

**Two unprecedented 3D metal-organic polyrotaxane frameworks
based on a new flexible tri(imidazole) ligand**

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Table S1. Selected bond lengths [Å] and angles [deg] for **1** and **2**.^[a]

Compound 1			
Cd(1)-O(4)	2.690(6)	Cd(1)-N(5)#1	2.309(7)
Cd1-O2#2	2.671(9)	Cd(1)-O(5)	2.239(5)
Cd(1)-O(3)#2	2.310(6)	Cd(1)-N(7)#3	2.312(7)
Cd(1)-N(3)	2.346(8)	N(5)#1-Cd(1)-N(3)	93.7(3)
N(5)#1-Cd(1)-N(7)#3	91.8(3)	N(5)#1-Cd(1)-O(3)#2	86.8(3)
N(7)#3-Cd(1)-N(3)	174.2(3)		
Compound 2			
Cd(1)-N(7)	2.286(4)	Cd(1)-N(7)#1	2.286(4)
Cd(1)-N(5)#2	2.374(4)	Cd(1)-N(5)#3	2.374(4)
Cd(1)-Cl(1)#4	2.6695(13)	Cd(1)-Cl(1)#5	2.6695(13)
Cd(2)-O(1)	2.245(4)	Cd(2)-N(3)	2.249(4)
Cd(2)-O(3)	2.261(3)	Cd(2)-O(4)	2.483(4)
Cd(2)-O(2)	2.512(4)	Cd(2)-Cl(1)	2.5367(14)
N(7)-Cd(1)-N(7)#1	180	N(7)-Cd(1)-N(5)#2	89.29(15)
N(7)#1-Cd(1)-N(5)#2	90.71(15)	N(7)-Cd(1)-N(5)#3	89.29(15)
N(7)#1-Cd(1)-N(5)#3	90.71(15)	N(5)#2-Cd(1)-N(5)#3	180
N(7)-Cd(1)-Cl(1)#4	88.64(12)	N(7)#1-Cd(1)-Cl(1)#4	91.36(12)
N(5)#2-Cd(1)-Cl(1)#4	95.80(11)	N(5)#3-Cd(1)-Cl(1)#4	84.20(11)
N(7)-Cd(1)-Cl(1)#5	91.36(12)	N(7)#1-Cd(1)-Cl(1)#5	88.64(12)
N(5)#2-Cd(1)-Cl(1)#5	84.20(11)	N(5)#3-Cd(1)-Cl(1)#5	95.80(11)
Cl(1)#4-Cd(1)-Cl(1)#5	180		

[a] Symmetry operations: for **1**: #1 -x+2, -y, -z+1; #2 x-1, y-1, z+1; #3 x+1, y+1, z-1; for **2**: #1 -x+3/2, y-1/2, -z+3/2; #2 x+1, y, z; #3 x, y-1, z.

