

Supplementary Material

Table S1. Selected bond lengths and angles of the complexes

1		3		4	
Bond distances (Å) with esd's in parentheses					
Cu1 O10	1.946(2)	O1 Cu1	1.9274(16)	Cu17 O6	1.9269(16)
Cu1 O17	1.942(3)	O2 C1	1.274(3)	Cu17 O4	1.9268(17)
Cu1 N9	2.012(3)	O2 Cu1	1.9214(16)	Cu17 N2	1.989(2)
Cu1 N2	2.001(3)	N4 C23	1.318(3)	Cu17 N3	1.999(2)
Cu1 O31	2.299(3)	N4 Cu1	2.004(2)	Cu17 O8	2.327(2)
O10 C11	1.283(4)	N3 Cu1	2.0026(19)	O6 C19	1.274(3)
O17 C16	1.263(4)	N2 N1	1.398(3)	O4 C15	1.270(3)
N9 C8	1.351(5)	O6 Cu1	2.303(2)	N2 C31	1.344(3)
N9 C25	1.317(5)	N5 O5	1.229(3)	N2 C27	1.344(3)
N2 C3	1.363(4)	N5 O7	1.229(3)	N7 C13	1.314(3)
N2 C28	1.331(5)	O6 N5	1.258(3)	N7 N11	1.395(3)
O34 N32	1.211(4)	N2 C1	1.356(3)	N12 O8	1.248(3)
O31 N32	1.209(4)	N2 C16	1.424(3)	N12 O1	1.235(3)
N32 O5	1.158(6)	N1 C3	1.298(3)	N12 O7	1.234(3)
Bond angles(Å)with esd's in parentheses					
O17 Cu1 O10	96.83(10)	C5 O1 Cu1	128.02(15)	O6 Cu17 O4	94.13(7)
N9 Cu1 O10	166.62(11)	C1 O2 Cu1	120.76(15)	O6 Cu17 N2	173.11(8)
N9 Cu1 O17	89.40(11)	C23 N4 C27	118.1(2)	O6 Cu17 N3	93.74(8)
N2 Cu1 O10	90.68(10)	C23 N4 Cu1	129.47(18)	O6 Cu17 O8	89.37(7)
N2 Cu1 O17	170.72(11)	C27 N4 Cu1	112.24(16)	O4 Cu17 N2	90.03(7)
N2 Cu1 N9	82.15(12)	C28 N3 Cu1	112.23(16)	O4 Cu17 N3	168.45(8)
O31 Cu1 O10	92.48(10)	C29 N3 C28	118.1(2)	O4 Cu17 O8	88.52(8)
O31 Cu1 O17	94.04(13)	C29 N3 Cu1	129.56(19)	N2 Cu17 N3	81.36(8)
O31 Cu1 N9	98.91(12)	N1 N2 C16	119.0(2)	N2 Cu17 O8	96.23(8)
O31 Cu1 N2	91.07(13)	C1 N2 N1	111.3(2)	N3 Cu17 O8	100.01(8)
C11 O10 Cu1	119.1(2)	O1 Cu1 N4	90.17(8)	C19 O6 Cu17	120.55(15)
C16 O17 Cu1	124.3(2)	O1 Cu1 N3	170.39(8)	C15 O4 Cu17	128.13(16)
C8 N9 Cu1	111.8(2)	O1 Cu1 O6	88.83(9)	C31 N2 Cu17	126.18(16)
C25 N9 Cu1	129.1(3)	O2 Cu1 O1	94.64(7)	O1 N12 O8	119.4(2)
C3 N2 Cu1	112.7(2)	O2 Cu1 N4	170.46(8)	O7 N12 O8	120.4(3)
C28 N2 Cu1	129.8(2)	O2 Cu1 N3	92.05(8)	O7 N12 O1	120.2(3)
N32 O31 Cu1	120.6(3)	O2 Cu1 O6	89.38(8)	N12 O8 Cu17	123.05(17)
C14 N13 N33	106.5(3)	N4 Cu1 O6	98.97(8)	N11 C19 C8	105.64(19)
O31 N32 O34	124.6(4)	N3 Cu1 N4	82.25(8)	O4 C15 C8	122.3(2)
O5 N32 O34	118.9(4)	N3 Cu1 O6	98.15(9)	N2 C31 C30	122.2(2)
O5 N32 O31	116.2(4)	O5 N5 O7	120.9(3)	N3 C26 C27	115.1(2)

Table S2. Analysis of Short Ring-Interactions with Cg-Cg distances < 6.0 Angstrom and Beta < 60.0 Deg. for complexes 1 & 4.

