Electronic Supplementary Material (ESI) for Dalton Transactions

A series of novel zinc(II) entangled coordination polymers based on carboxyphenyl-terpyridine ligands

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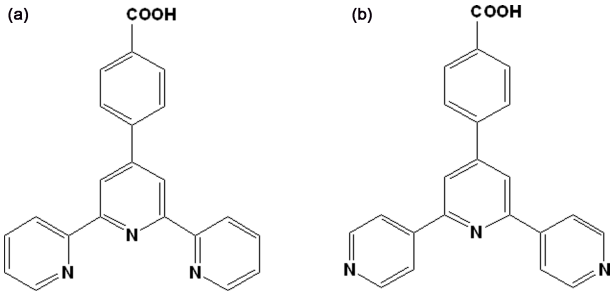

Scheme 1 Representation of the ligands HL_1 (a) and HL_2 (b).

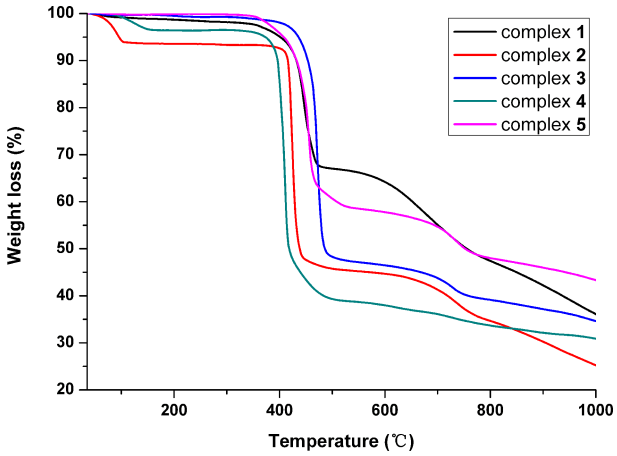

Figure S1. TGA diagrams of complexes **1-5**

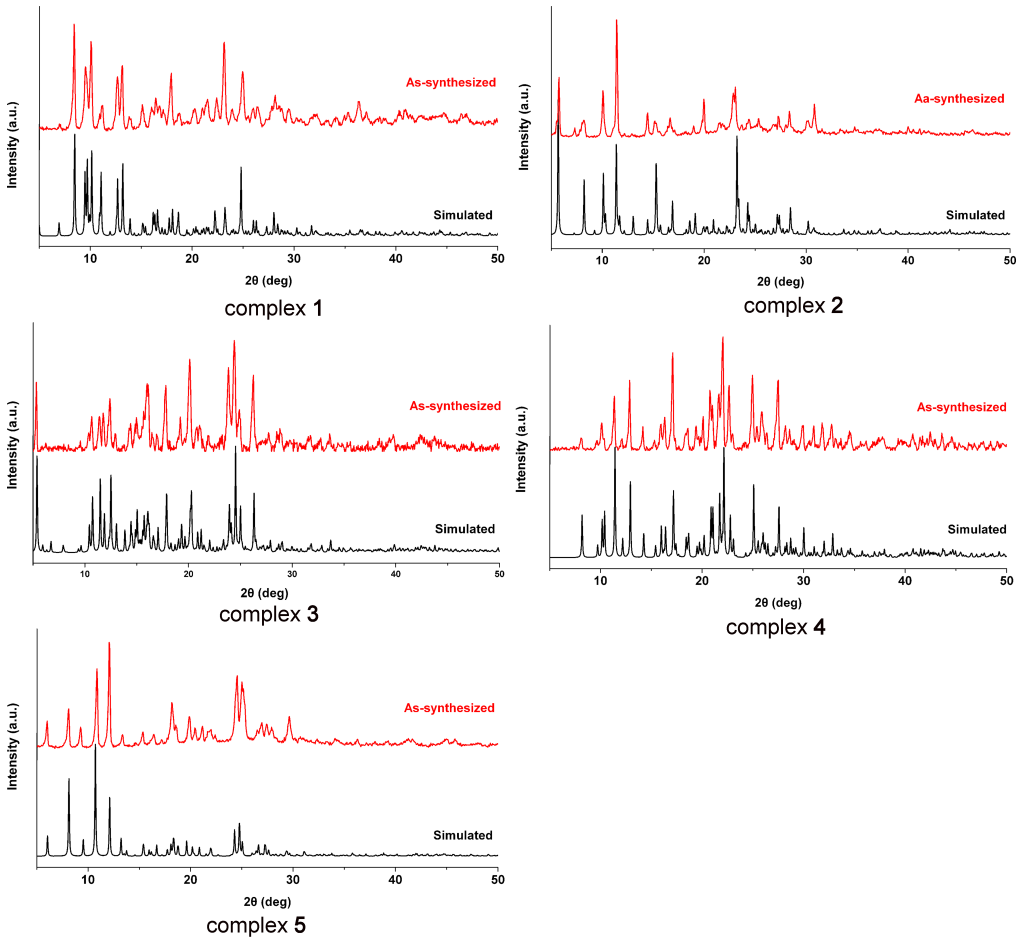

Figure S2. PXRD patterns of complexes **1-5**

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for **1-5**

complex **1**

Bond	Dist.	Bond	Dist.
Zn1—O1	1.947 (3)	Zn2—N5	2.094 (4)
Zn1—N2	2.077 (4)	Zn2—N4	2.170 (4)
Zn1—N3	2.174 (4)	Zn2—N6	2.194 (5)
Zn1—N1	2.233 (4)	Zn2—Cl2	2.2810 (16)
Zn1—Cl1	2.2420 (15)	Zn2—O4i	2.468 (5)
Zn2—O3i	2.047 (4)		
Angle	(º)	Angle	(º)
O1—Zn1—N2	113.60 (16)	N5—Zn2—O4i	81.59 (15)
O1—Zn1—N3	107.23 (15)	N4—Zn2—O4i	85.35 (17)
N2—Zn1—N3	75.35 (14)	N6—Zn2—O4i	89.56 (16)
O1—Zn1—N1	88.29 (16)	Cl2—Zn2—O4i	161.66 (11)
N2—Zn1—N1	74.21 (14)	N1—Zn1—Cl1	96.12 (12)
N3—Zn1—N1	149.35 (14)	O3i—Zn2—N5	138.15 (18)
O1—Zn1—Cl1	120.53 (13)	O3i—Zn2—N4	97.19 (17)
N2—Zn1—Cl1	124.67 (11)	N5—Zn2—N4	74.89 (14)
N3—Zn1—Cl1	98.14 (12)	O3i—Zn2—N6	104.93 (18)

N5—Zn2—N6	74.68 (14)	N4—Zn2—Cl2	97.30 (13)
N4—Zn2—N6	149.56 (15)	N5—Zn2—Cl2	116.66 (11)
O3i—Zn2—O4i	56.65 (18)	O3i—Zn2—Cl2	105.03 (16)
N6—Zn2—Cl2	96.86 (12)		

Symmetry codes: (i) x, 1+y, 1+z; (ii) x, -1+y, -1+z.

complex **2**

Bond	Dist.	Bond	Dist.
Zn1—O3i	1.933 (2)	Zn1—N6	2.181 (3)
Zn1—O1	1.946 (2)	Zn1—N4	2.181 (3)
Zn1—N5	2.074 (2)		
Angle	(º)	Angle	(º)
O3i—Zn1—O1	95.74 (12)	N5—Zn1—N6	75.68 (9)
O3i—Zn1—N5	132.05 (10)	O3i—Zn1—N4	93.82 (10)
