SUPPORTING INFORMATION

Multifarious zinc coordination polymers based on biphenyl-3,3',5,5'-tetracarboxylate and different flexibility of N-donor ligands

Qipeng Li[a,b*] and Jinjie Qian[a,b]

[a]*State Key Laboratory of Structure Chemistry, State Key Laboratory of Structure Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, China*

[b]*University of Chinese Academy of Sciences, Beijing, 100049, China*

**To whom correspondence should be addressed: E-mail: qpli@fjirsm.ac.cn; Fax: (+86) 591-83709847.*

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1. Crystallographic Data Tables

Table S1. Crystallographic Data for 1-4.

Items	1	2	3	4
formula	$C_{13}H_{11}NO_6Zn$	$C_{28}H_{22}N_2O_{10}Zn$	$C_{25}H_{24}N_4O_6Zn$	$C_{36}H_{36}N_8O_9Zn_2$
weight	342.60	611.85	514.85	855.47
crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
space group	$P2_1/c$	P-1	$P2_1/c$	$P2_1/c$
a (Å)	7.277(3)	11.470 (2)	10.1877 (9)	20.848 (2)
b (Å)	9.581 (4)	11.555 (2)	12.789 (1)	9.5471 (9)
c (Å)	18.528 (8)	12.047 (2)	17.693 (2)	19.181 (2)
α (°)	90.00	67.634 (8)	90.00	90.00
β(°)	95.204 (8)	70.48 (1)	99.720 (4)	99.637 (5)
γ(°)	90.00	65.664 (9)	90.00	90.00
V(Å^3)	1288 (1)	1314.9 (4)	2271.6 (4)	3816.8 (6)
Z	4	2	4	4
T/K	298 (2)	298 (2)	298 (2)	298 (2)
D_C (g cm^{-3})	1.769	1.545	1.505	1.489
μ(mm^{-1})	1.944	1.00	1.126	1.32
F(000)	696	628	1068	1760
θ range (°)	2.21–27.49	2.02–27.5	2.03-27.43	2.35-27.40
parameters	185	370	313	488
Gof on F^2	1.045	0.982	1.039	1.900
R_1[a]	0.0544	0.0437	0.0464	0.099
wR_2[b]	0.1560	0.1112	0.1489	0.2865

$R_1 = \Sigma||F0| - |Fc||/\Sigma|F0|$. $wR2 = [\Sigma w(Fo^2 - Fc^2)^2 / \Sigma w(F0)^2]^{1/2}$.

