

Electronic Supplementary Information (ESI) for Dalton Transactions

**Eight Zn(II) coordination networks based on flexible
1,4-di(1H-imidazol-1-yl)butane and different dicarboxylates:
Crystal structures, water clusters, and topologies**

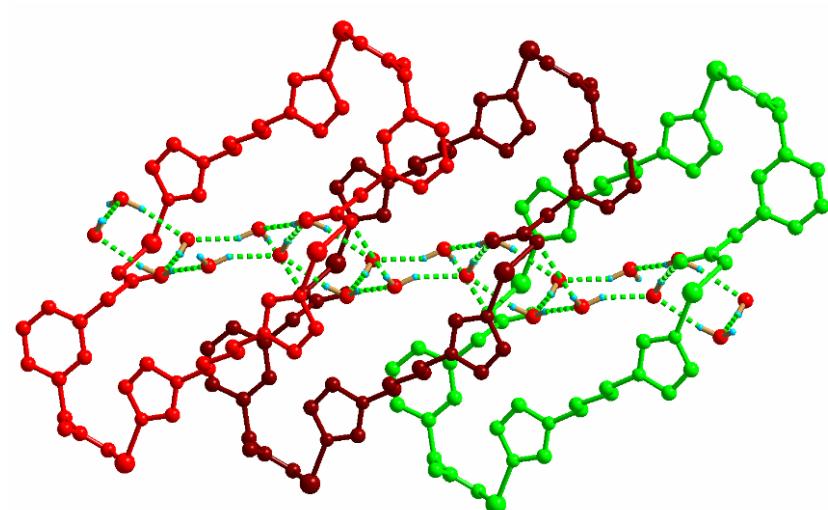
Di Sun,* Meng-Zhen Xu, Shan-Shan Liu, Shuai Yuan, Hai-Feng Lu, Sheng-Yu Feng,
Dao-Feng Sun

*Key Lab of Colloid and Interface Chemistry, Ministry of Education, School of Chemistry and Chemical
Engineering, Shandong University, Jinan, 250100, P. R. China. E-mail: dsun@sdu.edu.cn.*

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(1) Figure S1: The T4(2)6(2) water tape penetrates the windows of the 2D network of 2.



(2) Figure S2: The structural graphics for structure of 2.

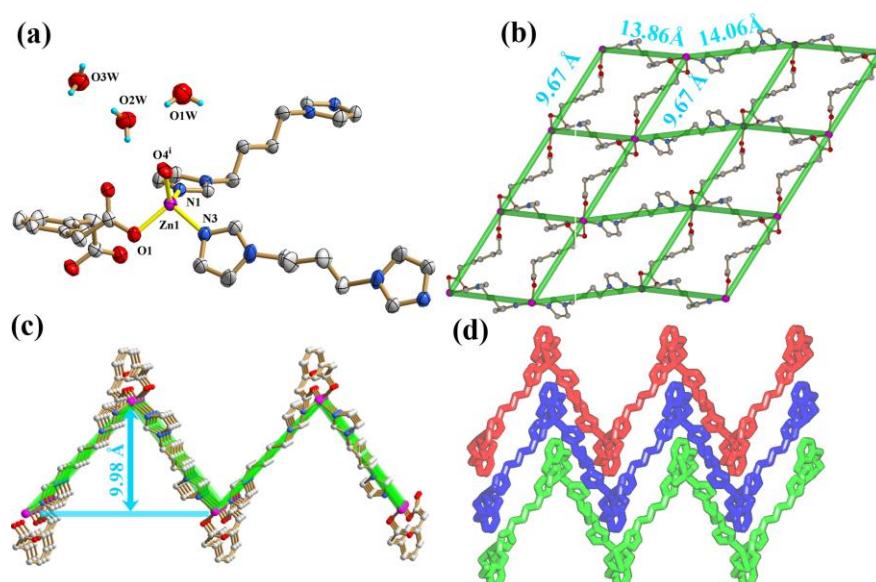


Figure S2 (a) The coordination environment of Zn(II) ion in **2** with the thermal ellipsoids at 50% probability level. (b) Ball-and-Stick view of the 2D 4⁴-sql net (Purple ball: Zn; Blue ball: N; Red ball: O; Gray: C). (c) Side view of the undulated 4⁴-sql net in the structure of **2**. (d) The packing of 2D nets in the crystal. (networks individually colored)

(3) Figure S3: The structural graphics for structure of 4.

