Supporting information

Table S1. Selected bond lengths and bond angles for complexes **1** and **2**.

1			
Cu(1)-N(2)	2.044(13)	N(2)-Cu(1)-N(8)	129.7(5)
Cu(1)-N(8)	2.018(13)	N(2)-Cu(1)-N(5)	109.4(5)
Cu(1)-N(5)	2.086(13)	N(8)-Cu(1)-N(5)	111.4(5)
Cu(1)-N(1)	2.145(13)	N(2)-Cu(1)-N(1)	79.3(5)
Cu(1)-Cl(1)	2.247(5)	N(8)-Cu(1)-N(1)	80.3(5)
Cu(2)-N(18)	1.994(14)	N(5)-Cu(1)-N(1)	79.6(5)
Cu(2)-N(12)	2.036(14)	N(2)-Cu(1)-Cl(1)	100.0(4)
Cu(2)-N(15)	2.120(13)	N(8)-Cu(1)-Cl(1)	100.5(4)
Cu(2)-N(11)	2.167(13)	N(5)-Cu(1)-Cl(1)	100.3(4)
Cu(2)-Cl(2)	2.225(5)	N(1)-Cu(1)-Cl(1)	179.1(4)
Cu(3)-N(14)	2.018(14)	N(18)-Cu(2)-N(12)	132.6(6)
Cu(3)-N(7)	2.011(12)	N(18)-Cu(2)-N(15)	106.7(5)
Cu(3)-Cl(5)	2.325(5)	N(12)-Cu(2)-N(15)	111.2(5)
Cu(3)-Cl(4)	2.332(5)	N(18)-Cu(2)-N(11)	80.6(5)
Cu(3)-Cl(3)	2.499(5)	N(12)-Cu(2)-N(11)	79.1(5)
Cu(4)-N(17)	2.035(13)	N(15)-Cu(2)-N(11)	80.2(5)
Cu(4)-N(4)	2.031(13)	N(18)-Cu(2)-Cl(2)	100.3(4)
Cu(4)-Cl(6)	2.317(5)	N(12)-Cu(2)-Cl(2)	97.3(4)
Cu(4)-Cl(7)	2.324(5)	N(15)-Cu(2)-Cl(2)	103.6(4)
Cu(4)-Cl(8)	2.530(5)	N(11)-Cu(2)-Cl(2)	175.6(4)
Cu(5)-N(10)	1.973(16)	N(14)-Cu(3)-N(7)	173.0(5)
Cu(5)-N(20)	1.992(15)	N(14)-Cu(3)-Cl(5)	91.9(4)
Cu(5)-Cl(9)	2.175(11)	N(7)-Cu(3)-Cl(5)	91.2(4)
Cu(5)-Cl(10)	2.378(8)	N(14)-Cu(3)-Cl(4)	87.3(4)
Cu(5)-Cl(11)	2.392(10)	N(7)-Cu(3)-Cl(4)	86.7(4)