2. Powder X-ray Diffraction

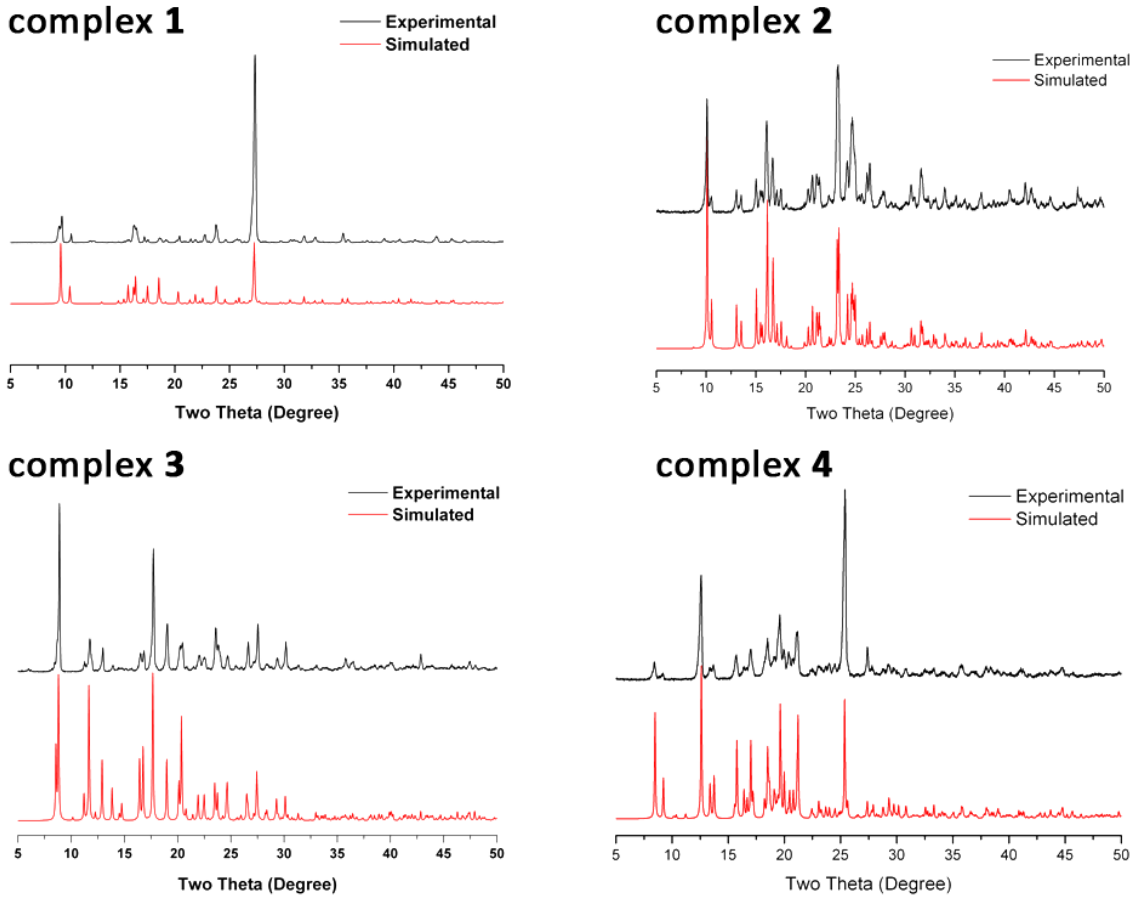

Figure S1: Experimental PXRD patterns for complex **1-4**, and their pattern simulated from single crystal X-ray structural data.

3. Thermogravimetric Analysis

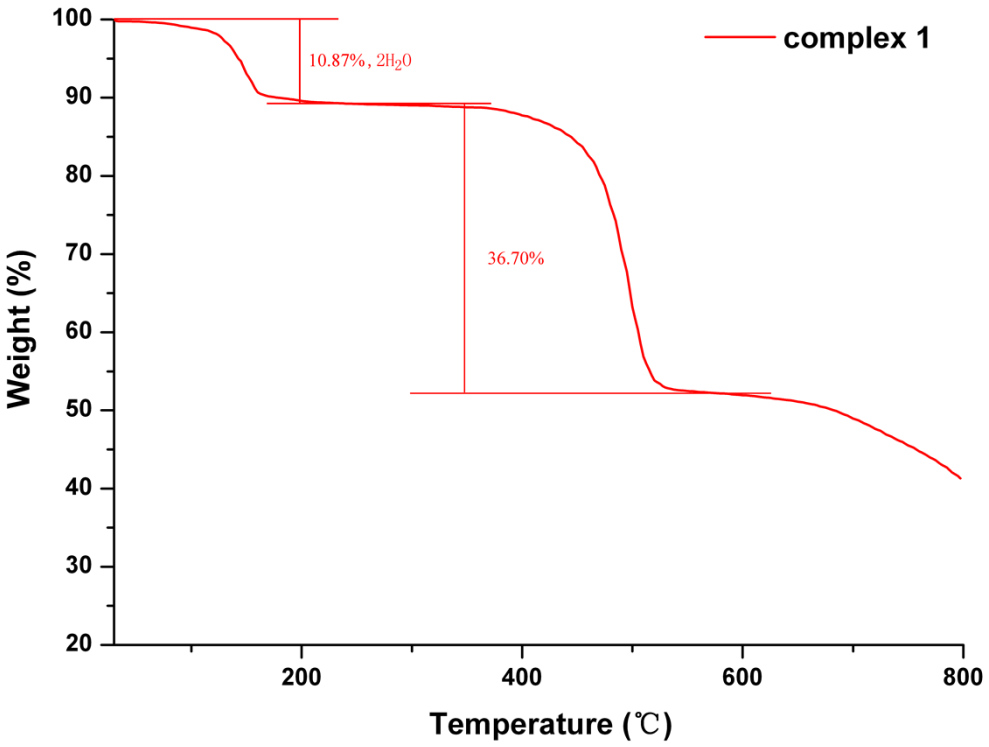

Figure S2. TGA data for the as-synthesized **1**.

