Supporting Information

A series of coordination polymers based on a 5-(3'-amine-1'*H*-pyrazol-4'-yl)-1*H*-tetrazole ligand: synthesis, structure and properties

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Table S1. Selected Bond Lengths(Å) and Bond Angles (° deg) for 1-4

		1			
Co(1)-N(1)	2.107(11)	N(1)-Co(1)-N(4)#1	176.2(4)	N(4)#1-Co(1)-N(14)	91.7(4)
Co(1)- N(8)	2.112(11)	N(8)-Co(1)-N(4)#1	87.0(4)	N(11)#2-Co(1)-N(14)	94.1(4)
Co(1)-N(4)#1	2.160(12)	N(1)-Co(1)-N(11)#2	86.0(4)	N(1)-Co(1)-N(7)	82.9(4)
Co(1)-N(11)#2	2.166(10)	N(8)-Co(1)-N(11)#2	175.1(5)	N(8)-Co(1)-N(7)	87.8(4)
Co(1)-N(14)	2.232(11)	N(4)#1-Co(1)-N(11)#2	97.8(4)	N(4)#1-Co(1)-N(7)	97.2(4)
Co(1)-N(7)	2.258(13)	N(1)-Co(1)-N(14)	87.8(4)	N(11)#2-Co(1)-N(7)	92.0(4)
N(1)-Co(1)-N(8)	89.2(4)	N(8)-Co(1)-N(14)	85.3(4)	N(14)-Co(1)-N(7)	168.4(5)
		2			
Zn(1)-N(8)	2.136(11)	N(4)#1-Zn(1)-N(11)#2	98.9(4)	N(1)-Zn(1)-N(14)	87.1(4)
Zn(1)-N(4)#1	2.160(10)	N(8)-Zn(1)-N(1)	88.4(4)	N(8)-Zn(1)-N(7)	86.4(4)
Zn(1)-N(11)#2	2.162(11)	N(4)#1-Zn(1)-N(1)	175.0(4)	N(4)#1-Zn(1)-N(7)	97.7(4)
Zn(1)-N(14)	2.217(11)	N(11)#2-Zn(1)-N(1)	86.2(4)	N(11)#2-Zn(1)-N(7)	92.0(4)
Zn(1)-N(7)	2.307(12)	N(8)-Zn(1)-N(14)	85.2(4)	N(1)-Zn(1)-N(7)	82.2(4)
N(8)-Zn(1)-N(4)#1	86.6(4)	N(4)#1-Zn(1)-N(14)	92.2(4)	N(14)-Zn(1)-N(7)	166.5(4)
N(8)-Zn(1)-N(11)#2	174.5(4)	N(11)#2-Zn(1)-N(14)	95.5(4)		
		3			
Cd(1)-N(11)#2	2.319(7)	N(11)#2-Cd(1)-N(8)	172.3(3)	N(8)-Cd(1)-N(14)	80.4(2)
Cd(1)-N(4)#3	2.325(7)	N(4)#3-Cd(1)-N(8)	84.9(2)	N(1)-Cd(1)-N(14)	88.3(3)
Cd(1)-N(8)	2.327(7)	N(11)#2-Cd(1)-N(1)	85.7(2)	N(11)#2-Cd(1)-N(7)	91.7(2)
Cd(1)-N(1)	2.373(7)	N(4)#3-Cd(1)-N(1)	171.5(2)	N(4)#3-Cd(1)-N(7)	101.9(2)
Cd(1)-N(14)	2.410(7)	N(8)-Cd(1)-N(1)	86.6(2)	N(8)-Cd(1)-N(7)	87.0(2)
Cd(1)-N(7)	2.486(8)	N(11)#2-Cd(1)-N(14)	98.8(2)	N(1)-Cd(1)-N(7)	77.2(2)
N(11)#2-Cd(1)-N(4)#3	102.8(2)	N(4)#3-Cd(1)-N(14)	90.7(3)	N(14)-Cd(1)-N(7)	161.4(3)
		4			
Cu(1)-N(1)	1.990(2)	N(1)-Cu(1)-N(7)#1	87.99(10)	N(1)#1-Cu(1)-N(3)#2	93.54(8)
Cu(1)-N(1)#1	1.990(2)	N(1)#1-Cu(1)-N(7)#1	92.01(10)	N(7)#1-Cu(1)-N(3)#2	90.09(9)
Cu(1)-N(7)#1	2.069(2)	N(1)-Cu(1)-N(7)	92.01(10)	N(7)-Cu(1)-N(3)#2	89.91(9)
Cu(1)-N(7)	2.069(2)	N(1)#1-Cu(1)-N(7)	87.99(10)	N(1)-Cu(1)-N(3)#3	86.46(8)
Cu(1)-N(3)#2	2.462(2)	N(7)#1-Cu(1)-N(7)	180.0	N(7)#1-Cu(1)-N(3)#3	89.91(9)
Cu(1)-N(3)#3	2.462(2)	N(1)-Cu(1)-N(7)	174.70(10)	N(7)-Cu(1)-N(3)#3	90.09(9)
N(1)-Cu(1)-N(1)#1	180.000(9)	N(1)-Cu(1)-N(3)#2	86.46(8)	N(3)#2-Cu(1)-N(3)#3	180.00

