

**Supporting information:**

# Syntheses, Structures, and Optical Properties of Novel Zinc(II) Complexes with Multicarboxylate and N-donor Ligands

**Qian Chu, Guang-Xiang Liu, Yong-Qing Huang, Xiao-Feng Wang, Wei-Yin Sun\***

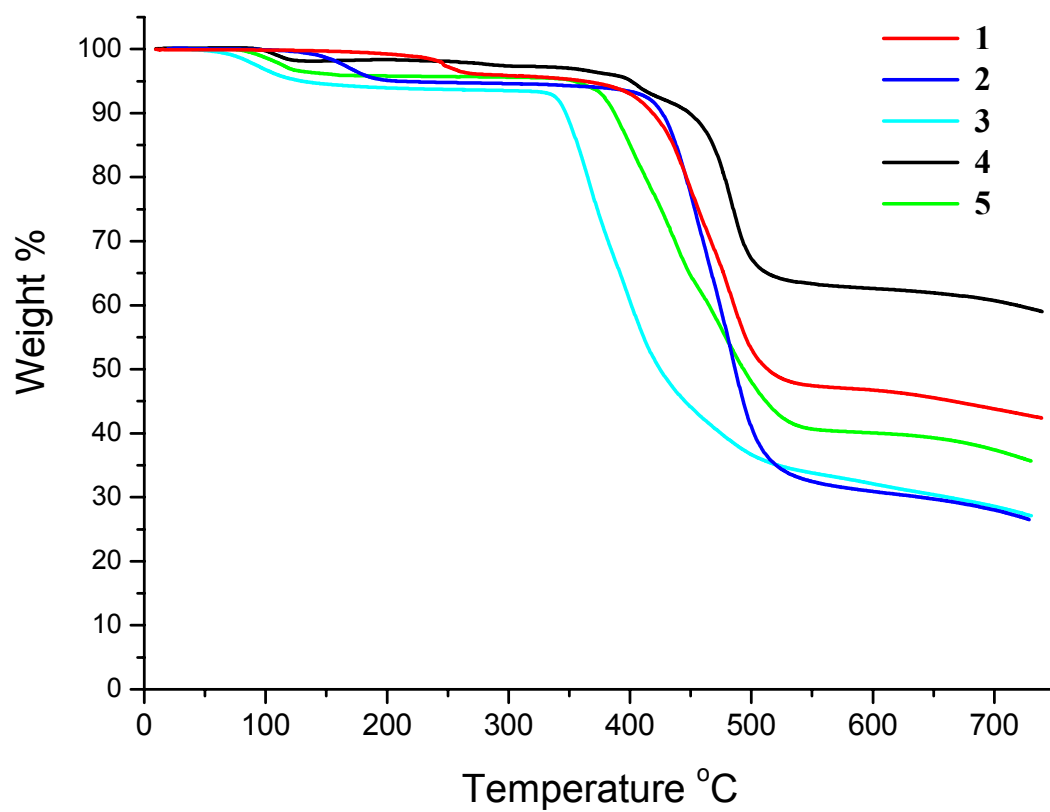
*Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China*