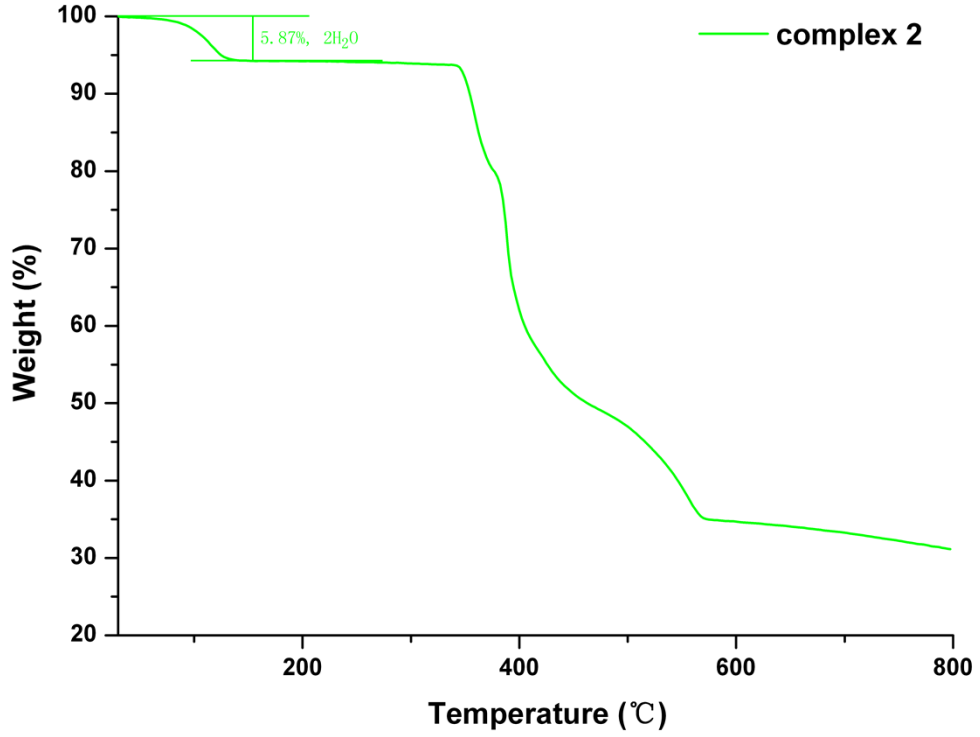

Figure S3. TGA data for the as-synthesized **2**.

