Electronic Supplementary Information

A Carbon-free Inorganic-metal Complex Consisting of All-nitrogen Pentazole Anion, Zn(II) Cation and H_2O

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Table S1. Bond lengths of complex **2**.

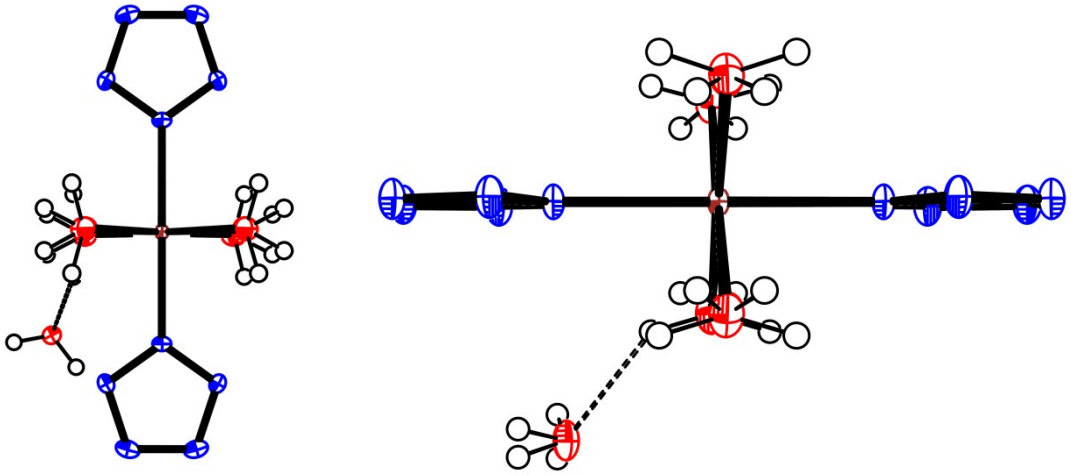
parameter		bond length (Å)
Zn1	O1	2.105(3)
Zn1	O1	2.105(3)
Zn1	O1	2.105(3)
Zn1	O1	2.105(3)
Zn1	N1	2.155(5)
Zn1	N1	2.155(5)
O2	H2A	0.86
O2	H2B	0.8603
O1	H1A	0.896
O1	H1B	0.8961
N1	N2	1.329(4)
N1	N2	1.329(4)
N2	N3	1.328(5)
N3	N3	1.326(7)

Table S2. Bond angles of complex **2**.

parameter			bond angle (°)
O1	Zn1	O1	91.6(2)
O1	Zn1	O1	88.4(2)
O1	Zn1	O1	180
O1	Zn1	O1	88.4(2)
O1	Zn1	O1	180
O1	Zn1	O1	91.6(2)
O1	Zn1	N1	90
O1	Zn1	N1	90
O1	Zn1	N1	90
O1	Zn1	N1	90
O1	Zn1	N1	90
O1	Zn1	N1	90
O1	Zn1	N1	90
O1	Zn1	N1	90
N1	Zn1	N1	180
H2A	O2	H2B	109.5
Zn1	O1	H1A	111.7
Zn1	O1	H1B	111.7
H1A	O1	H1B	107.1
N2	N1	Zn1	125.4(2)
N2	N1	Zn1	125.4(2)
N2	N1	N2	109.2(5)
N3	N2	N1	106.9(3)
N3	N3	N2	108.5(2)

Table S3. Hydrogen bonds of complex **2**.

Donor-H…Acceptor	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (°)
O(1)-H(1A)…O(2)	0.9	2.01	2.797(4)	145
O(1)-H(1B)…O(1)	0.9	2.49	3.145(5)	130
O(2)-H(2A)…N(2)	0.86	2.24	3.002(5)	148
O(2)-H(2B)…N(3)	0.86	2.07	2.891(5)	160



(a) (b)

Fig. S1 (a) ORTEP representation of the molecular structure of **2** viewed normal to (001). (b) ORTEP representation of the molecular structure of **2** viewed normal to (100).

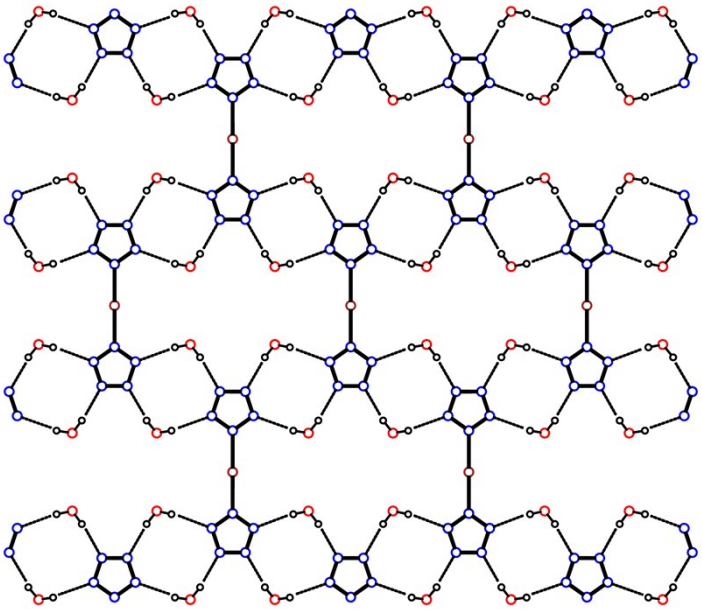


Fig. S2 2D layered intermolecular interactions in the crystal structure of **2** viewed normal to (001) (coordinated waters are omitted for clarity).