Symmetry transformations used to generate equivalent atoms:

1, #1 *x*, -*y*+3/2, *z*-1/2 #2 *x*+1, -*y*+3/2, *z*+1/2 #3 *x*, -*y*+3/2, *z*+1/2 #4 *x*-1, -y+3/2, *z*-1/2

2, #1 *x*+1, -*y*+3/2, *z*+1/2 #2 *x*, -*y*+3/2, *z*-1/2 #3 *x*-1, -*y*+3/2, *z*-1/2 #4 *x*, -*y*+3/2, *z*+1/2

3, #1 *x*+1, -*y*+3/2, *z*+1/2 #2 *x*, -*y*+3/2, *z*-1/2 #3 *x*, -*y*+3/2, *z*+1/2 #4 *x*-1, -*y*+3/2, *z*-1/2

4, #1 -*x*, -*y*+1, -*z*+1 #2 -*x*, *y*+1/2, -*z*+1/2 #3 *x*, -*y*+1/2, *z*+1/2 #4 -*x*, *y*-1/2, -*z*+1/2

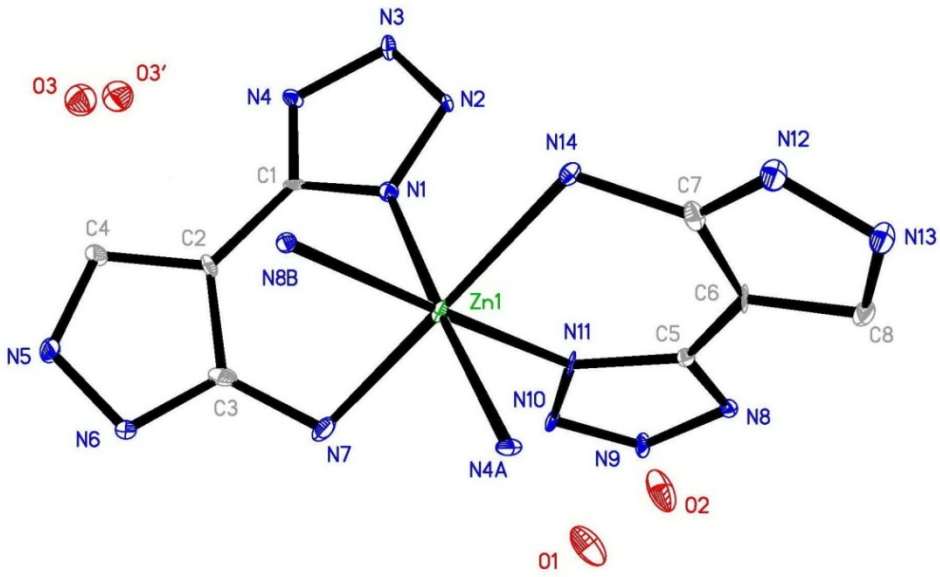

Figure S1. Molecule structure of **2**, showing the coordination environments of Zn^{II} and H_2apt ligands. Symmetry operator: A = *x*, 1.5–*y*, –0.5+*z*; B = 1+*x*, 1.5–*y*, 0.5+*z*.