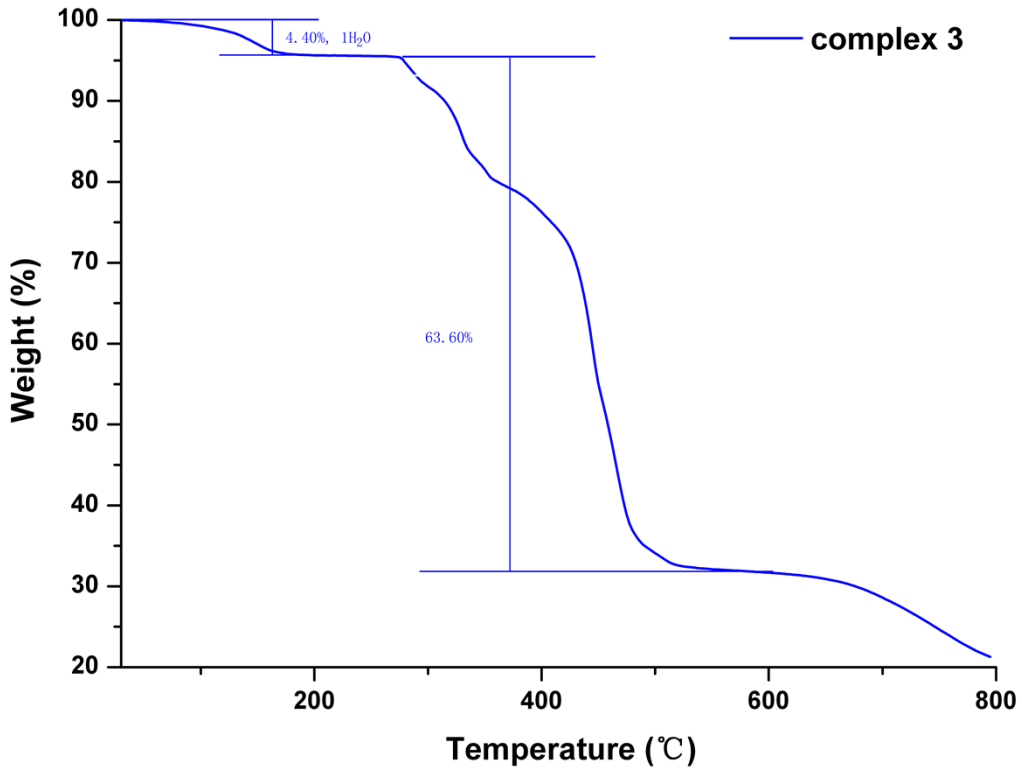

Figure S4. TGA data for the as-synthesized **3**.

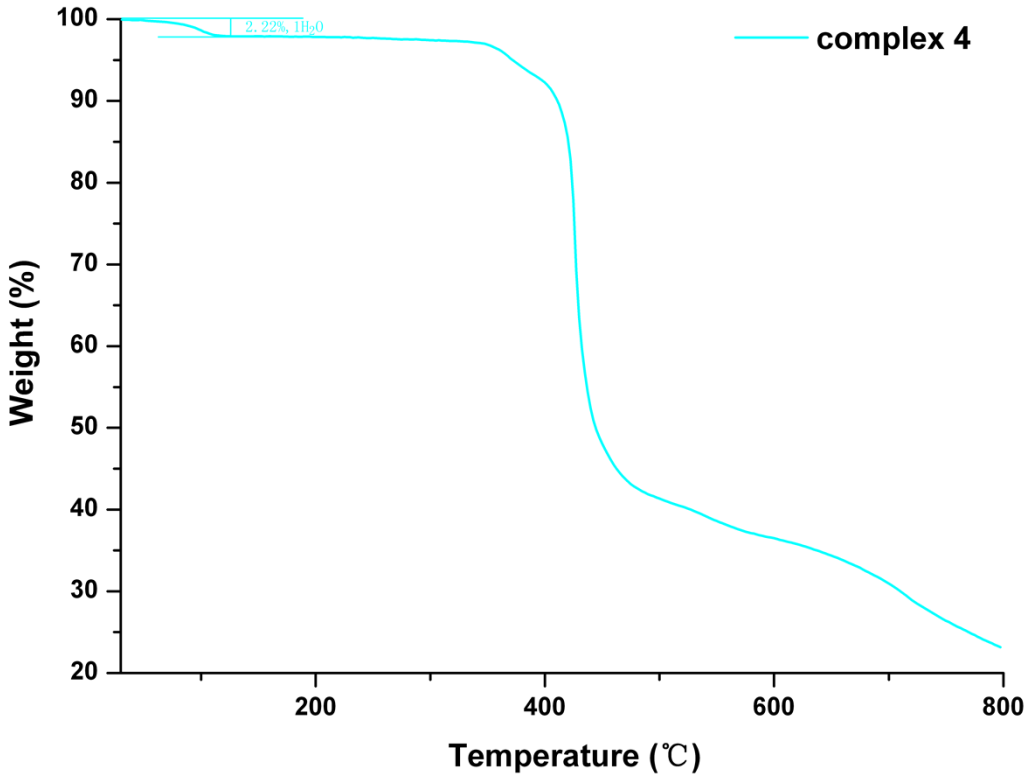

Figure S5. TGA data for the as-synthesized **4**.