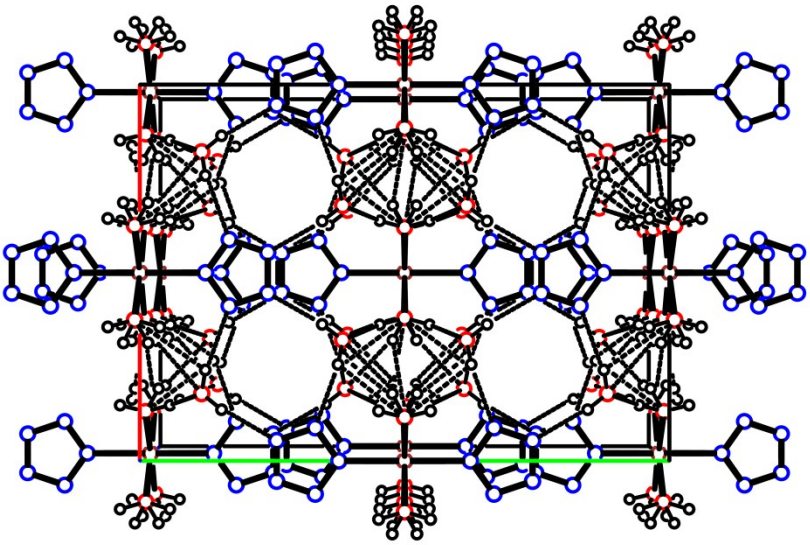


Fig. S3 Ball-and-stick packing diagrams of **2** viewed normal to (001) with hydrogen bonds.

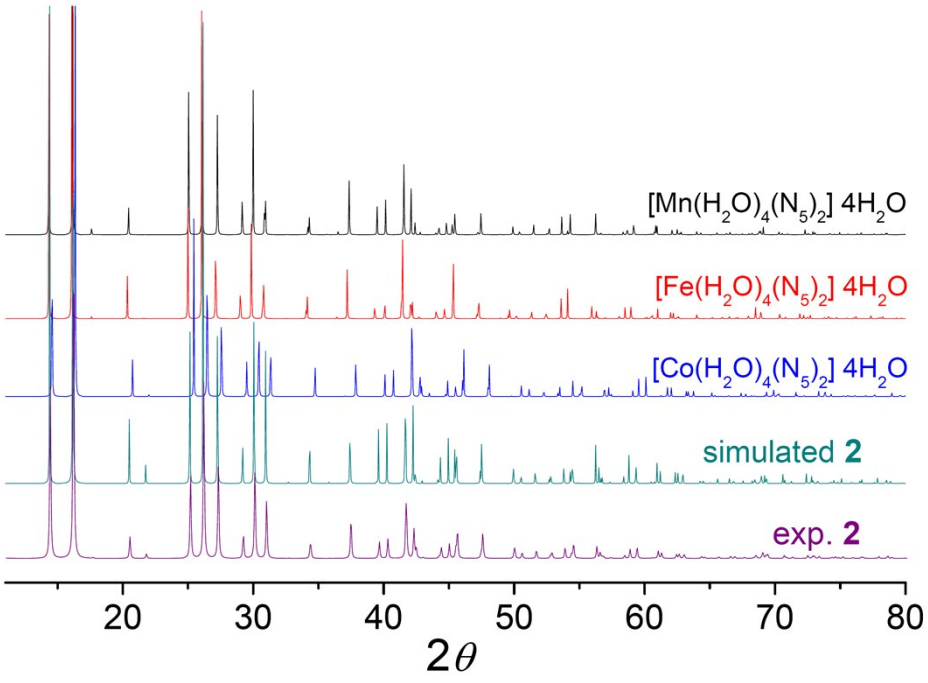


Fig. S4 Powder X-ray diffraction pattern of complex **2** (purple). The patterns in black ($[Mn(H_2O)_4(N_5)_2]\cdot 4H_2O$), red ($[Fe(H_2O)_4(N_5)_2]\cdot 4H_2O$), blue ($[Co(H_2O)_4(N_5)_2]\cdot 4H_2O$), and dark green (**2**) are the calculated patterns from their single crystal structures.