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Coordination polymers with mixed 4,4'-bipyridine-2,2',6,6'-tetracarboxylate and imidazole-containing ligands: synthesis, structure and property†

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Table S1. Selected bond lengths (Å) and angles (deg) for complexes **1** - **3**.[a]

Complex **1**			
Mn(1)–O(17)	2.156(6)	Mn(1)–O(18)	2.171(6)
Mn(1)–N(11)	2.243(7)	Mn(1)–O(19)	2.258(7)
Mn(1)–O(3)	2.311(5)	Mn(1)–O(5)#1	2.317(6)
Mn(1)–O(1)	2.436(6)	Mn(2)–O(20)	2.193(8)
Mn(2)–O(26)	2.204(8)	Mn(2)–N(112)	2.222(8)
Mn(2)–N(21)	2.265(7)	Mn(2)–O(3)#2	2.333(5)
Mn(2)–O(5)	2.354(6)	Mn(2)–O(7)	2.470(6)
Mn(3)–O(21)	2.182(6)	Mn(3)–N(132)	2.218(8)
Mn(3)–N(31)	2.262(6)	Mn(3)–O(9)	2.271(8)
Mn(3)–O(7)#3	2.320(5)	Mn(3)–O(11)	2.337(6)

Mn(3)–O(8)#3	2.487(6)	Mn(4)–O(22)	2.187(6)
Mn(4)–N(152)#4	2.209(8)	Mn(4)–N(41)	2.264(7)
Mn(4)–O(13)	2.277(6)	Mn(4)–O(1)#5	2.371(6)
Mn(4)–O(15)	2.383(6)	Mn(4)–O(2)#5	2.421(6)
O(17)–Mn(1)–O(18)	99.5(2)	O(17)–Mn(1)–N(11)	97.8(2)
O(18)–Mn(1)–N(11)	137.8(2)	O(17)–Mn(1)–O(19)	178.2(3)
N(11)–Mn(1)–O(19)	83.9(3)	O(18)–Mn(1)–O(19)	78.7(3)
O(18)–Mn(1)–O(3)	144.7(2)	O(17)–Mn(1)–O(3)	95.2(2)
O(19)–Mn(1)–O(3)	86.2(3)	N(11)–Mn(1)–O(3)	70.4(2)
O(18)–Mn(1)–O(5)#1	79.5(2)	O(17)–Mn(1)–O(5)#1	84.0(2)
O(19)–Mn(1)–O(5)#1	95.3(2)	N(11)–Mn(1)–O(5)#1	140.7(2)
O(17)–Mn(1)–O(1)	88.9(2)	O(3)–Mn(1)–O(5)#1	70.3(2)
N(11)–Mn(1)–O(1)	67.2(2)	O(18)–Mn(1)–O(1)	74.9(2)
O(3)–Mn(1)–O(1)	137.6(2)	O(19)–Mn(1)–O(1)	91.0(3)
O(20)–Mn(2)–O(26)	100.2(4)	O(5)#1–Mn(1)–O(1)	151.8(2)
O(26)–Mn(2)–N(112)	175.1(4)	O(20)–Mn(2)–N(112)	83.4(3)
O(26)–Mn(2)–N(21)	94.7(3)	O(20)–Mn(2)–N(21)	139.3(3)
O(20)–Mn(2)–O(3)#2	80.8(3)	N(112)–Mn(2)–N(21)	84.4(3)
N(112)–Mn(2)–O(3)#2	95.7(3)	O(26)–Mn(2)–O(3)#2	81.9(3)
O(20)–Mn(2)–O(5)	146.6(3)	N(21)–Mn(2)–O(3)#2	139.1(2)
N(112)–Mn(2)–O(5)	84.9(2)	O(26)–Mn(2)–O(5)	90.3(4)
O(3)#2–Mn(2)–O(5)	69.3(2)	N(21)–Mn(2)–O(5)	70.0(2)
O(26)–Mn(2)–O(7)	91.3(3)	O(20)–Mn(2)–O(7)	73.9(2)
N(21)–Mn(2)–O(7)	68.0(2)	N(112)–Mn(2)–O(7)	92.7(2)
O(5)–Mn(2)–O(7)	138.0(2)	O(3)#2–Mn(2)–O(7)	152.2(2)
O(21)–Mn(3)–N(31)	93.6(2)	O(21)–Mn(3)–N(132)	165.4(3)
O(21)–Mn(3)–O(9)	94.6(3)	N(132)–Mn(3)–N(31)	88.9(3)
N(31)–Mn(3)–O(9)	69.9(2)	N(132)–Mn(3)–O(9)	99.8(3)
N(132)–Mn(3)–O(7)#3	95.3(2)	O(21)–Mn(3)–O(7)#3	89.7(2)
O(9)–Mn(3)–O(7)#3	80.3(2)	N(31)–Mn(3)–O(7)#3	150.2(2)
N(132)–Mn(3)–O(11)	84.9(2)	O(21)–Mn(3)–O(11)	82.7(2)
O(9)–Mn(3)–O(11)	137.5(2)	N(31)–Mn(3)–O(11)	68.0(2)
O(21)–Mn(3)–O(8)#3	86.5(2)	O(7)#3–Mn(3)–O(11)	141.7(2)