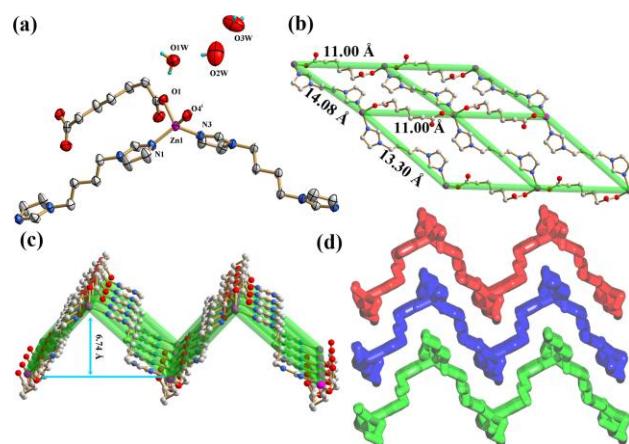


Figure S3 (a) The coordination environment of Zn(II) ion in **4** (Symmetry code: (iii) $-x+1, -y+1, -z+1$). (b) Ball-and-Stick view of the 2D 4^4 -sql net. (c) Side view of the undulated 4^4 -sql net in the structure of **4** (Purple ball: Zn; Blue ball: N; Red ball: O; Gray: C). (d) The packing of 2D nets in the crystal. (networks individually colored)

(4) Figure S4: The structural graphics for structure of 7.

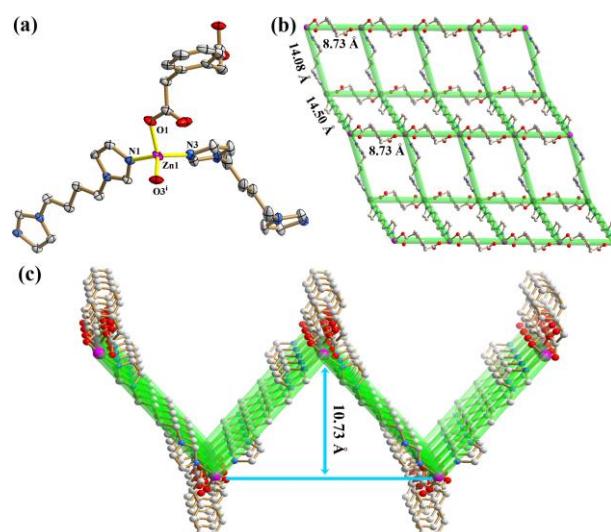


Figure S4 (a) The coordination environment of Zn(II) ion in **7** (Symmetry code: (i) $x, y-1, z$). (b) Ball-and-Stick view of the 2D 4^4 -sql net. (c) Side view of the undulated 4^4 -sql net in the structure of **7** (Purple ball: Zn; Blue ball: N; Red ball: O; Gray: C).

(5) Figure S5: The structural graphics for structure of 8.

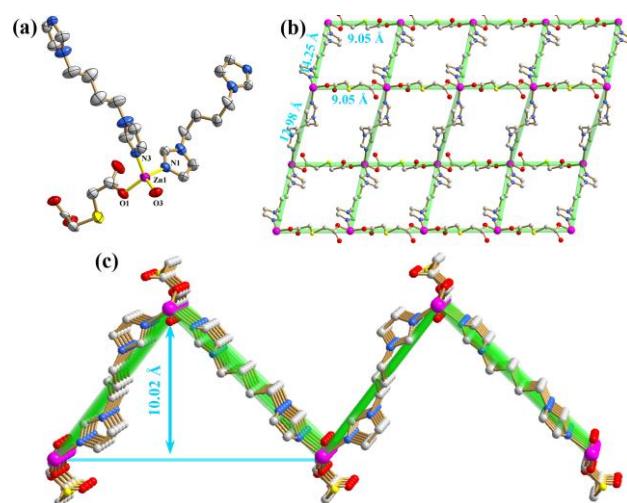
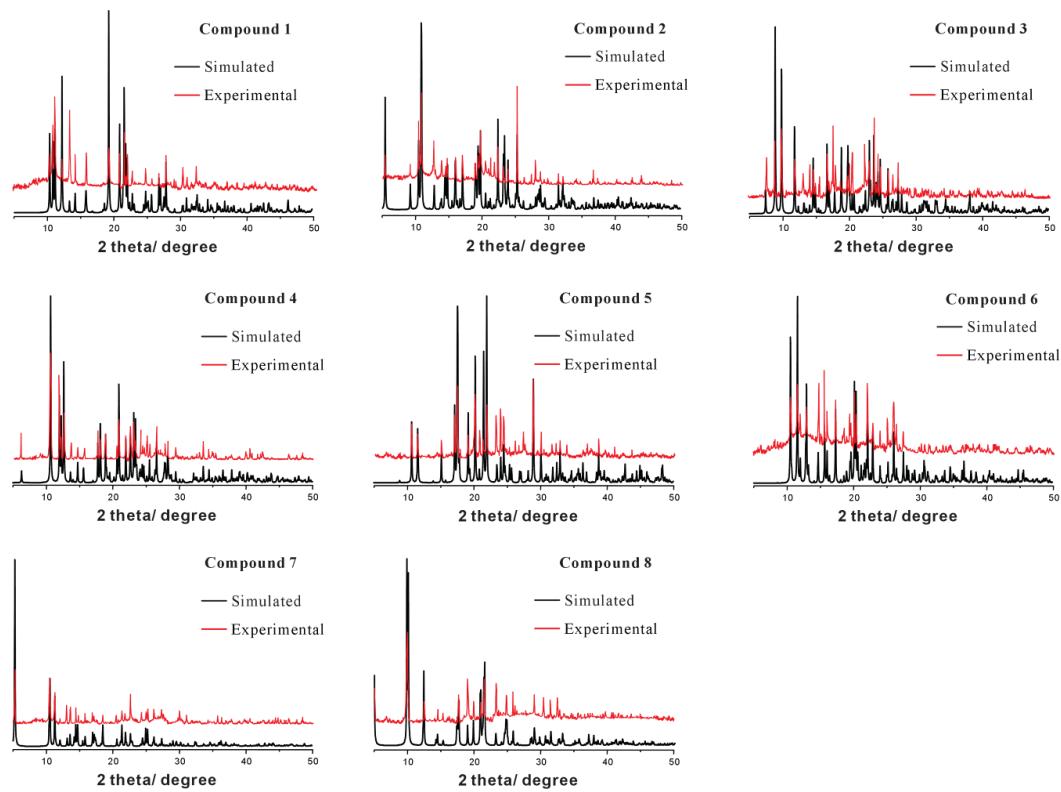