O1—Zn1—N5	131.94 (11)	O1—Zn1—N4	100.80 (12)
O3i—Zn1—N6	103.28 (10)	N5—Zn1—N4	74.94 (9)
O1—Zn1—N6	101.30 (12)	N6—Zn1—N4	150.41 (9)

Symmetry codes: (i) x, 1+y, z; (ii) x, -1+y, z.

complex **3**

Bond	Dist.	Bond	Dist.
Zn1—O1i	1.951 (4)	Zn2—O5iv	1.923 (5)
Zn1—N1	2.074 (4)	Zn2—O8i	2.002 (5)
Zn1—N4	2.093 (4)	Zn2—N10	2.069 (4)
Zn1—O3ii	2.109 (3)	Zn2—N7	2.078 (4)
Zn1—O4ii	2.252 (3)		
Angle	(º)	Angle	(º)
O1i—Zn1—N1	124.07 (17)	N4—Zn1—O4ii	150.07 (14)
O1i—Zn1—N4	104.83 (17)	O3ii—Zn1—O4ii	59.17 (12)
N1—Zn1—N4	101.05 (17)	O5iv—Zn2—O8i	103.0 (3)
O1i—Zn1—O3ii	125.18 (15)	O5iv—Zn2—N10	107.3 (2)
N1—Zn1—O3ii	102.49 (15)	O8i—Zn2—N10	123.8 (2)
N4—Zn1—O3ii	91.38 (15)	O5iv—Zn2—N7	125.5 (3)
O1i—Zn1—O4ii	89.99 (15)	O8i—Zn2—N7	100.07 (19)
N1—Zn1—O4ii	91.30 (15)	N10—Zn2—N7	99.15 (17)

Symmetry codes: (i) 1+x, y, z; (ii) x, -1+y, z; (iii) -1+x, y, z; (iv) x, 1+y, z.

complex **4**

Bond	Dist.	Bond	Dist.
Zn1—O5i	1.9451 (15)	Zn1—N3ii	2.0446 (17)
Zn1—O3	1.9989 (14)	Zn1—N1	2.0676 (16)
Angle	(º)	Angle	(º)
O5i—Zn1—O3	114.56 (7)	O5i—Zn1—N1	104.28 (7)

O5i—Zn1—N3ii	136.88 (7)	O3—Zn1—N1	100.75 (6)
O3—Zn1—N3ii	97.52 (6)	N3ii—Zn1—N1	96.67 (7)

Symmetry codes: (i) 3/2-x, -1/2+y, 1/2-z; (ii) 3/2-x, 1/2+y, -1/2-z; (iii) 3/2-x, 1/2+y, 1/2-z; (iv) 3/2-x, -1/2+y, -1/2-z

complex **5**

Bond	Dist.	Bond	Dist.
Zn1—O3	1.918 (5)	Zn1—O2i	1.996 (4)
Zn1—O1	1.977 (4)	Zn1—N3ii	2.025 (5)
Angle	(º)	Angle	(º)
O3—Zn1—O1	103.0 (2)	O3—Zn1—N3ii	125.9 (2)
O3—Zn1—O2i	112.1 (2)	O1—Zn1—N3ii	115.99 (18)
O1—Zn1—O2i	93.90 (16)	O2i—Zn1—N3ii	101.48 (16)

Symmetry codes: (i) 1-x, -1/2+y, 1/2-z; (ii) -1+x, 3/2-y, -1/2+z; (iii) 1-x, 1/2+y, 1/2-z; (iv) 1+x, 3/2-y, 1/2+z; (v) 1-x, 2-y, -z.