**Table S1** Distance [ $\text{\AA}$ ] and Angles [deg] of Hydrogen Bonding for Complexes **1** – **5**

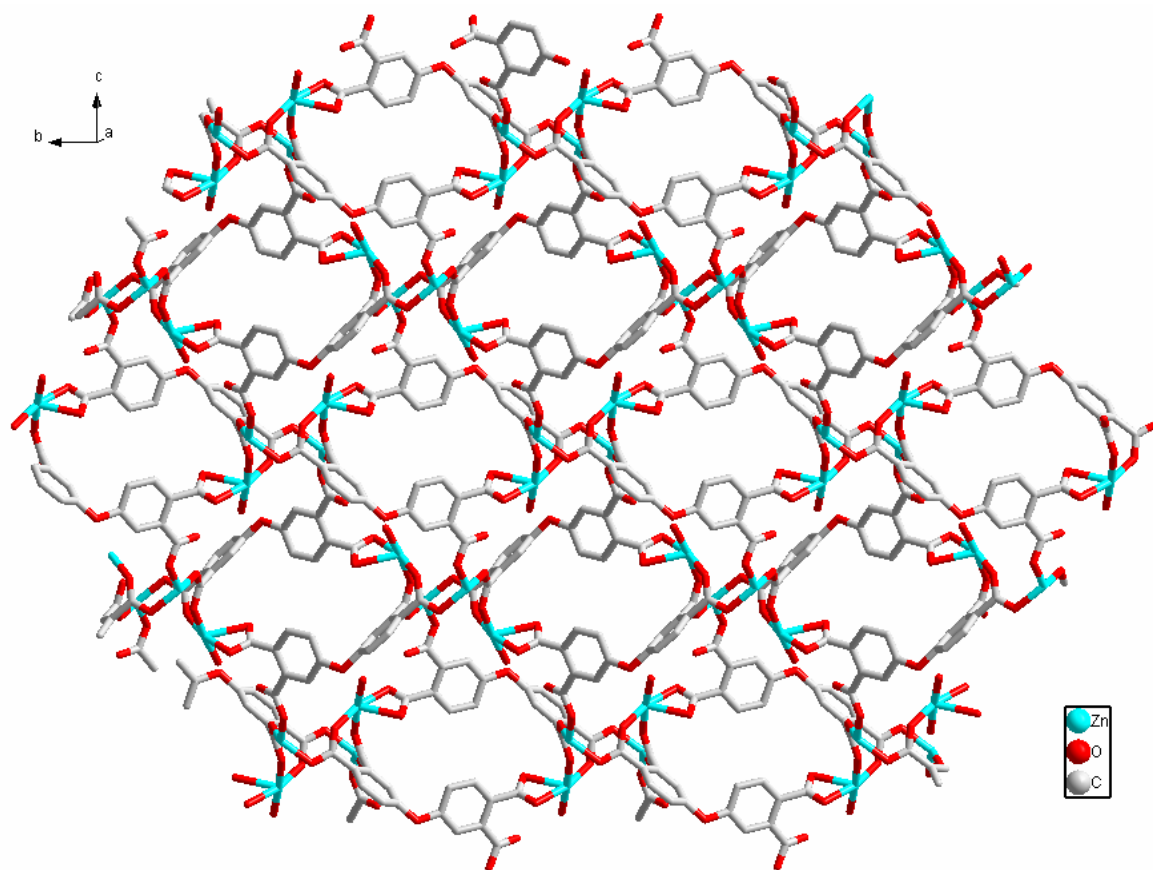
D-H...A	Distance of D...A ( $\text{\AA}$ )	Angle of D-H-A (deg.)
[Zn <sub>2</sub> (OA)(bipy)(H <sub>2</sub> O)]·0.5(bipy) ( <b>1</b> )		
O1W-H1WA-N3#1	2.807(5)	154
O1W-H1WB-O7#2	2.731(3)	157
C24-H24-O3#3	3.320(4)	142
C27-H27-O7#4	3.274(6)	145
[Zn <sub>2</sub> (OA)(dib)(H <sub>2</sub> O)]·H <sub>2</sub> O ( <b>2</b> )		
O2W-H2WA-O1#5	2.730(7)	145
O2W-H2WB-O1W#6	2.513(9)	170
C19-H19-O1#7	3.255(6)	156
C22-H22-O4#5	3.417(6)	166
C26-H26-O8#8	3.381(5)	152
C28-H28-O7#9	3.374(5)	169
[Zn <sub>2</sub> (OA)(bbi) <sub>2</sub> ]·3H <sub>2</sub> O ( <b>3</b> )		
C6-H6A-O8#10	3.409(6)	171
C17-H17A-O9#11	3.101(6)	131
C17-H17A-O1W#12	3.284(6)	142
C20-H20A-O3W#12	3.213(9)	127