Cg(I) Res(I)Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_perp	CgJ_perp
Complex-1							
Cg(1) -> Cg(2)	[-1+X,Y,Z]	4.8061(20)	15.59	47.46	34.98	3.938	3.249
Cg(1) -> Cg(7)	[-1+X,Y,Z]	4.4230(22)	12.85	40.05	29.92	3.834	3.386
Cg(2) -> Cg(6)	[1+X,Y,Z]	4.2423(22)	12.50	35.81	37.03	3.387	3.440
Cg(2) -> Cg(7)	[1-X,-Y,-Z]	3.6874(23)	3.75	24.58	28.30	3.247	3.353
Cg(3) -> Cg(5)	[1+X,Y,Z]	4.5309(19)	9.34	39.42	48.75	2.987	3.500
Cg(3) -> Cg(6)	[1+X,Y,Z]	4.9640(19)	10.21	46.18	53.53	2.951	3.437
Cg(3) -> Cg(7)	[1-X,-Y,-Z]	3.4441(22)	3.53	12.34	13.57	3.348	3.365
Cg(4) -> Cg(7)	[-1+X,Y,Z]	3.7968(24)	10.51	24.49	15.24	3.663	3.455
Cg(5) -> Cg(2)	[-1+X,Y,Z]	3.6216(22)	11.58	20.51	9.13	3.576	3.392
Cg(6) -> Cg(7)	[-1+X,Y,Z]	3.7205(23)	9.89	21.74	23.18	3.420	3.456
Complex-4							
Cg(1) -> Cg(8)	[1-X,-Y,1-Z]	4.1501(15)	11.60	32.72	43.27	3.022	3.491
Cg(2) -> Cg(5)	[1-X,-Y,1-Z]	4.4596(16)	11.50	38.30	49.78	2.880	3.500
Cg(4) -> Cg(5)	[1/2-X,1/2+Y,1/2-Z]	4.5561(17)	16.96	49.94	33.34	3.806	2.933

Table S3. Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.4 Ang. - Gamma < 30.0 Deg) for complexes 1 & 4

X--H(I) Res(I) Cg(J)	[ARU(J)]	H..Cg	X-H..Cg	X..Cg
Complex-1				
C(22)-H(22) [1] -> Cg(6)	[1-X,-1/2+Y,1/2-Z]	3.0299	158.37	3.9095(50)
C(27)-H(27) [1]-> Cg(3)	[-1+X,Y,Z]	3.2055	108.83	3.6145(39)
Complex-4				
C(1)-H(1)-> Cg(8)	[3/2-X,1/2+Y,1/2-Z]	3.3401	127.44	3.9748(33)
C(11)-H(11)-> Cg(2)	[3/2-X,1/2+Y,1/2-Z]	2.8120	159.90	3.6990(38)
C(25)-H(25)-> Cg(1)	[1-X,-Y,1-Z]	3.1192	98.72	3.3873(30)
C(28)-H(28)-> Cg(6)	[-1+X,Y,Z]	3.0856	133.26	3.7840(31)
C(30)-H(30)-> Cg(5)	[1/2-X,1/2+Y,1/2-Z]	3.1688	111.71	3.6176(32)
C(37)-H(37)-> Cg(2)	[1-X,-Y,1-Z]	3.0940	111.48	3.5419(29)
C(43)-H(43C)-> Cg(7)	[X,-1+Y,Z]	2.8751	146.39	3.7128(36)

