11)	22(1)	31(1)	15(1)	0(1)	-1(1)	2(1)
N(12)	35(2)	55(2)	12(1)	-2(1)	1(1)	0(1)
O(11)	47(2)	45(2)	15(1)	-1(1)	-10(1)	-8(1)
N(100)	42(2)	60(2)	34(2)	-3(2)	7(1)	7(2)
O(101)	64(2)	151(4)	32(2)	-12(2)	15(1)	16(2)
O(102)	42(2)	142(4)	65(2)	-6(2)	-5(2)	28(2)
O(103)	40(2)	94(2)	31(1)	-7(2)	9(1)	10(2)
C(11)	26(2)	31(2)	13(1)	-1(1)	-2(1)	-1(1)
C(12)	20(2)	32(2)	16(2)	-2(1)	-1(1)	3(1)
C(13)	27(2)	40(2)	18(2)	2(1)	4(1)	0(1)
C(14)	20(2)	43(2)	27(2)	1(2)	-1(1)	1(1)
C(15)	23(2)	39(2)	22(2)	2(1)	-5(1)	1(1)
C(16)	34(2)	29(2)	14(2)	0(1)	-3(1)	6(1)
C(17)	44(2)	59(3)	20(2)	4(2)	8(1)	6(2)

Table 3.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1W)	11478	7166	8842	100(20)
H(2W)	11426	8239	9660	86(18)
H(3W)	8585	7031	10833	45(12)
H(4W)	9144	8312	10320	60(14)
H(12)	9877	6137	6511	41
H(12A)	9682	5066	7881	28
H(13)	7093	5369	9581	34
H(14)	5370	5609	8324	37
H(15)	5828	5551	6799	35
H(17A)	10173	6967	5037	49
H(17B)	8822	5978	4630	49

Fig. S4: TGA of complex **2**



Supplementary Material (ESI) for Chemical Communications

Experimental

Synthesis of 2: 1.0 mL of acetonitrile was layered on to an EtOH(0.2 mL)/$CHCl_3$(5.0 mL) solution (5.2 mL) of **1** (15.0 mg, 0.056 mmol). Over this solution an acetonitrile solution (1.0 mL) of CuI (10.5 mg, 0.055mmol) was carefully layered. Bright-yellow colored crystals of **2** were exclusively formed after 3-4 days. Similar type of crystals were formed when the metal to ligand ratio was changed from 1:2 to 1:1 and 2:1, keeping the amounts of the solvents constant. The crystals loose the solvent at room temperature, however the diffraction data was collected at room temperature by immersing the crystals in oil and covering with glue.

Synthesis of 3: 2.0 mL of acetonitrile was layered on to an EtOH(1.0 mL)/$CHCl_3$ (5.0mL) solution (6.0 mL) of **1** (15.0 mg, 0.056 mmol). Over this solution an acetonitrile (3.0 mL) solution of CuI (5.3 mg, 0.028 mmol) was carefully layered. Needle-shaped dark-yellow colored crystals of **3** were formed after 3-4 days. On keeping the solution for a longer time (15-20 days), few bright-yellow colored crystals of **2** were formed. Crystals of **3** were also found to form even with different metal to ligand ratios (1:1 and 2:1). Further the use of nitrobenzene in place of $CHCl_3$ resulted in the exclusive formation of **3**.

Elemental analysis: for **2**, found: C, 28.62%; H, 2.21%; N, 8.96%; calcd: C, 29.07%; H, 2.42%, N, 8.75%; for **3**, found: C, 25.97%; H, 1.82%; N, 8.61%; calcd: C, 25.80%; H, 2.15%; N, 8.60%.