Figure S5 (a) The coordination environment of Zn(II) ion in **8** Symmetry code: (i) x , $y-1$, z . (b) Ball-and-Stick view of the 2D 4^4 -sql net. (c) Side view of the undulated 4^4 -sql net in the structure of **7** (Purple ball: Zn; Blue ball: N; Red ball: O; Gray: C).

(6) Figure S6: PXRD patterns of 1-8



(7) Figure S7: Solid-State Photoluminescences of CPs 1-8 at 77 K (black line) and 298 K (red line)

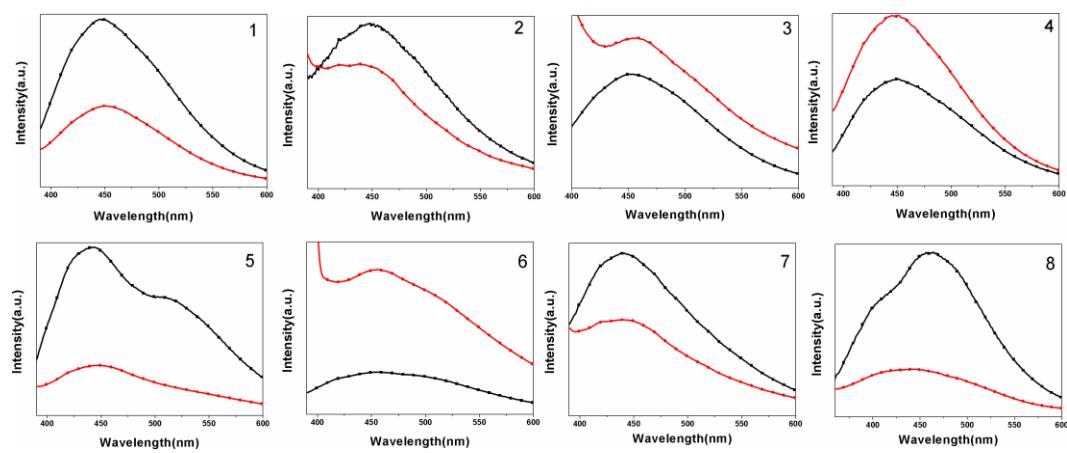


Figure S7 Solid-State Photoluminescences of CPs 1-8 at 77 K (black line) and 298 K (red line).

(8) Table S1: Selected bond lengths (Å) and angle (°) for 1-8.