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above

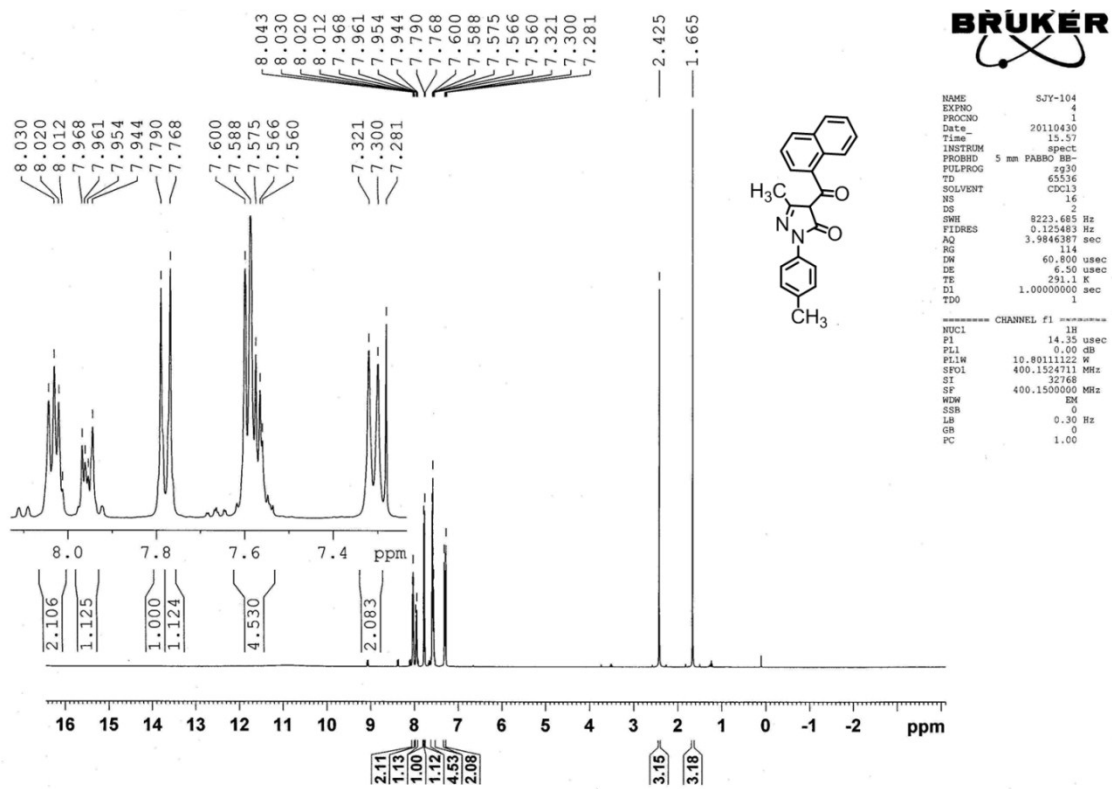


Fig. S1. ¹H NMR spectrum of L2