C24-H24A-O7#11	3.219(6)	138
C27-H27A-O2	3.131(6)	168
C29-H29A-O1W#13	3.309(6)	160
C34-H34A-O4#13	3.193(6)	154
C36-H36A-O2W#14	3.291(9)	140
<b>[Zn<sub>2</sub>(OA)(phen)<sub>2</sub>(H<sub>2</sub>O)] (4)</b>		
C1-H1-O1#15	3.312(5)	135
O1W-H1WA-O8#16	3.319(6)	163
O1W-H1WB-O2	2.762(5)	170
C10-H10-O1W	3.060(6)	121
C15-H15-O4#17	3.080(5)	120
C18-H18-O8#18	3.322(6)	164
<b>[Zn<sub>4</sub>(OA)<sub>2</sub>(2,2'-bipy)<sub>2</sub>(H<sub>2</sub>O)]·2H<sub>2</sub>O (5)</b>		
O1W-H1WA-O16#19	2.606(6)	127
O2W-H2WA-O9#20	2.908(8)	177
O2W-H2WB-O2#21	3.014(8)	140
O3W-H3WA-O12#22	2.859(10)	177
O3W-H3WB-O17#23	3.092(10)	127
C6-H6-O14#24	3.404(7)	169
C30-H30-O5#25	3.393(8)	171
C36-H36-O3W#26	3.269(13)	174
C39-H39-O3W#26	3.483(12)	174
C43-H43-O10	3.270(9)	133
C46-H46-O2W#27	3.416(10)	175
C49-H49-O2W#27	3.249(10)	174
C50-H50-O8#28	3.208(8)	133
C52-H52-O1W	3.066(8)	120

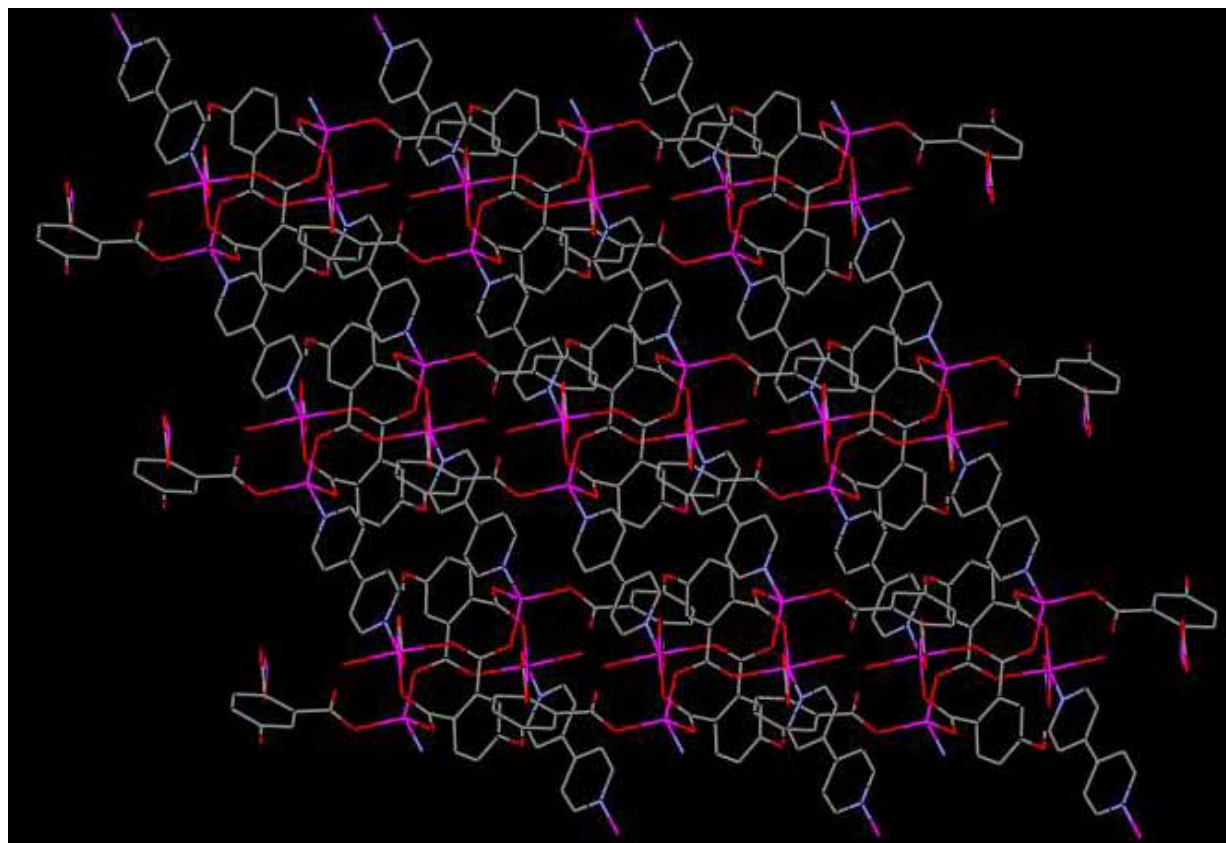
Symmetry transformations are used to generate equivalent atoms: #1 1+x,y,z; #2 2-x, 2-y,2-z; #3 3/2-x,-1/2+y,3/2-z; #4 1-x, 2-y,2-z; #5 1-x,-1/2+y,1/2-z; #6 x,y,-1+z; #7 1+x,y,z; #8 2-x,-1/2+y,1/2-z; #9 2-x,2-y,1-z; #10 3-x,1-y,-2-z; #11 x,y,1+z; #12 2-x,1-y,-1-z; #13 1/2+x,1/2-y,1/2+z; #14 -1/2+x,1/2-y,1/2+z; #15 1/2-x,-1/2+y,1/2-z; #16 -1/2+x,3/2-y,-1/2+z; #17 -1/2-x,1/2+y,1/2-z; #18 1/2-x,1/2+y,-1/2+z; #19 1/2+x,1/2-y,-1/2+z; #20 1+x,1+y,z; #21 1/2+x,1/2+y,z; #22 x,y,-1+z; #23 1/2+x,1/2+y,-1+z; #24 -1/2+x,1/2-y,-1/2+z; #25 1/2+x,1/2-y,1/2+z; #26 -1+x,y,z; #27 1/2+x,3/2-y,1/2+z; #28 3/2+x,1/2-y,1/2+z.