N(31)–Mn(3)–O(8)#3	154.8(2)	N(132)–Mn(3)–O(8)#3	85.3(3)
O(7)#3–Mn(3)–O(8)#3	54.9(2)	O(9)–Mn(3)–O(8)#3	135.2(2)
O(22)–Mn(4)–N(152)#4	177.9(3)	O(11)–Mn(3)–O(8)#3	87.1(2)
N(152)#4–Mn(4)–N(41)	88.5(3)	O(22)–Mn(4)–N(41)	90.8(2)
N(152)#4–Mn(4)–O(13)	92.9(3)	O(22)–Mn(4)–O(13)	85.0(2)
O(22)–Mn(4)–O(1)#5	91.6(2)	N(41)–Mn(4)–O(13)	71.2(2)
N(41)–Mn(4)–O(1)#5	145.1(2)	N(152)#4–Mn(4)–O(1)#5	90.1(3)
O(22)–Mn(4)–O(15)	90.6(2)	O(13)–Mn(4)–O(1)#5	143.6(2)
N(41)–Mn(4)–O(15)	67.8(2)	N(152)#4–Mn(4)–O(15)	91.0(2)
O(1)#5–Mn(4)–O(15)	77.4(2)	O(13)–Mn(4)–O(15)	138.7(2)
N(152)#4–Mn(4)–O(2)#5	91.9(2)	O(22)–Mn(4)–O(2)#5	88.1(2)
O(13)–Mn(4)–O(2)#5	88.1(2)	N(41)–Mn(4)–O(2)#5	159.3(2)
O(15)–Mn(4)–O(2)#5	132.8(2)	O(1)#5–Mn(4)–O(2)#5	55.5(2)