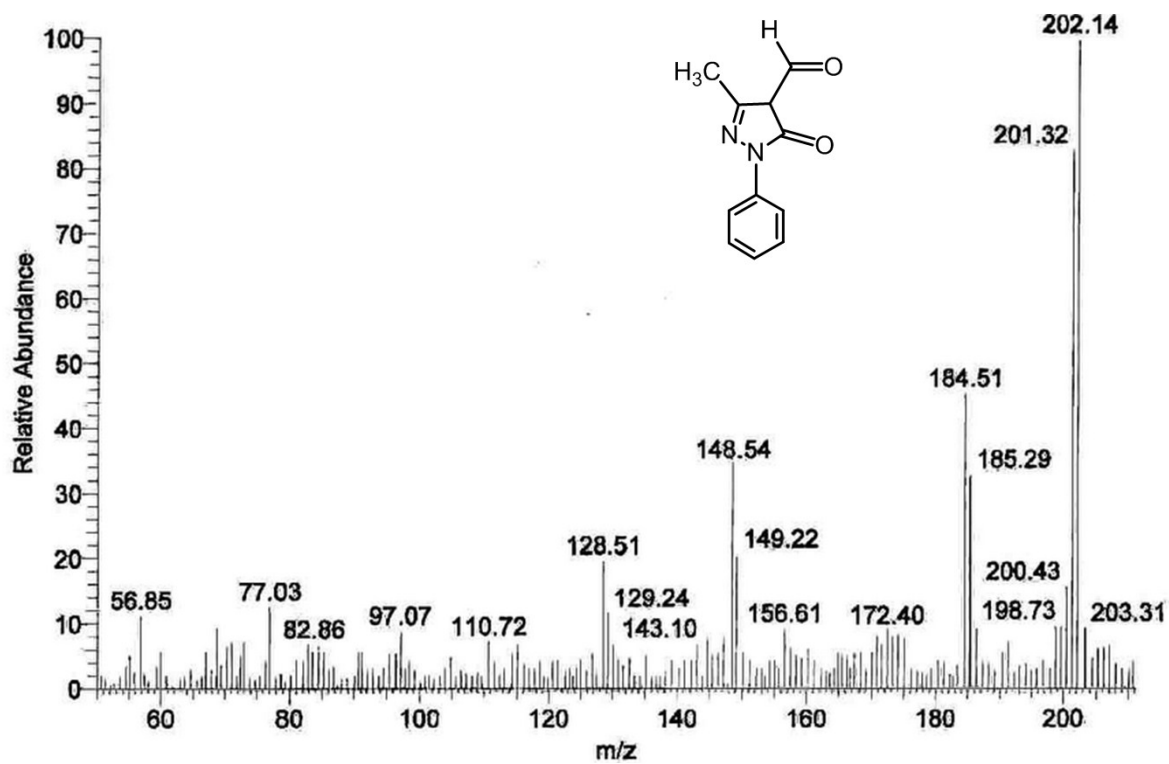


Fig. S2. Mass spectrum of L1

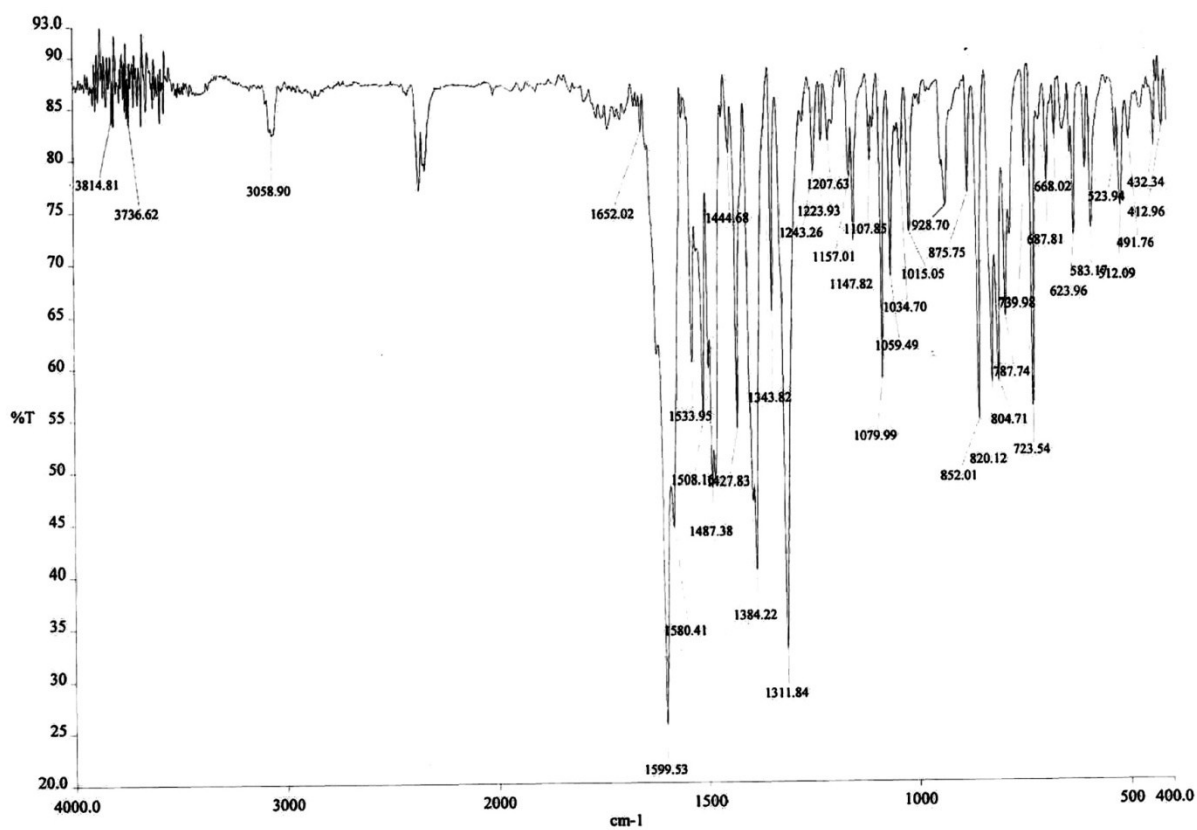


Fig. S3. FTIR spectrum of Complex-3

