Electronic Supplementary Information (ESI)

Probing the coordination chemistry of a reactive 2,2′-bipyridyl-3,3′-*bis*-imine ligand by X-ray crystallography.

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Table S1. Selected bond lengths (Å) and bond/torsion angles (°) for $\mathbf{L_3}$

Bond Lengths			
N3-C11	1.270(2)	N5-C18	1.345(2)
N4-C17	1.274(2)	N5-C22	1.339(3)
N3-C4	1.421(2)	N6-C12	1.345(2)
N4-C7	1.415(2)	N6-C16	1.344(3)
N1-C1	1.339(2)	C5-C6	1.490(2)
N1-C5	1.343(2)	C11-C12	1.476(2)
N2-C6	1.340(2)	C17-C18	1.472(2)
N2-C10	1.337(2)		
Bond angles			
N2-C6-C5	116.53(14)	N4-C17-C18	120.68(16)
N1-C5-C6	117.11(14)	N3-C4-C5	118.06(15)
C4-N3-C11	117.95(15)	N4-C7-C6	118.91(15)
C7-N4-C17	119.05(15)	N5-C18-C19	122.96(16)
N3-C11-C12	122.42(16)	N6-C12-C11	114.32(15)
Dihedral angles			
C4-C5-C6-C7	64.4(2)	N3-C11-C12-C13	3.7(3)
C11-N3-C4-C5	130.96(17)	N4-C17-C18-C19	8.2(3)
C17-N4-C7-C6	143.54(17)		

Table S2. Selected bond lengths (Å) and bond/torsion angles (°) for $\mathbf{L_4}$

Bond lengths			
O1-C6	1.435(2)	C4B-C5	1.488(7)
O1-C12	1.434(3)	C5-C6	1.524(3)
N1A-N1B	0.583(15)	C7-C8	1.399(3)
N3-H2	1.81(3)	N2-C7	1.382(3)
N2-C6	1.431(3)	C(6)-O(1)	1.435(2)
Bond angles			
N3-H2-N2	140.42(2)	C7-N2-H2	111.3(15)
C6-N2-C7	122.62(19)	O1-C6-C5	110.34(15)
C6-N2-H2	123.3(16)	O1-C6-N2	113.62(17)
Dihedral angles			
N3-C11-C11a-N3a*	−180.0(2)	N1A-C5-C6-N2	−11.8(6)
N2-C7-C11-C11a*	−1.8(3)	N1B-C5-C6-N2	15.0(6)
C7-N2-C6-C5	−160.08(19)	C7-N2-C6-O1	76.0(2)

* Symmetry code is 2-x,1-y,-z.

Table S3. Selected bond lengths (Å) and bond/torsion angles (°) for $\mathbf{L_5}$

Bond lengths			
N3-C11	1.433(3)	N23-C31	1.460(3)
N4-C11	1.474(3)	N24-C31	1.451(3)
Bond angles			
N3-C11-N4	113.18(19)	N23-C31-N24	112.68(19)
N3-C11-C12	113.3(2)	N23-C31-C32	114.0(2)
N4-C11-C12	111.53(18)	N24-C31-C32	111.6(2)
Dihedral angle			
C4-C5-C6-C7	24.5(4)	C24-C25-C26-C27	33.5(4)

Table S4. Selected bond lengths (Å) and bond/torsion angles (°) for $\mathbf{C_3}$

Bond lengths			
Cu1-O1	2.210(2)	Cu1-O3	2.016(3)
Cu1-O2	1.941(3)	Cu1-N1	1.954(3)
Cu1-N2	1.986(3)	N4-C11	1.427(5)
N3-C11	1.454(5)	N3-C11	1.454(5)
N4-C11	1.427(5)		
Bond angles			
O1-Cu1-O2	89.39(11)	O2-Cu1-O3	86.86(12)
O1-Cu1-O3	87.73(11)	O1-Cu1-N1	95.10(11)
O1-Cu1-N2	118.18(12)	O2-Cu1-N1	173.03(13)
O3-Cu1-N1	98.63(13)	O2-Cu1-N2	92.33(12)

N1-Cu1-N2	80.85(13)	O3-Cu1-N2	154.08(13)
N4-C11-C12	111.8(3)	N3-C11-N4	111.8(3)
N3-C11-C12	108.3(3)		
Dihedral angle			
C4-C5-C6-C7	−3.9(6)		