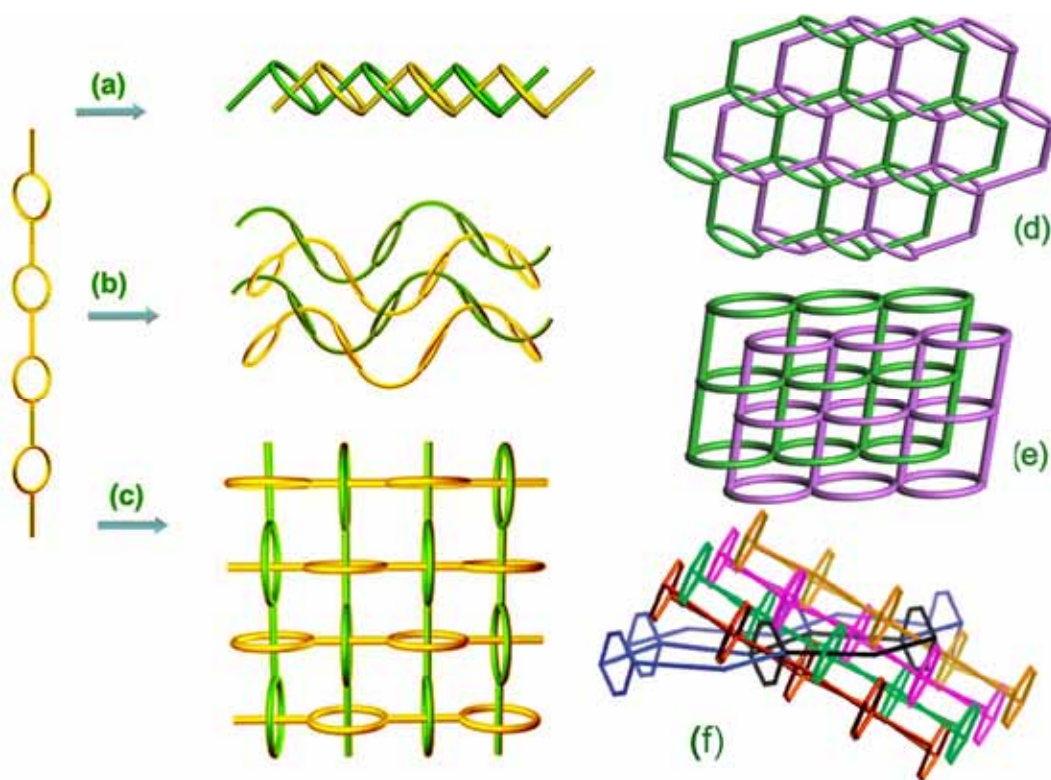


Chart S1. Schematic representations of the known (a) 1D \rightarrow 1D, (b) inclined 1D \rightarrow 2D, (c) parallel 1D \rightarrow 2D, (d) and (e) parallel 2D \rightarrow 2D, and (f) inclined 2D \rightarrow 3D polyrotaxane networks.

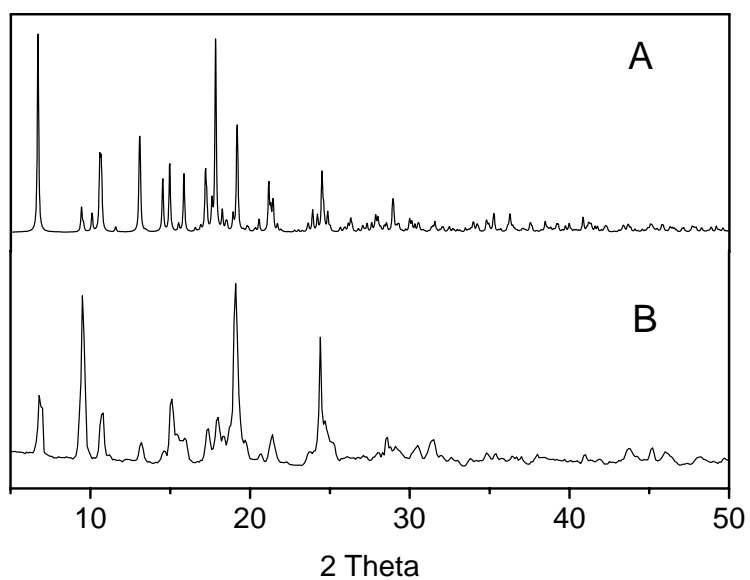


Fig. S1. Simulated (A) and measured (B) PXR patterns of **1**.

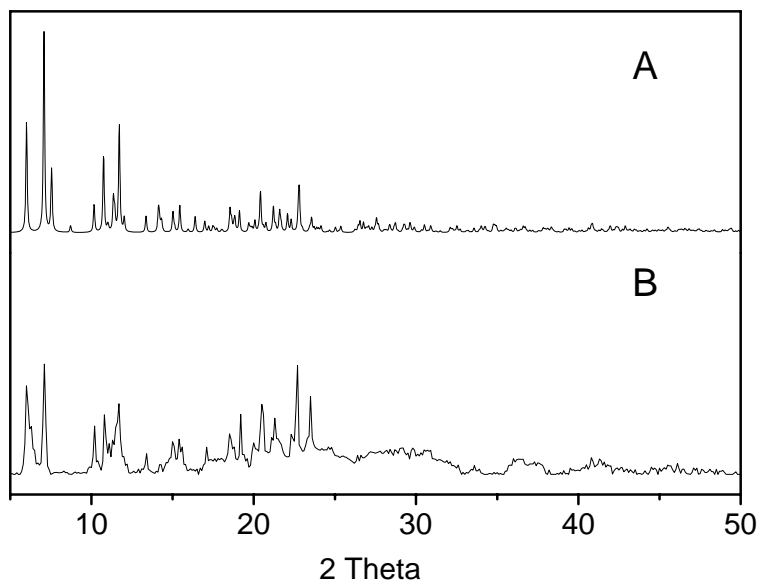


Fig. S2. Simulated (A) and measured (B) PXRD patterns of **2**.