Electronic Supporting Information (ESI)

A (3,6)-connected layer with unprecedented adeninate nucleobase-derived heptanuclear disc

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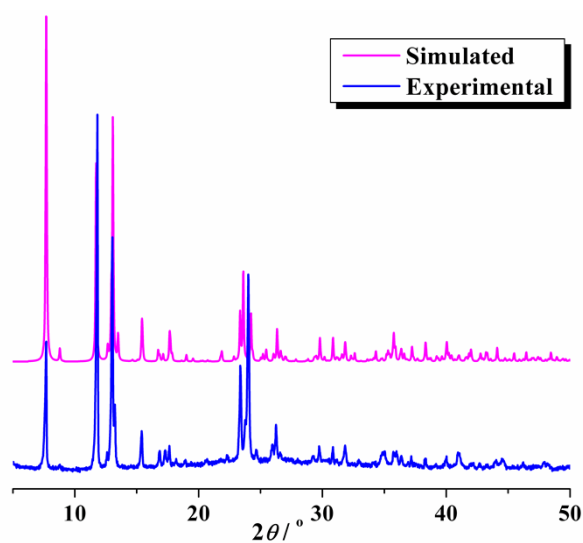[b] *Collaborative Center of Chemical Science and Engineering (Tianjin), Tianjin 300071, China*

Fig. S1 Simulated (purple) and experimental (blue) PXRD patterns for **1**.
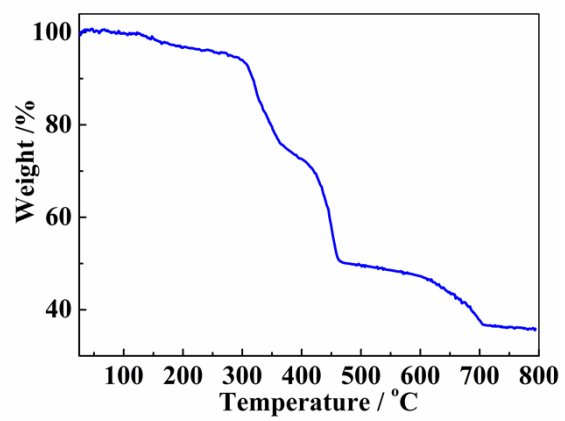
Fig. S2 TG curve of **1**.