Table S5. Selected bond lengths (Å) and angles (˚) for $\mathbf{C_5}$

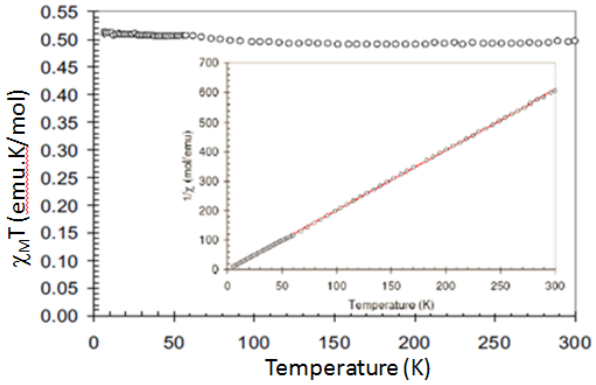
Bond lengths			
Zn1-O1	2.110(3)	Zn1-O2	2.074(3)
Zn1-O3	2.086(3)	Zn1-O4	2.118(3)
Zn1-N1	2.155(3)	Zn1-N2	2.127(3)
N3-C11	1.257(5)	N4-C11	1.438(5)
N4-C17	1.374(5)		
Bond angle			
O1-Zn1-O3	90.39(11)	O1-Zn1-O2	87.21(11)
O1-Zn1-N1	87.22(11)	O1-Zn1-O4	172.51(11)
O2-Zn1-O3	92.43(11)	O1-Zn1-N2	91.79(11)
O2-Zn1-N1	93.93(10)	O2-Zn1-O4	86.05(11)
O3-Zn1-O4	86.63(10)	O2-Zn1-N2	172.16(11)
O3-Zn1-N2	95.35(10)	O3-Zn1-N1	173.09(11)
O4-Zn1-N2	95.34(11)	O4-Zn1-N1	96.51(10)
C11-N4-C17	129.0(3)	N1-Zn1-N2	78.25(10)
C7-N4-C11	111.6(3)	C7-N4-C17	118.3(3)
N3-C11-C12	119.9(3)	N3-C11-N4	123.2(3)
N4-C11-C12	116.2(3)		
Dihedral angle			
C4-C5-C6-C7	28.4(6)		

Table S6. Selected bond lengths (Å) and angles (˚) for complex $\mathbf{C_6}$

Bond lengths			
Co1-O1	2.145(6)	Co1-N3	2.107(7)
Co1-N1	2.154(7)	Co1-N4	2.160(7)
Co1-N2	2.112(8)	Co1-N5	2.086(7)
Bond angles			
N1-Co1-N2	76.5(3)	N3-Co1-N5	92.2(3)
N1-Co1-N3	150.6(3)	N4-Co1-N5	90.5(3)
N1-Co1-N4	133.4(3)	O1-Co1-N1	88.5(3)
N1-Co1-N5	90.2(3)	O1-Co1-N2	92.4(3)
N2-Co1-N3	74.2(3)	O1-Co1-N3	91.9(2)
N2-Co1-N4	150.0(3)	O1-Co1-N4	85.9(3)
N2-Co1-N5	93.3(3)	O1-Co1-N5	173.7(3)
N3-Co1-N4	75.9(3)		
Dihedral angles			
N1-C5-C6-N2	−0.5(11)	N3-C17-C18-N4	1.0(11)
N2-C10-C11-N3	−1.0(10)		

Magnetic measurements

Variable temperature dc magnetic susceptibility data were collected on single crystals of complex **8** on a Quantum Design MPMS SQUID magnetometer in an applied field of 0.1 T from 5-300 K. Pascal's constants were used to estimate the diamagnetic corrections, which were subtracted from the experimental susceptibilities to give the molar paramagnetic susceptibilities (χ_M). The magnetic properties of complex **8** were examined on a SQUID magnetometer in an applied field of 0.1 T between 5 and 300 K, Fig. 11. The sample was corrected for diamagnetism associated with the capsule and sample holder. The sample exhibited Curie Weiss behaviour across the entire temperature range with C = 0.490 emu.K.mol^{-1} and θ = +1.15 K (Figure 3.14, inset). The value of C is consistent with an S = ½ paramagnet with g = 2.29 which falls in the expected range for Cu^{II} complexes (ca. 2.0 – 2.3).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0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
χM T (emu.K/mol)
0
50
100
150
200
250
300
Temperature (K)
700
600
500
400
300
200
100
0
1/χ (mol/emu)
0
50
100
150
200
250
300
Temperature (K)