Complex **2**

Ni(1)–N(81)	1.988(2)	Ni(1)–N(112)	2.057(3)
Ni(1)–N(12)	2.078(3)	Ni(1)–N(32)#1	2.090(3)
Ni(1)–O(5)	2.128(2)	Ni(1)–O(7)	2.206(2)
Ni(2)–N(71)#2	1.977(3)	Ni(2)–N(52)	2.025(3)
Ni(2)–N(132)#3	2.093(3)	Ni(2)–N(152)	2.114(3)
Ni(2)–O(1)#2	2.151(3)	Ni(2)–O(3)#2	2.184(2)
N(81)–Ni(1)–N(112)	175.2(1)	N(81)–Ni(1)–N(12)	92.5(1)
N(112)–Ni(1)–N(12)	91.9(1)	N(81)–Ni(1)–N(32)#1	89.0(1)
N(112)–Ni(1)–N(32)#1	86.8(1)	N(12)–Ni(1)–N(32)#1	174.1(1)
N(81)–Ni(1)–O(5)	78.0(1)	N(112)–Ni(1)–O(5)	99.8(1)
N(12)–Ni(1)–O(5)	93.1(1)	N(32)#1–Ni(1)–O(5)	92.9(1)
N(81)–Ni(1)–O(7)	76.1(1)	N(112)–Ni(1)–O(7)	106.0(1)
N(12)–Ni(1)–O(7)	88.2(1)	N(32)#1–Ni(1)–O(7)	86.6(1)
O(5)–Ni(1)–O(7)	154.1(1)	N(71)#2–Ni(2)–N(52)	176.1(1)
N(71)#2–Ni(2)–N(132)#3	90.3(1)	N(52)–Ni(2)–N(132)#3	92.6(1)
N(71)#2–Ni(2)–N(152)	89.8(1)	N(52)–Ni(2)–N(152)	87.5(1)
N(132)#3–Ni(2)–N(152)	175.7(1)	N(71)#2–Ni(2)–O(1)#2	77.7(1)
N(52)–Ni(2)–O(1)#2	99.7(1)	N(132)#3–Ni(2)–O(1)#2	93.0(1)
N(152)–Ni(2)–O(1)#2	91.3(1)	N(71)#2–Ni(2)–O(3)#2	77.3(1)

N(52)–Ni(2)–O(3)#2	105.3(1)	N(132)#3–Ni(2)–O(3)#2	88.0(1)
N(152)–Ni(2)–O(3)#2	87.6(1)	O(1)#2–Ni(2)–O(3)#2	154.9(1)
		Complex **3**	
Co(1)–N(11)#1	2.053(3)	Co(1)–N(212)	2.091(3)
Co(1)–N(132)#2	2.118(3)	Co(1)–N(112)	2.140(3)
Co(1)–O(5)#1	2.144(3)	Co(1)–O(7)#1	2.213(3)
Co(2)–N(21)	2.028(3)	Co(2)–N(152)#2	2.051(3)
Co(2)–N(252)#3	2.134(4)	Co(2)–N(232)	2.154(4)
Co(2)–O(3)	2.180(3)	Co(2)–O(1)	2.208(3)
N(11)#1–Co(1)–N(212)	174.3(1)	N(11)#1–Co(1)–N(132)#2	92.4(1)
N(212)–Co(1)–N(132)#2	92.4(1)	N(11)#1–Co(1)–N(112)	88.6(1)
N(212)–Co(1)–N(112)	87.1(1)	N(132)#2–Co(1)–N(112)	173.9(1)
N(11)#1–Co(1)–O(5)#1	75.8(1)	N(212)–Co(1)–O(5)#1	100.9(1)
N(132)#2–Co(1)–O(5)#1	92.9(1)	N(112)–Co(1)–O(5)#1	93.2(1)
N(11)#1–Co(1)–O(7)#1	74.5(1)	N(212)–Co(1)–O(7)#1	108.7(1)
N(132)#2–Co(1)–O(7)#1	88.4(1)	N(112)–Co(1)–O(7)#1	86.1(1)
O(5)#1–Co(1)–O(7)#1	150.3(1)	N(21)–Co(2)–N(152)#2	174.9(1)
N(21)–Co(2)–N(252)#3	89.4(1)	N(152)#2–Co(2)–N(252)#3	94.1(1)
N(21)–Co(2)–N(232)	89.2(1)	N(152)#2–Co(2)–N(232)	87.7(1)
N(252)#3–Co(2)–N(232)	175.0(1)	N(21)–Co(2)–O(3)	76.0(1)
N(152)#2–Co(2)–O(3)	100.1(1)	N(252)#3–Co(2)–O(3)	93.9(1)
N(232)–Co(2)–O(3)	90.4(2)	N(21)–Co(2)–O(1)	75.8(1)
N(152)#2–Co(2)–O(1)	108.0(1)	N(252)#3–Co(2)–O(1)	87.5(1)
N(232)–Co(2)–O(1)	87.5(1)	O(3)–Co(2)–O(1)	151.7(1)