Cu(6)-N(22)	1.991(14)	Cl(5)-Cu(3)-Cl(4)	146.8(2)
Cu(6)-N(28)	2.033(14)	N(14)-Cu(3)-Cl(3)	91.7(4)
Cu(6)-N(25)	2.078(14)	N(7)-Cu(3)-Cl(3)	93.6(4)
Cu(6)-N(21)	2.191(13)	Cl(5)-Cu(3)-Cl(3)	103.72(19)
Cu(6)-Cl(12)	2.236(5)	Cl(4)-Cu(3)-Cl(3)	109.48(18)
Cu(7)-N(35)	1.998(14)	N(17)-Cu(4)-N(4)	172.0(5)
Cu(7)-N(38)	2.011(14)	N(17)-Cu(4)-Cl(6)	90.8(4)
Cu(7)-N(31)	2.109(12)	N(4)-Cu(4)-Cl(6)	92.7(4)
Cu(7)-N(32)	2.090(14)	N(17)-Cu(4)-Cl(7)	85.5(4)
Cu(7)-Cl(13)	2.247(5)	N(4)-Cu(4)-Cl(7)	87.6(4)
Cu(8)-N(34)	2.005(14)	Cl(6)-Cu(4)-Cl(7)	146.7(2)
Cu(8)-N(24)	2.029(14)	N(17)-Cu(4)-Cl(8)	94.3(4)
Cu(8)-Cl(15)	2.317(5)	N(4)-Cu(4)-Cl(8)	91.9(4)
Cu(8)-Cl(14)	2.326(5)	Cl(6)-Cu(4)-Cl(8)	103.77(18)
Cu(8)-Cl(16)	2.493(5)	Cl(7)-Cu(4)-Cl(8)	109.46(18)
Cu(9)-N(37)	2.017(14)	N(10)-Cu(5)-N(20)	175.8(7)
Cu(9)-N(27)	2.008(13)	N(10)-Cu(5)-Cl(9)	87.7(6)
Cu(9)-Cl(19)	2.318(5)	N(20)-Cu(5)-Cl(9)	88.9(5)
Cu(9)-Cl(17)	2.341(5)	N(10)-Cu(5)-Cl(10)	83.3(5)
Cu(9)-Cl(18)	2.456(5)	N(20)-Cu(5)-Cl(10)	95.8(5)
Cu(10)-N(30)	2.019(18)	Cl(9)-Cu(5)-Cl(10)	113.1(4)
Cu(10)-N(40)	2.00(2)	N(10)-Cu(5)-Cl(11)	92.2(6)
Cu(10)-O(9W)	2.17(2)	N(20)-Cu(5)-Cl(11)	91.6(5)
Cu(10)-Cl(21)	2.292(13)	Cl(9)-Cu(5)-Cl(11)	117.4(4)
Cu(10)-Cl(20)	2.560(11)	Cl(10)-Cu(5)-Cl(11)	129.1(3)

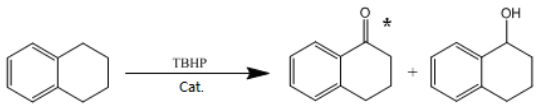
2

Cu(1)-N(8)	2.050(4)	N(8)-Cu(1)-N(5)	118.89(16)
Cu(1)-N(5)	2.061(4)	N(8)-Cu(1)-N(2)	121.69(16)
Cu(1)-N(2)	2.067(4)	N(5)-Cu(1)-N(2)	110.32(17)
Cu(1)-N(1)	2.137(4)	N(8)-Cu(1)-N(1)	79.92(16)

Cu(1)-Cl(5)	2.2419(15)	N(5)-Cu(1)-N(1)	79.74(16)
Cu(2)-N(9)	1.990(5)	N(2)-Cu(1)-N(1)	80.01(16)
Cu(2)-N(10)#1	2.010(5)	N(8)-Cu(1)-Cl(5)	100.34(12)
Cu(2)-O(2)	2.085(4)	N(5)-Cu(1)-Cl(5)	100.93(13)
Cu(2)-Cl(4)	2.2970(17)	N(2)-Cu(1)-Cl(5)	99.06(12)
Cu(2)-Cl(8)	2.5015(17)	N(1)-Cu(1)-Cl(5)	179.01(12)
Cu(3)-N(4)	2.027(5)	N(9)-Cu(2)-N(10)#1	172.4(2)
Cu(3)-N(4)#2	2.027(5)	N(9)-Cu(2)-O(2)	87.18(18)
Cu(3)-Cl(6)#2	2.2804(13)	N(10)#1-Cu(2)-O(2)	86.80(19)
Cu(3)-Cl(6)	2.2804(13)	N(9)-Cu(2)-Cl(4)	88.03(14)
N(4)-Cu(3)-N(4)#2	180.000(1)	N(10)#1-Cu(2)-Cl(4)	94.51(15)
N(4)-Cu(3)-Cl(6)#2	91.54(13)	O(2)-Cu(2)-Cl(4)	146.68(14)
N(4)#2-Cu(3)-Cl(6)#2	88.46(13)	N(9)-Cu(2)-Cl(8)	92.43(14)
N(4)-Cu(3)-Cl(6)	88.46(13)	N(10)#1-Cu(2)-Cl(8)	93.75(15)
N(4)#2-Cu(3)-Cl(6)	91.54(13)	O(2)-Cu(2)-Cl(8)	107.64(14)
Cl(6)#2-Cu(3)-Cl(6)	180.00(8)	Cl(4)-Cu(2)-Cl(8)	105.50(6)