Complex 1							
Zn1-N1	2.0012(17)	Zn1-O2A	1.849(9)				
N1 ⁱ -Zn1-N1	117.51(10)	O2A ⁱ -Zn1-N1 ⁱ	106.3(3)	O2A-Zn1-N1 ⁱ	120.3(3)		
Symmetry code: (i) $-x+1, y, -z+3/2$.							
Complex 2							
Zn1-N1	1.9925(19)	Zn1-O1	1.9855(17)	Zn1-N3	2.024(2)	Zn1-O4 ⁱ	1.9577(18)
N1-Zn1-N3	110.49(8)	O4 ⁱ -Zn1-N1	118.57(8)	O1-Zn1-N1	106.96(8)	O4 ⁱ -Zn1-N3	107.32(9)
O1-Zn1-N3	98.37(8)	O4 ⁱ -Zn1-O1	113.28(8)				
Symmetry code: (i) $x, y+1, z$.							
Complex 3							
Zn1-N1	2.010(2)	Zn1-O1	1.945(2)	Zn1-N3 ⁱ	2.040(3)	Zn1-O3	1.982(2)
N1-Zn1-N3 ⁱ	102.79(10)	O1-Zn1-O3	103.26(9)	O1-Zn1-N1	128.50(10)	O3-Zn1-N1	110.39(10)
O1-Zn1-N3 ⁱ	109.18(11)	O3-Zn1-N3 ⁱ	99.06(10)				
Symmetry code: (i) $-x+2, -y, -z+1$.							
Complex 4							
Zn1-N1	1.995(3)	Zn1-O1	1.990(2)	Zn1-N3	2.007(3)	Zn1-O4 ⁱ	1.965(2)
N1-Zn1-N3	120.27(12)	O4 ⁱ -Zn1-N1	112.27(11)	O1-Zn1-N1	105.66(11)	O4 ⁱ -Zn1-N3	104.14(11)
O1-Zn1-N3	115.15(11)	O4 ⁱ -Zn1-O1	96.99(10)				
Symmetry code: (i) $x-1, y-1, z$.							
Complex 5							
Zn1-N1	1.966(3)	Zn1-O1W	1.993(3)	Zn1-O1	1.920(2)	Zn1-O4 ⁱ	1.922(3)
N1-Zn1-O1W	101.34(13)	O1-Zn1-O4 ⁱ	95.74(11)	O1-Zn1-N1	122.52(12)	O4 ⁱ -Zn1-N1	120.40(13)
O1-Zn1-O1W	108.81(12)	O4 ⁱ -Zn1-O1W	107.34(12)				
Symmetry code: (i) $x+1/2, y-1/2, -z+1/2$.							
Complex 6							
Zn1-N1	2.022(4)	Zn1-O1	1.954(4)	Zn1-N3	1.987(4)	Zn1-O4 ⁱ	1.958(4)
N3-Zn1-N1	103.26(17)	O1-Zn1-O4 ⁱ	109.02(17)	O1-Zn1-N1	113.61(17)	O4 ⁱ -Zn1-N1	96.34(18)
O1-Zn1-N3	118.40(18)	O4 ⁱ -Zn1-N3	113.97(18)				
Symmetry code: (i) $x+1/2, -y+1/2, z-1/2$.							
Complex 7							
Zn1-N1	2.004(3)	Zn1-O1	1.962(2)	Zn1-N3	1.984(3)	Zn1-O3 ⁱ	1.953(2)
N3-Zn1-N1	107.22(12)	O3 ⁱ -Zn1-N1	113.04(11)	O1-Zn1-N1	100.62(11)	O3 ⁱ -Zn1-N3	115.72(12)
O1-Zn1-N3	108.82(12)	O3 ⁱ -Zn1-O1	110.30(11)				
Symmetry code: (i) $x, y-1, z$.							
Complex 8							
Zn1-N1	2.043(5)	Zn1-O1	2.010(4)	Zn1-N3	2.043(5)	Zn1-O3 ⁱ	2.033(16)
N3-Zn1-N1	107.4(2)	O1-Zn1-O3 ⁱ	108.8(5)	O1-Zn1-N1	112.6(2)	O3 ⁱ -Zn1-N1	116.9(5)
O1-Zn1-N3	116.0(2)	O3 ⁱ -Zn1-N3	94.1(5)				
Symmetry code: (i) $x, y-1, z$.							

(9) Table S2: The Dimensions of the Windows and the Thickness of the 4^4 -sql Networks of 1, 2, 4, 7 and 8.

4^4 -sql net	1	2	4
Dimension	9.15×13.45	9.67×13.86	11.00×14.08
$L_{\text{dimb}} \times L_{\text{dicarboxylate}}/\text{\AA}$		9.67×14.06	11.00×13.30
Thickness/ \AA	3.94	9.98	6.74
4^4 -sql net	7	8	
Dimension	8.73×14.08	9.05×14.25	
$L_{\text{dimb}} \times L_{\text{dicarboxylate}}/\text{\AA}$	8.73×14.50	9.05×12.98	
Thickness/ \AA	10.73	10.02	