Table S1 Selected Bond Lengths (Å) and Angles (°) for **1** ^{a}

Cu(1)–O(9)	1.979(3)	Cu(3)–O(10)$^{\#1}$	1.981(3)
Cu(1)–O(10)	2.000(3)	Cu(3)–N(3)	2.103(4)
Cu(1)–O(8)	2.327(4)	Cu(3)–O(11W)	2.430(4)
Cu(2)–O(8)	1.924(3)	Cu(3)–O(5)	2.484(4)
Cu(2)–O(3)$^{\#2}$	1.973(4)	Cu(4)–N(9)	1.880(6)
Cu(2)–O(9)	1.982(4)	Cu(4)–O(8)$^{\#1}$	1.908(3)
Cu(2)–O(2)$^{\#3}$	1.994(4)	Cu(4)–O(1)$^{\#4}$	1.996(4)
Cu(2)–O(11W)	2.385(4)	Cu(4)–O(10)$^{\#1}$	2.001(4)
Cu(2)–O(12W)	2.438(4)	Cu(4)–O(5)	2.415(4)
Cu(3)–O(9)	1.945(3)	Cu(4)–O(12W)	2.576(3)
Cu(3)–O(4)$^{\#2}$	1.976(4)		
O(9)$^{\#1}$–Cu(1)–O(10)	79.66(14)	O(10)$^{\#1}$–Cu(3)–N(3)	89.78(19)
O(9)–Cu(1)–O(10)	100.34(14)	O(4)$^{\#2}$–Cu(3)–N(3)	95.7(2)
O(9)$^{\#1}$–Cu(1)–O(8)	105.08(13)	O(9)–Cu(3)–O(11W)	85.41(14)
O(9)–Cu(1)–O(8)	74.92(13)	O(4)$^{\#2}$–Cu(3)–O(11W)	81.88(15)
O(10)$^{\#1}$–Cu(1)–O(8)	105.67(13)	O(10)$^{\#1}$–Cu(3)–O(11W)	90.96(14)
O(10)–Cu(1)–O(8)	74.33(13)	N(3)–Cu(3)–O(11W)	99.89(18)
O(8)–Cu(2)–O(9)	84.79(15)	O(9)–Cu(3)–O(5)	89.28(13)
O(3)$^{\#2}$–Cu(2)–O(9)	94.37(15)	O(4)$^{\#2}$–Cu(3)–O(5)	104.93(15)
O(8)–Cu(2)–O(2)$^{\#3}$	93.95(16)	O(10)$^{\#1}$–Cu(3)–O(5)	81.87(14)
O(3)$^{\#2}$–Cu(2)–O(2)$^{\#3}$	88.96(15)	N(3)–Cu(3)–O(5)	84.37(18)
O(8)–Cu(2)–O(11W)	86.45(14)	N(9)–Cu(4)–Cu(2)$^{\#1}$	150.03(19)
O(3)$^{\#2}$–Cu(2)–O(11W)	84.59(15)	N(9)–Cu(4)–O(1)$^{\#4}$	90.9(2)
O(9)–Cu(2)–O(11W)	85.83(14)	O(8)$^{\#1}$–Cu(4)–O(1)$^{\#4}$	93.00(16)
O(2)$^{\#3}$–Cu(2)–O(11W)	107.77(15)	N(9)–Cu(4)–O(10)$^{\#1}$	93.8(2)
O(8)–Cu(2)–O(12W)	91.36(15)	O(8)$^{\#1}$–Cu(4)–O(10)$^{\#1}$	84.40(14)
O(3)$^{\#2}$–Cu(2)–O(12W)	97.35(16)	N(9)–Cu(4)–O(5)	86.5(2)
O(9)–Cu(2)–O(12W)	81.47(15)	O(8)$^{\#1}$–Cu(4)–O(5)	85.12(14)
O(2)$^{\#3}$–Cu(2)–O(12W)	84.90(15)	O(1)$^{\#4}$–Cu(4)–O(5)	112.19(16)
O(9)–Cu(3)–O(10)$^{\#1}$	80.97(14)	O(10)$^{\#1}$–Cu(4)–O(5)	83.24(14)
O(9)–Cu(3)–O(4)$^{\#2}$	94.09(15)		

^{a} Symmetry codes: $^{\#1}$ $1 - x$, $1 - y$, $2 - z$, $^{\#2}$ $2 - x$, $-y$, $2 - z$, $^{\#3}$ $x - 1$, y, $z + 1$, $^{\#4}$ $2 - x$, $1 - y$, $1 - z$.

Table S2 The geometric parameters involved in the superexchange pathways within the Cu^{II}_7 cluster of **1**.

Coupling constant	pathways	$r_{Cu\cdots Cu}$ (Å)		θ (°)	mediator	Overlap of the magnetic orbits	$\angle$Cu–O–Cu (°)
J_1	1	Cu1$\cdots$Cu4	3.1701(4)	61.197	μ_3-OH$^-$	dz^2–$d(x^2–y^2)$	96.437(6)
					μ_3-OH$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	104.797(6)
	2	Cu1$\cdots$Cu2	3.1473(3)	62.712	μ_3-OH$^-$	$d(x^2–y^2)$—$d(x^2–y^2)$	105.231(6)
					μ_3-OH$^-$	dz^2–$d(x^2–y^2)$	95.055(5)
J_2	3	Cu1$\cdots$Cu3	3.0199(4)	5.257	μ_3-OH$^-$	$d(x^2–y^2)$—$d(x^2–y^2)$	98.698(5)
					μ_3-OH$^-$	$d(x^2–y^2)$—$d(x^2–y^2)$	100.633(5)
J_3	4	Cu2$\cdots$Cu3	3.0922(4)	60.405	μ-H$_2$O	dz^2–dz^2	79.904(4)
					μ_3-OH$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	103.911(6)
					syn,syn-COO$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	
	5	Cu2$\cdots$Cu4	3.0141(4)	64.411	μ-H$_2$O	dz–dz^2	73.853(4)
					μ_3-OH$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	103.746(6)
					μ-syn,syn-COO$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	
J_4	6	Cu3$\cdots$Cu4	3.2306(3)	56.053	μ-SO$_3^-$	dz^2–dz^2	82.488(4)
					μ_3-OH$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	108.439(6)
					μ-N3, N9-ade$^-$	$d(x^2–y^2)$–$d(x^2–y^2)$	
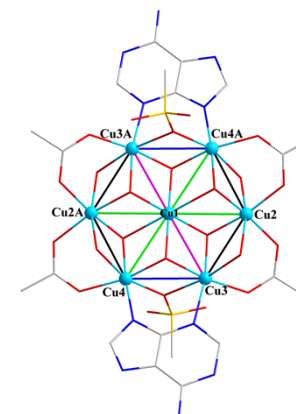
Table S3 Selected Hydrogen-bonding parameters (Å, °) for **1** [a]