Symmetry transformations used to generate equivalent atoms: #1 *x*, *y*, *z*+1; #2 *x*, *y*, *z*–1; #3 –*x*+1, *y*–1/2, –*z*+1; #4 –*x*+1, *y*+1/2, –*z*+1; #5 –*x* + 1, *y* + 1/2, –*z* + 2 for **1**; #1 –*x* + 1, *y*– 1/2, –*z* + 1/2; #2 *x*, –*y* + 1/2, *z*– 1/2; #3 *x*+1, *y*, *z* for **2**;#1 *x*,–*y*+1/2,*z*–1/2; #2 –*x*+1,*y*+1/2,–*z*+1/2; #3 *x*–1,*y*,*z*for **3**.

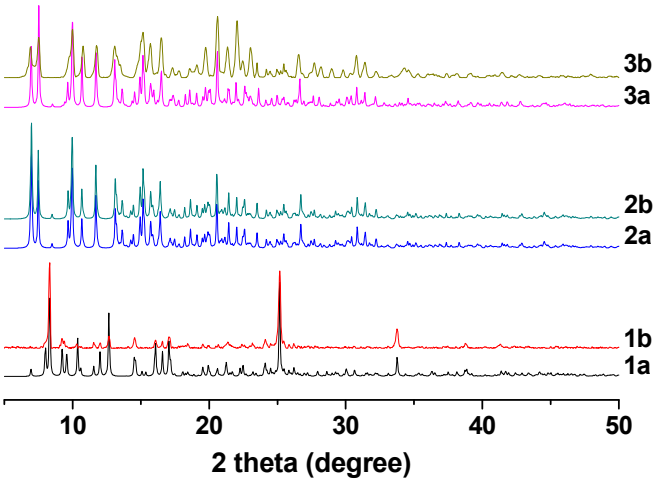

Fig. S1. The PXRD patterns of complexes **1-3**: a – simulated; b – as-synthesized**.**

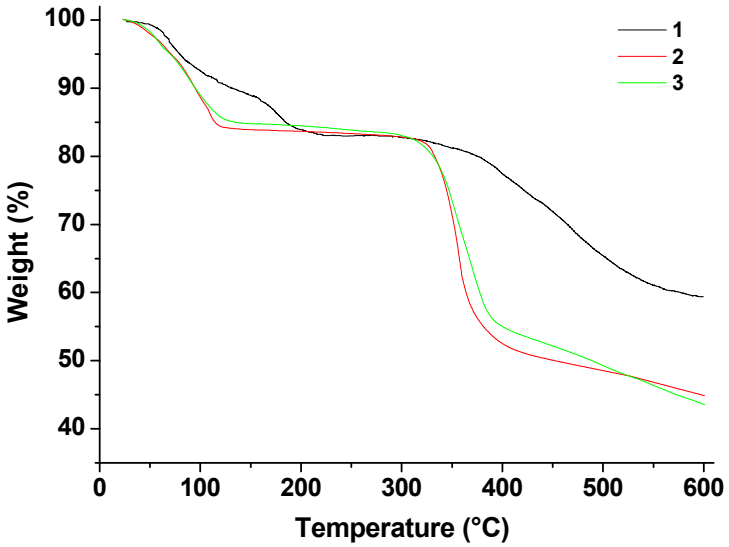

Fig. S2. The TGA curves of complexes **1 - 3**.