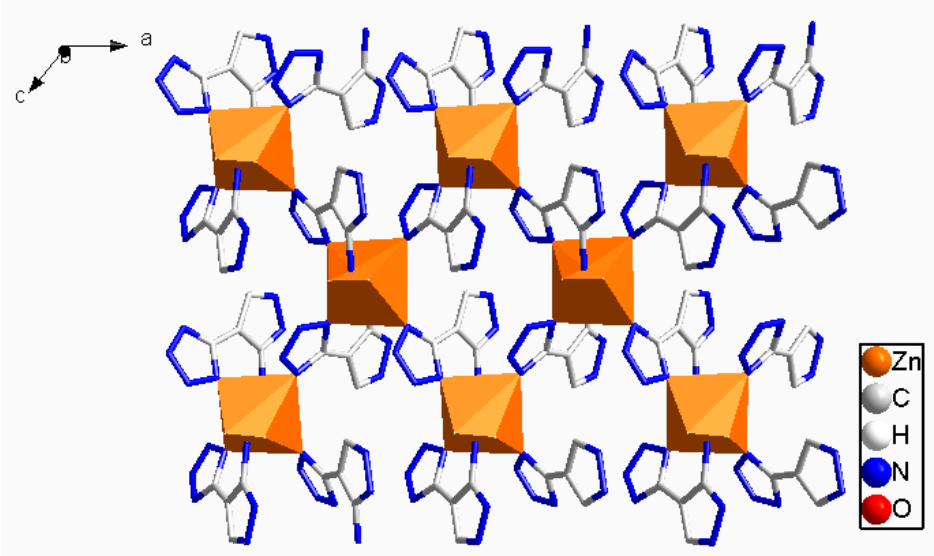

Figure S2. The 2D layer of **2**.

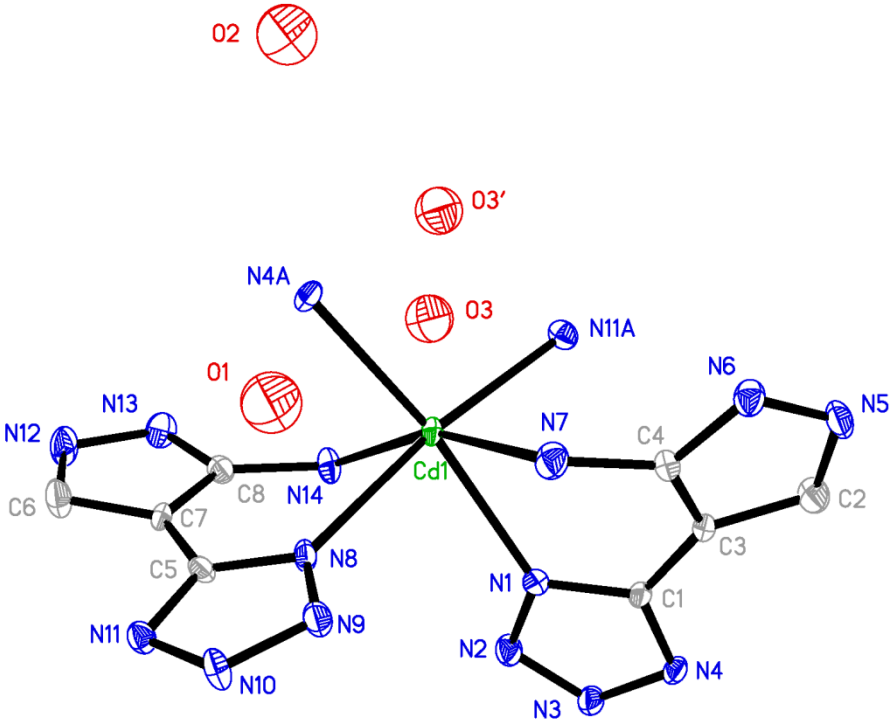

Figure S3. Molecule structure of **3**, showing the coordination environments of Cd^{II} and H_2apt ligands. Symmetry operator: A = –0.5+*x*, 0.5–*y*, –0.5+*z*; B = –0.5+*x*, 0.5–*y*, 0.5+*z*.

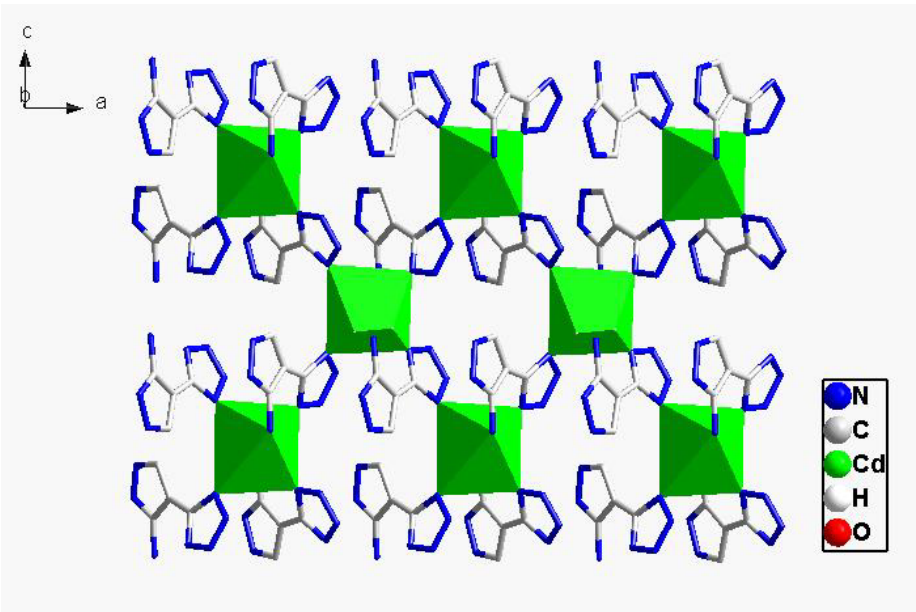

Figure S4. The 2D layer of **3**.