4. Additional Structural Figures

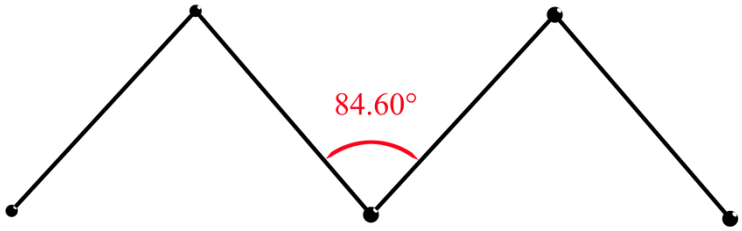

Figure S6. Dihedral angle of a 4^4-sql sheet in complex **2** viewed along *c* axis.

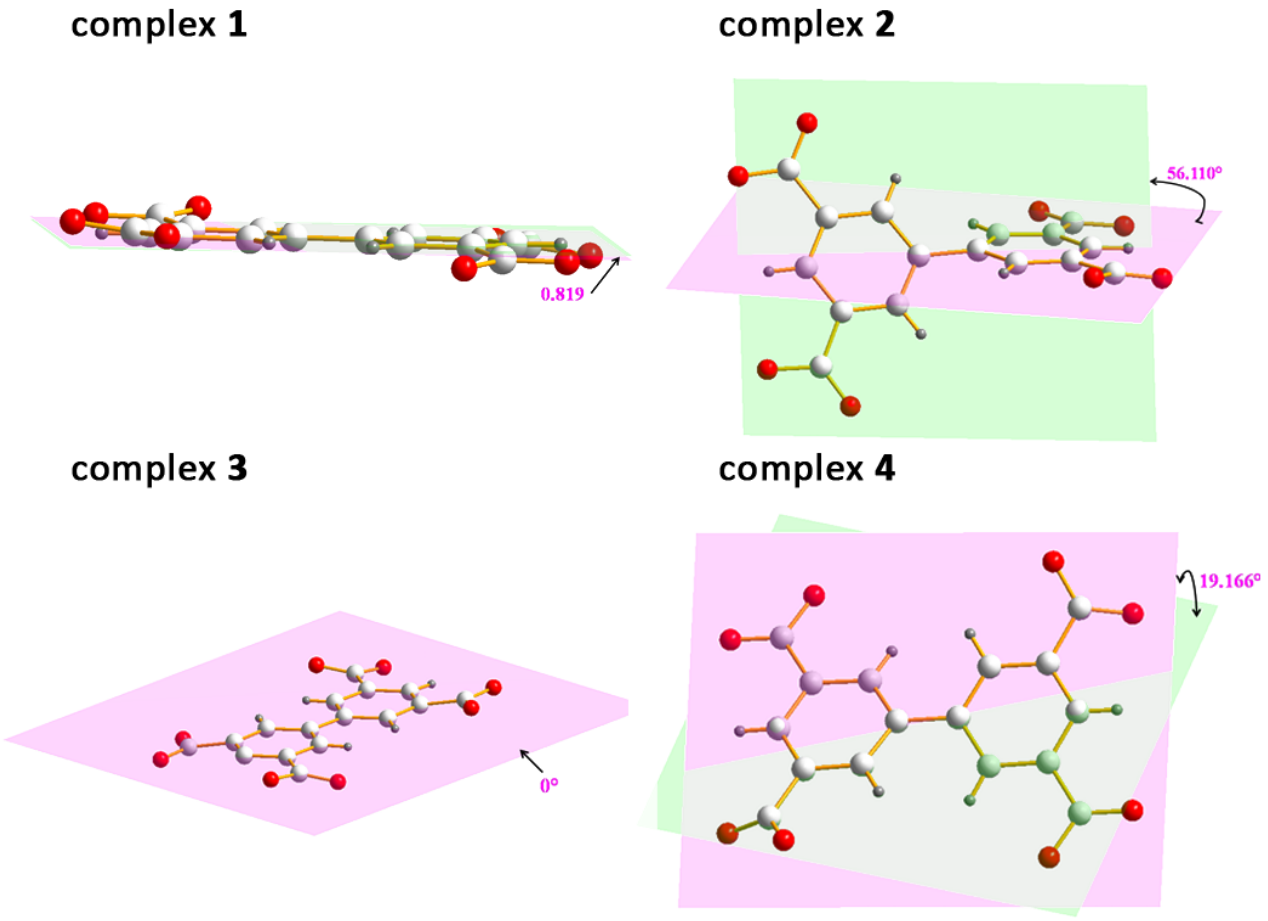

Figure S7. Dihedral angles are calculated for the $bptc^{4-}$ ligands in the complex **1**-**4**.