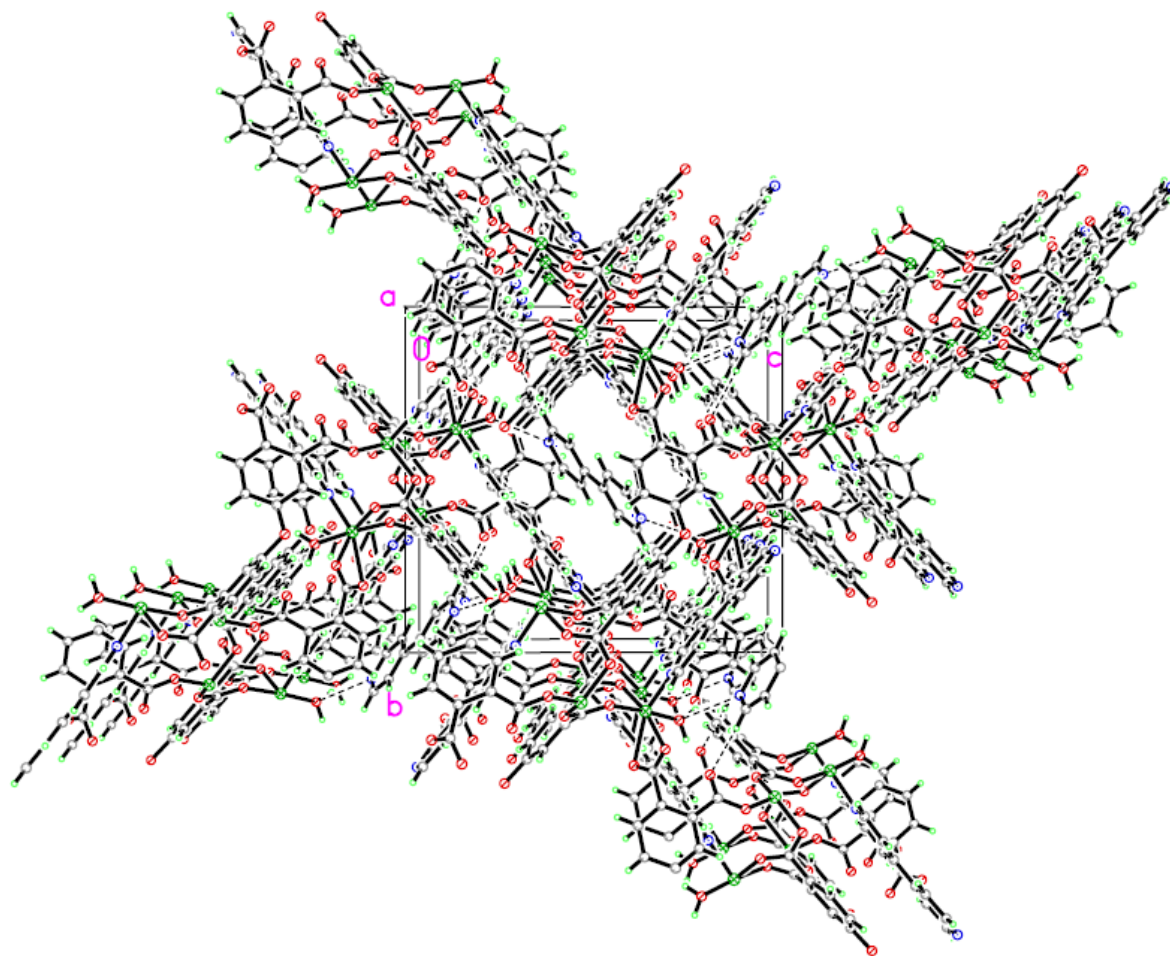
**Figure S1** Thermal gravimetric curves of complexes **1 - 5**