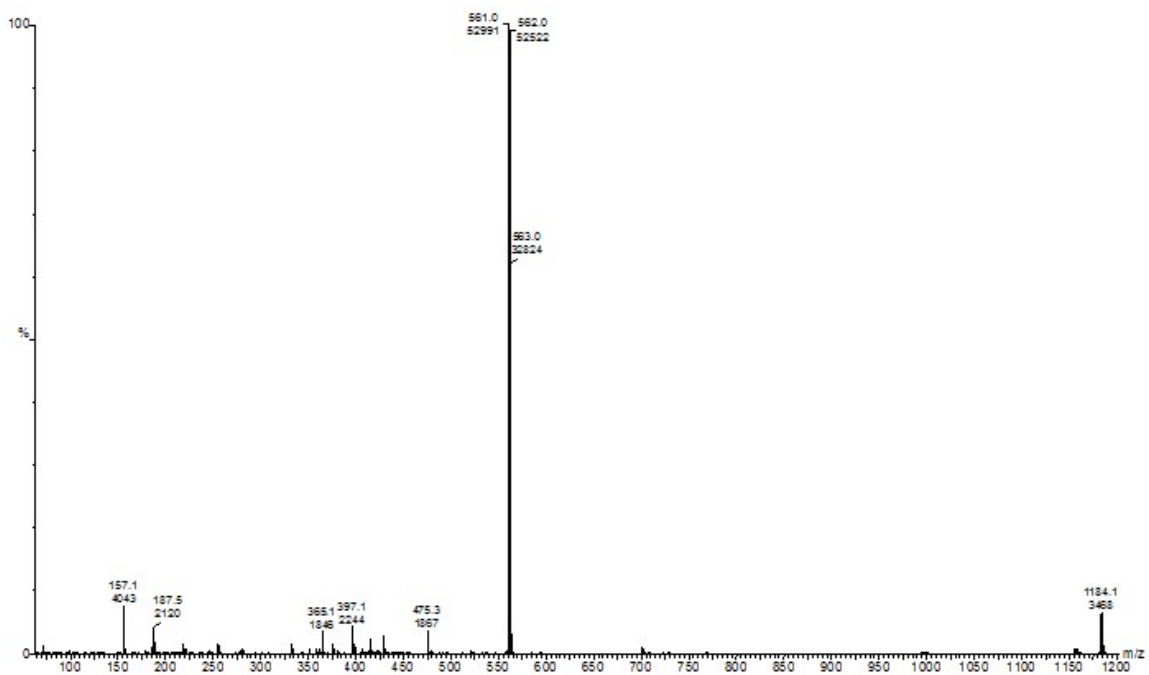


Fig. S4. Mass spectrum of Complex-4

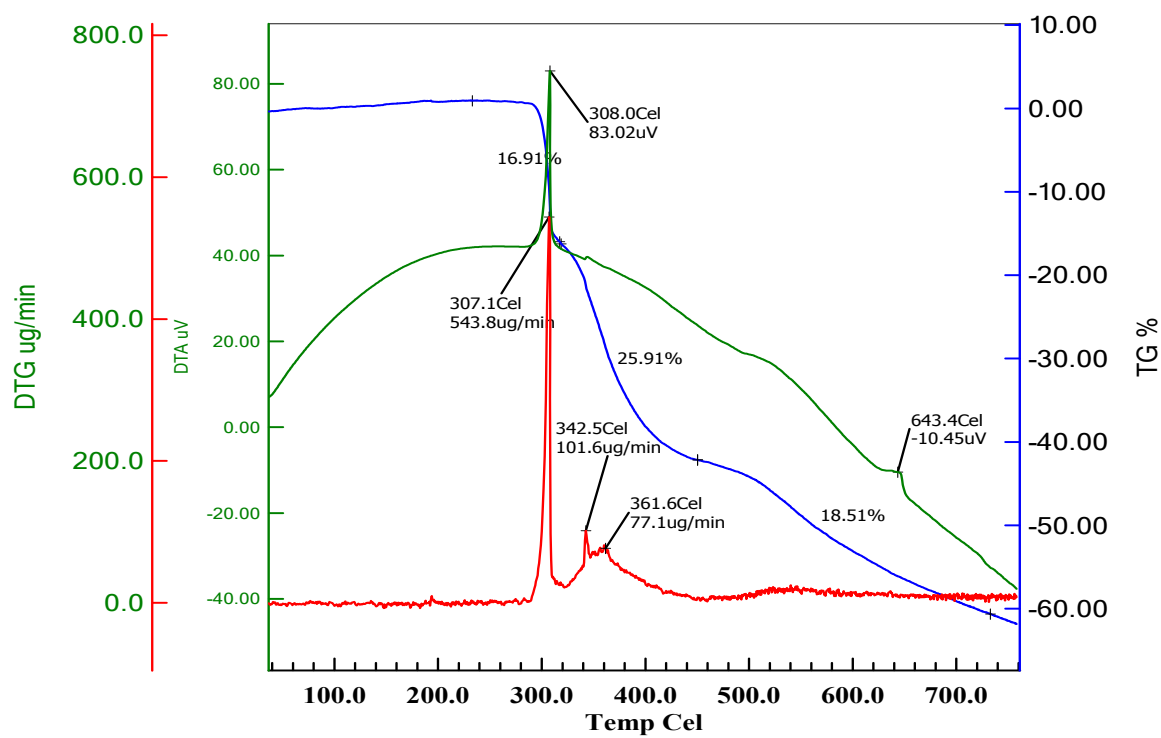


Fig. S5. TGA spectrum of Complex-3