5. IR Spectrum

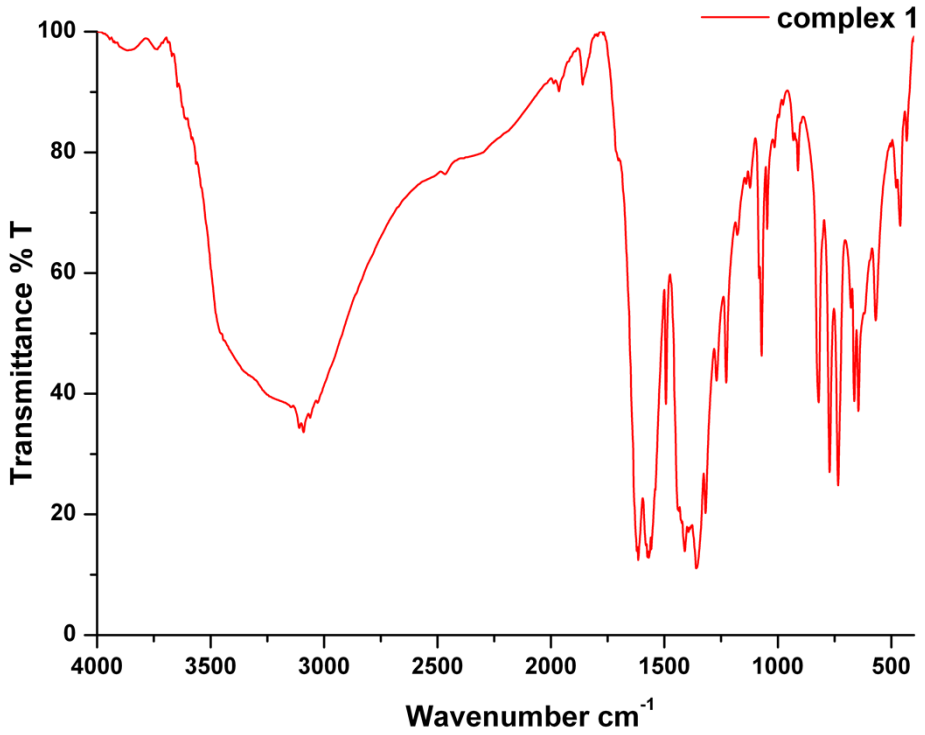

Figure S8. IR spectroscopy for complex **1**.