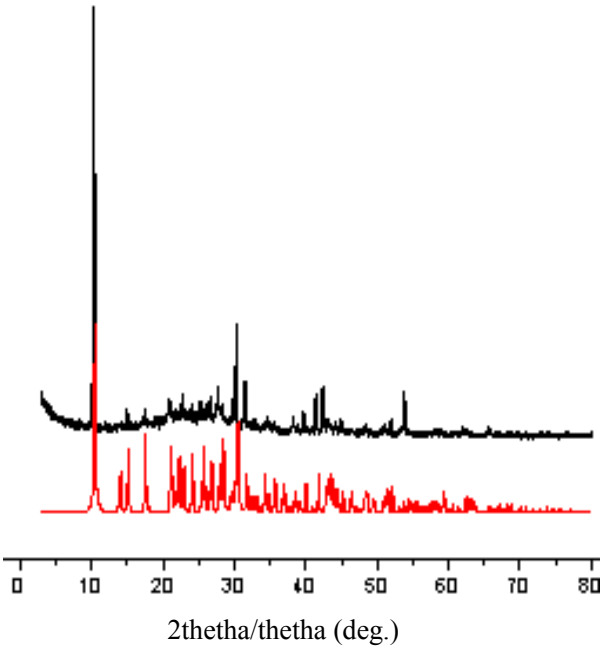

Figure S5. X-Ray powder diffraction patterns of **1**. Black line (experiment); red line (simulation) .

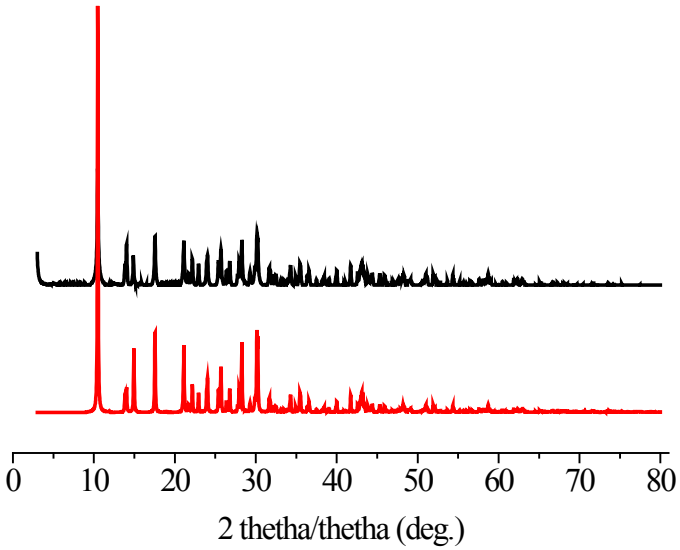

Figure S6. X-Ray powder diffraction patterns of **2**. Black line (experiment); red line (simulation) .

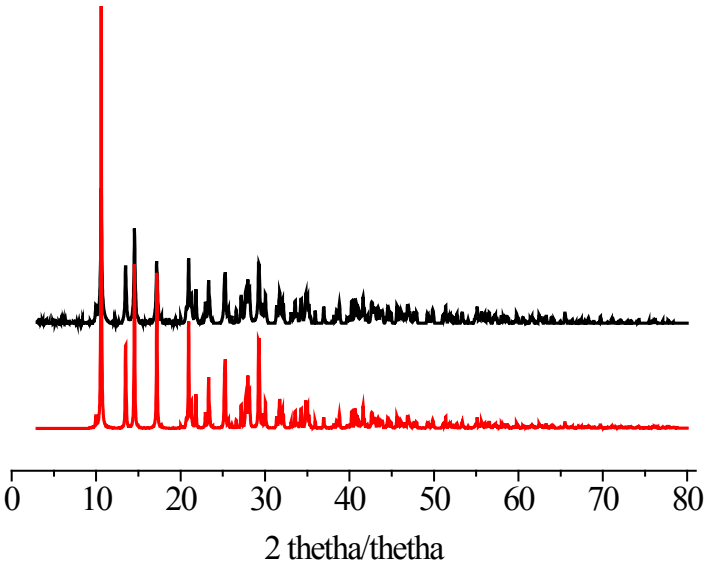

Figure S7. X-Ray powder diffraction patterns of **3**. Black line (experiment); red line (simulation) .