D–H⋯A	d (D–H)	d (H⋯A)	d (D⋯A)	∠DHA
O10–H10'⋯O6[#1]	0.850	1.982	2.790	158.43
O12W–H12A⋯O6[#1]	0.850	2.367	2.813	113.26
O12W–H12B⋯N7[#2]	0.850	2.062	2.880	161.44
O11W–H11A⋯O7[#3]	0.850	1.973	2.733	148.38
O11W–H11B⋯N1[#4]	0.850	1.742	2.585	170.60
N6–H6B⋯O2[#4]	0.860	2.379	3.183	155.84

[a] Symmetry codes: [#1] $1-x, 1-y, 1-z$, [#2] $1+x, y, z$, [#3] $x, y, z-1$, [#4] $-x, -y, 1-z$.
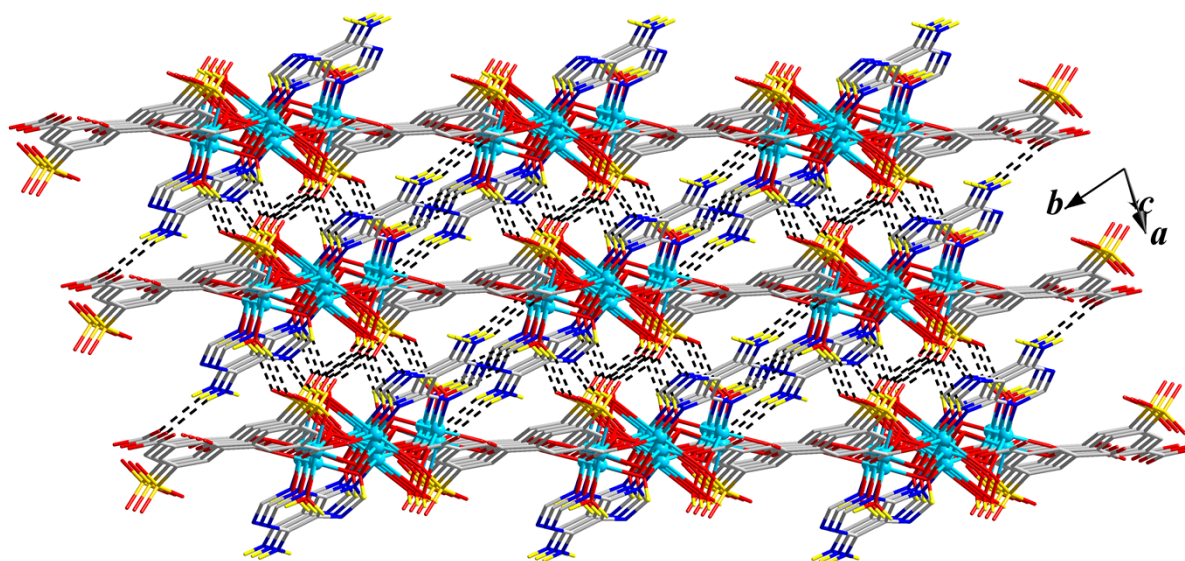
Fig. S3 3D supramolecular network of **1** generated by hydrogen-bonding interactions.