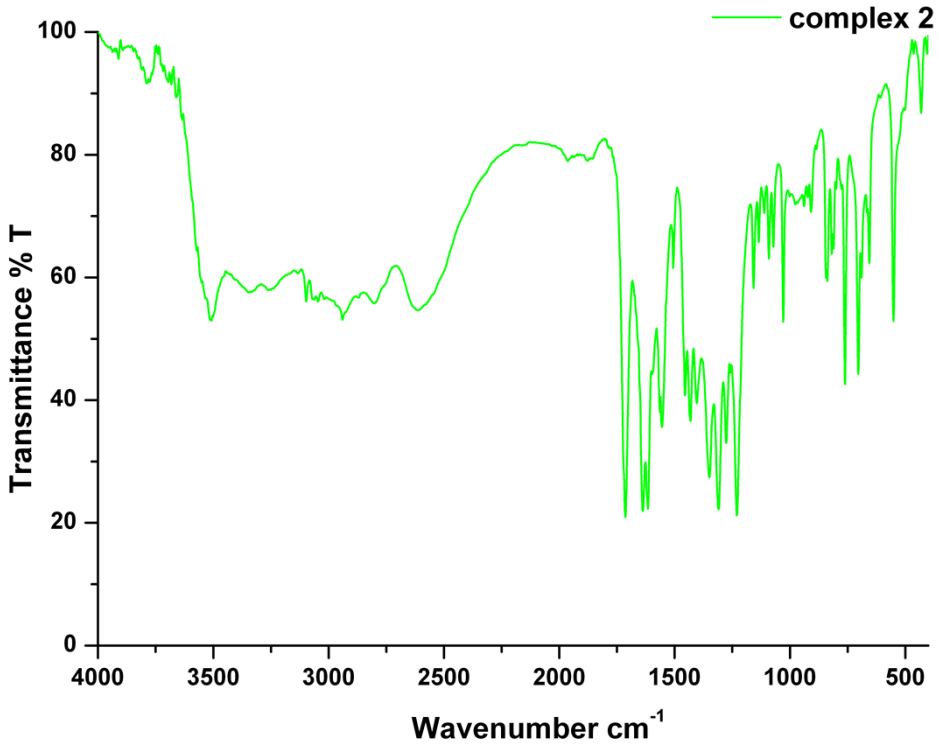

Figure S9. IR spectroscopy for complex **2**.

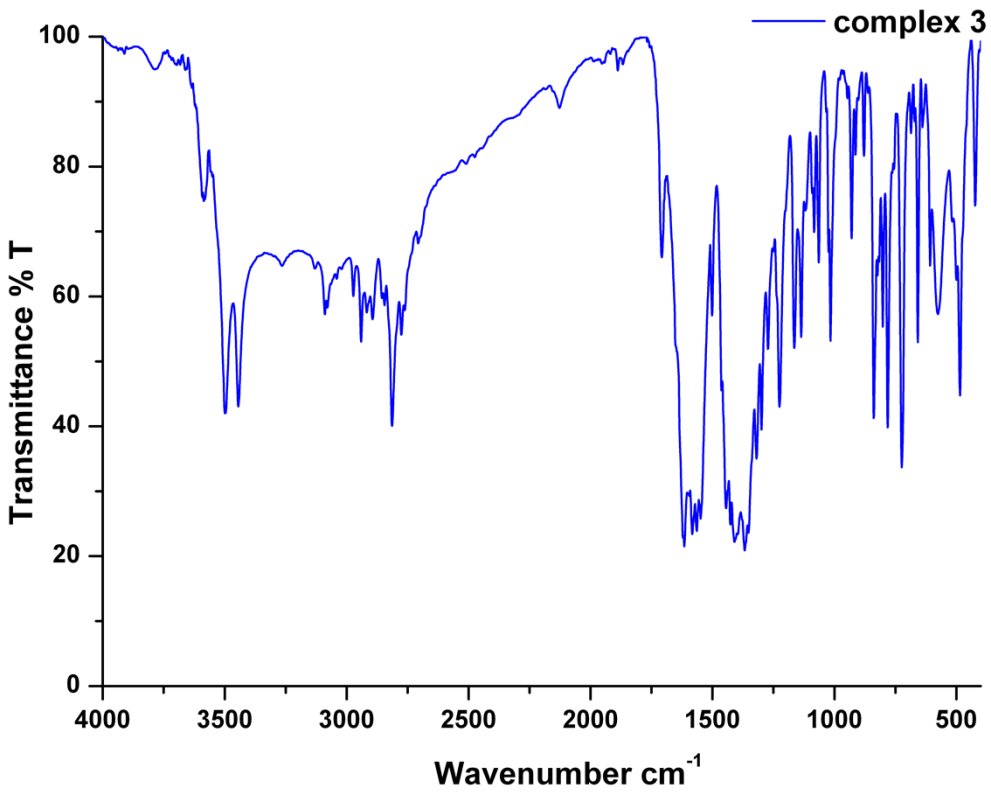

Figure S10. IR spectroscopy for complex **3**.