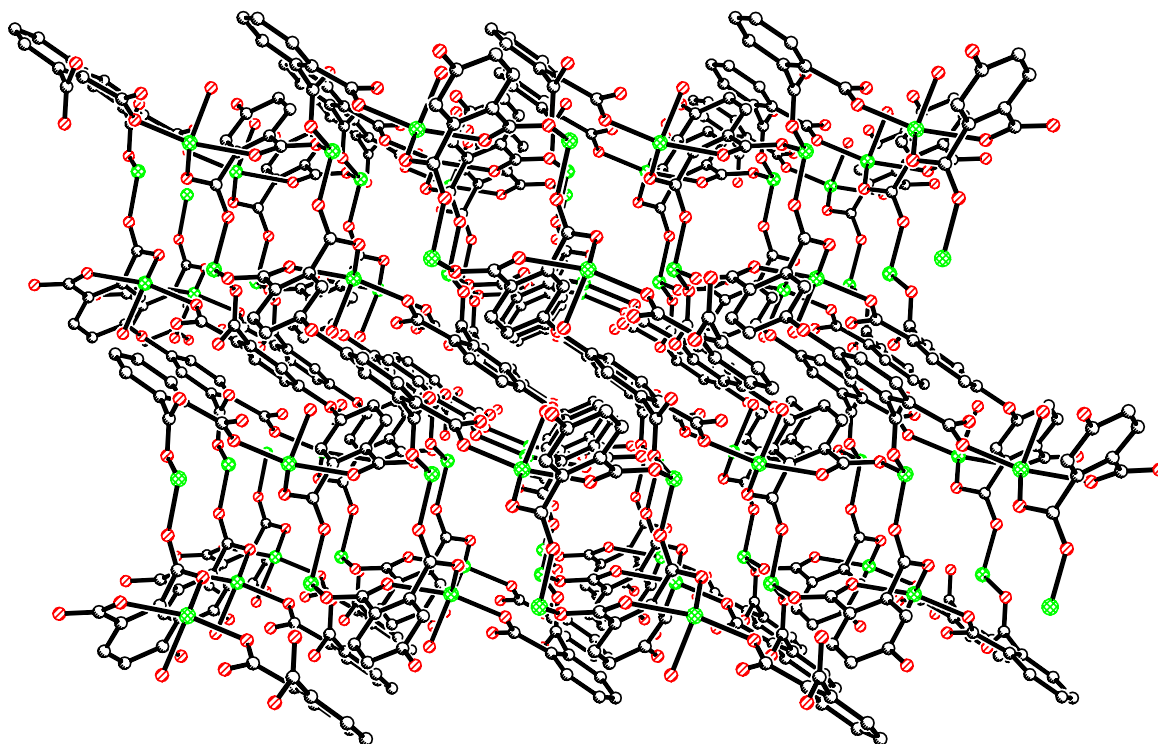
**Figure S2** Infinite 2D network structure of 1.