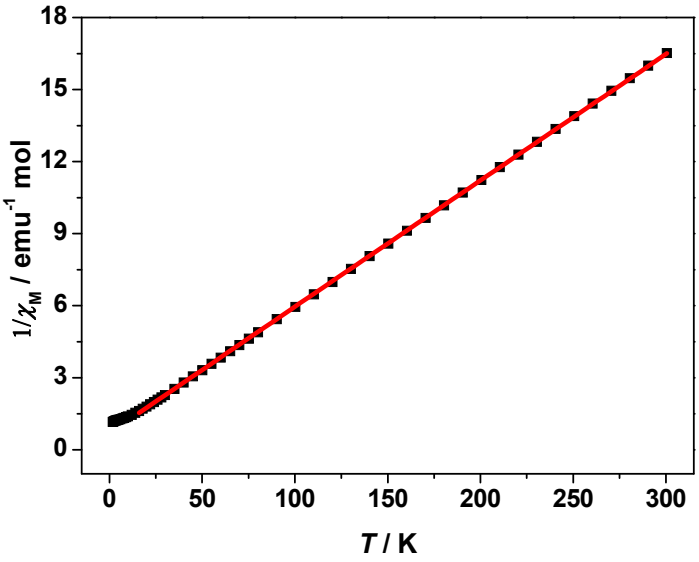

Fig. S3. Temperature dependence of $1/\chi_M$ for **1** in the range of ca. 14 - 300 K. The solid line shows the Curie–Weiss fitting.

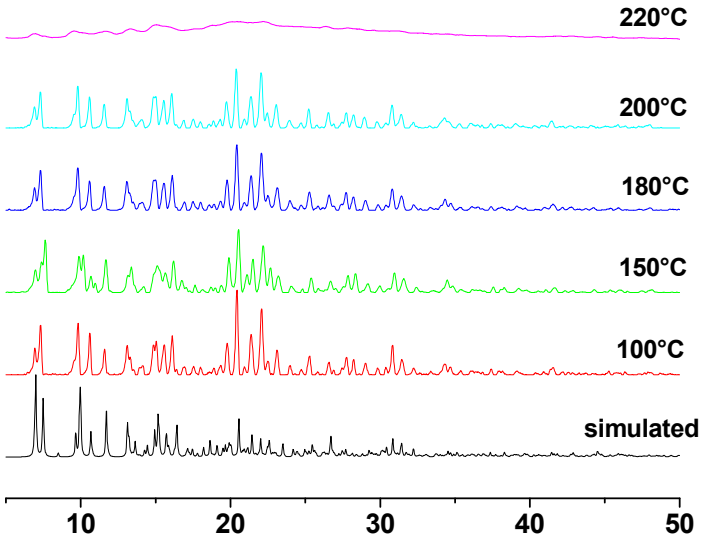

Fig. S4. Comparison of the PXRD patterns of **2** evacuated at different temperatures.

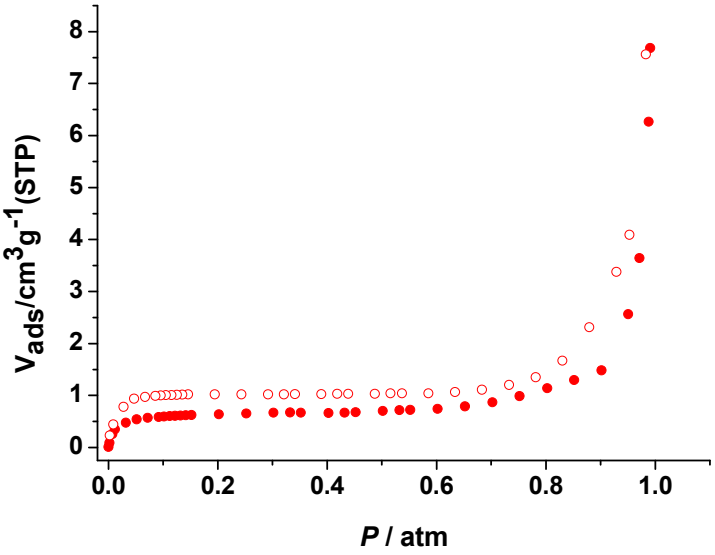

Fig. S5. N_2 adsorption isotherms for complex **2** at 77 K: filled shape, adsorption; open shape, desorption.