Symmetry transformations used to generate equivalent atoms: #1 -y+2,x-y+1,z; #2 -x+y+1,-x+2,z; #3 -x+y+1,-x+1,z; #4 -y+1,x-y,z; #5 x,x-y,-z+3/2; #6 -x+y+1,y,-z+3/2; #7 -y+1,-x+1,-z+3/2.

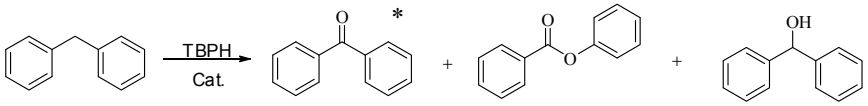
Table S2. Oxidation of tetralin with complexes **1** and **2** as catalysts ($CuCl_2$ as a reference).



Entry	Ctalyst	Time/h	Conversion(%)	Conversion of major product*(%)	Selectivity(%)
1	Complex **1**	1	12	7.6	64
		2	13	8.7	65
		3	17.8	11.8	66
		4	18.4	12	67
		5	21.7	14.6	67
		6	22.2	15.2	68
		10	26.5	18.5	70
		24	37	28	76
		48	50.6	41	82
2	Complex **2**	1	0.65	0.46	71
		2	2.3	1.5	65
		3	10.7	6.7	62
		4	15.6	10	63
		5	24.6	16	65
		6	27	18	67
		10	32.6	22.8	70
		24	45.8	36	78
		48	52	44	84

3	$CuCl_2$	1	1.7	1.1	67
		2	8.4	5.8	69
		3	9.6	6.9	71
		4	13.2	10	72
		5	14.9	9.9	66
		6	15.4	10.4	72
		10	22.9	16.7	73
		24	46	35	77
		48	55	43	78

Table S3. Oxidation of diphenyl methane with complexes **1** and **2** as catalysts ($CuCl_2$ as a reference).



Entry	Ctalyst	Time/h	Conversion(%)	Conversion of major product*(%)	Selectivity(%)
1	Complex **1**	1	4.9	3.6	74
		2	6.6	5.1	76
		3	7.6	5.7	75
		4	8.8	6.7	76
		5	9.2	6.9	75
		6	11.6	8.7	75
		24	12.7	9.7	76
		48	17.2	12.8	75
2	Complex **2**	1	0.29	0.25	86
		2	0.41	0.32	78
		3	0.75	0.63	84
		4	1.6	1.3	81
		5	2.7	2.0	74
		6	4.2	3.1	74
		24	8.0	5.9	74
		48	8.1	5.9	73
3	$CuCl_2$	1	11.6	8.1	70
		2	11.9	8.3	70
		3	11.7	8.3	71
		4	13.2	9.3	70
		5	12.9	9.1	70