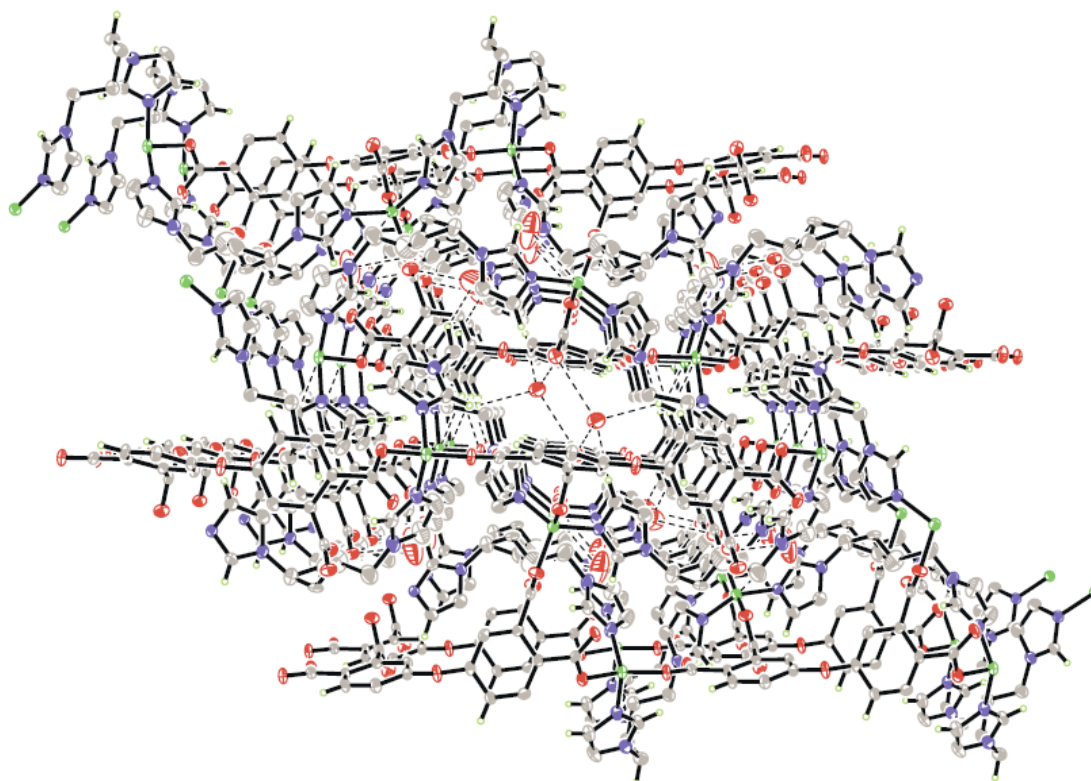
**Figure S3** 3D structure of **1** pillared by 4,4'-bipy ligands.



**Figure S4** Crystal packing diagram of **1** with hydrogen bonds indicated by dashed lines.



**Figure S5** 3D structure of **2** formed by connection of the  $Zn_4$  units through the  $OA^{4-}$  ligands.



**Figure S6** Crystal packing diagram of **3** with hydrogen bonds indicated by dashed lines.