6	13.4	9.4	70
24	13.0	9.3	71
48	12.4	8.6	69

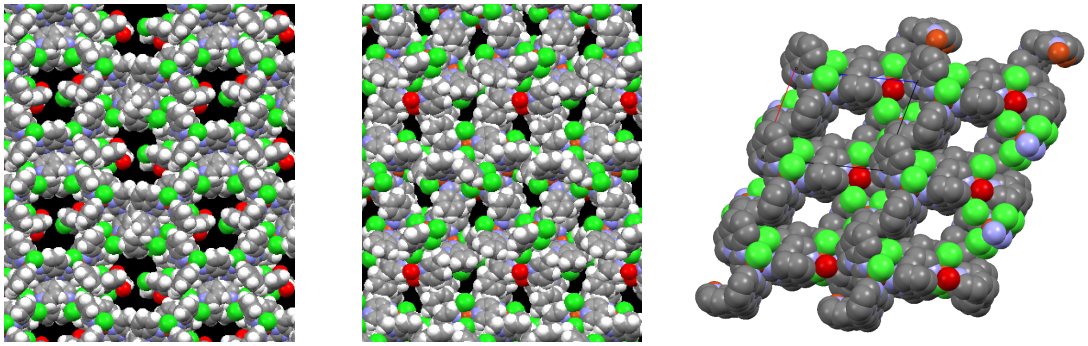
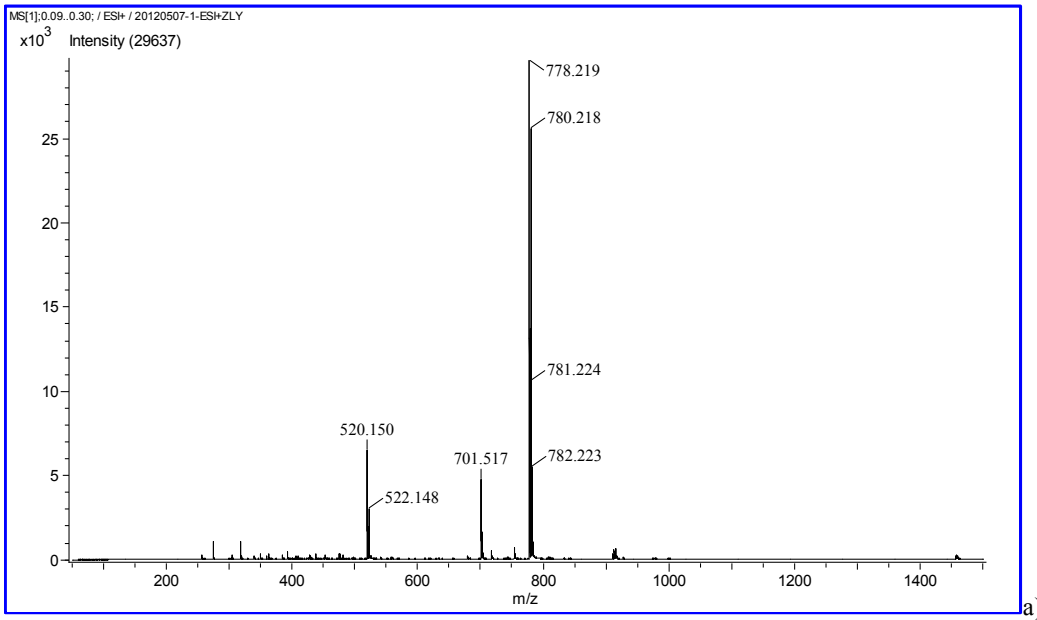
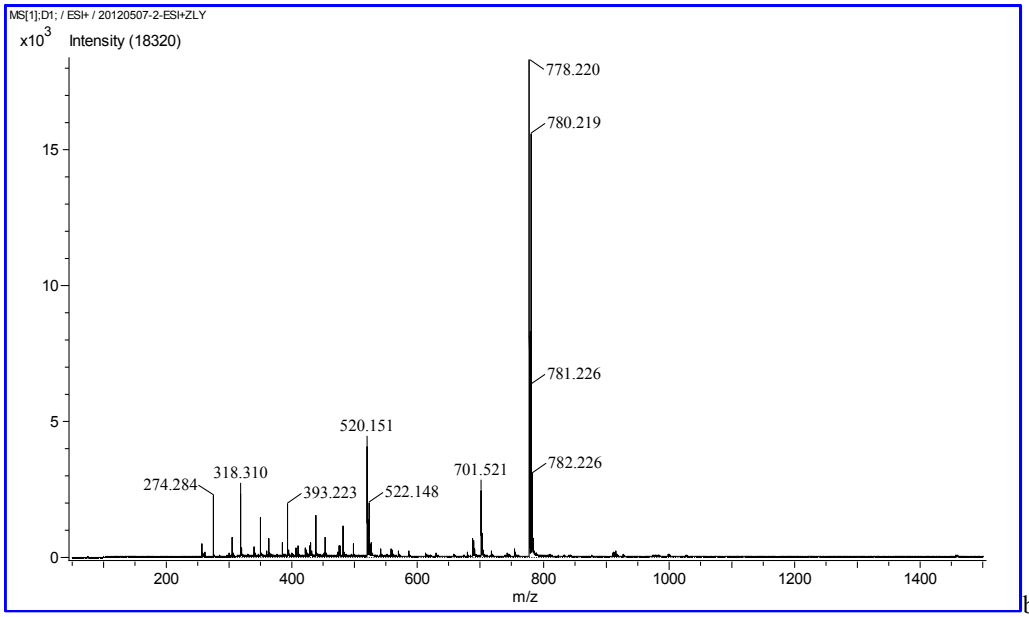


Figure S1. Spacefilling modes in the crystal packing of complex **1** along *a* (left) and *c* (middle) directions, and complex **2** along *b* direction (right). The solvent molecules are omitted for clarity.



a)



b)

Figure S2. ESI-MS spectra of complexes **1** (a) and **2** (b).

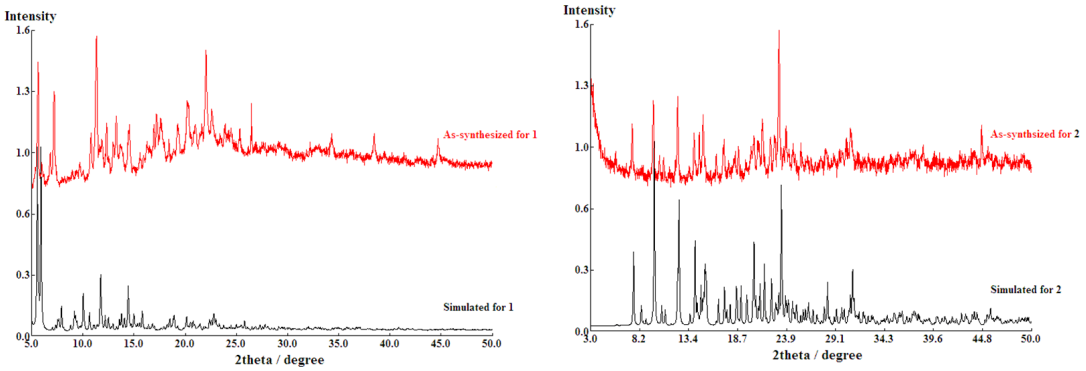


Figure S3. PXRD patterns of complexes**1** (left) and **2** (right).

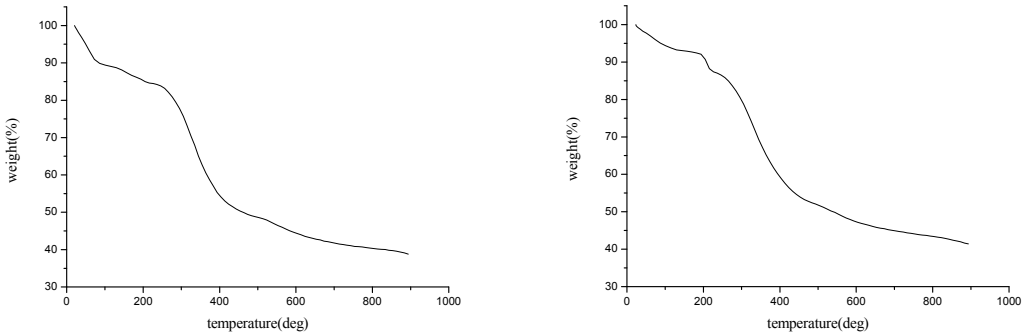


Figure S4. TGA curves of complexes **1** (left) and **2** (right).