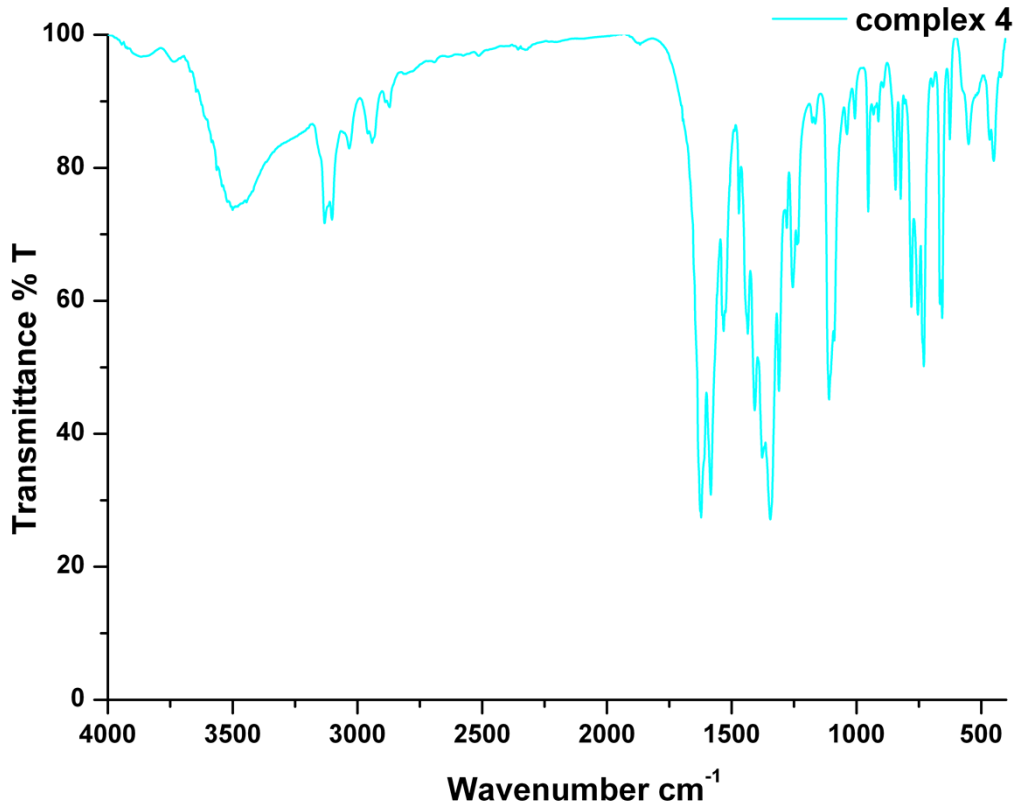

Figure S11. IR spectroscopy for complex **4**.

6. Crystallographic Data Tables

Table S2. Bond lengths [Å] and angles [°] for complex **1**.

Zn1—O1	**1.905(3)**	**Zn1—O5**	**2.040(3)**
Zn1—O3^{i}	**1.947(3)**	**Zn1—N1**	**2.043(3)**
O1—Zn1—O3^{i}	**119.26(13)**	**O3^{i}—Zn1—N1**	**101.24(12)**
O1—Zn1—O5	**107.22(14)**	**O5—Zn1—N1**	**94.77(13)**
O3^{i}—Zn1—O5	**105.06(13)**	**C7—O1—Zn1**	**121.9(3)**
O1—Zn1—N1	**125.22(13)**		

Symmetry transformations used to generate equivalent atoms:

(i) *x, -1+y, z*.

Table S3. Bond lengths [Å] and angles [°] for complex **2**.

Zn1—O1	**1.976(3)**	**Zn1—O5^{i}**	**2.146(3)**
Zn1—N1	**2.059(3)**	**Zn1—O6^{i}**	**2.248(4)**
Zn1—N2	**2.063(3)**	**O1—Zn1—N1**	**128.88(13)**
N2—Zn1—O5^{i}	**92.38(13)**	**O1—Zn1—N2**	**101.44(13)**
O1—Zn1—O6^{i}	**93.29(12)**	**N1—Zn1—N2**	**98.43(13)**
N1—Zn1—O6^{i}	**91.52(13)**	**O1—Zn1—O5^{i}**	**116.64(14)**
N2—Zn1—O6^{i}	**150.74(13)**	**N1—Zn1—O5^{i}**	**108.97(15)**
O5^{i}—Zn1—O6^{i}	**58.36(12)**		

Symmetry transformations used to generate equivalent atoms:

(i) *x, y, 1+z*.

Table S4. Bond lengths [Å] and angles [°] for complex **3**.

Zn1—O1	**2.0568(18)**	**Zn1—N4^{ii}**	**2.140(2)**
Zn1—O2^{i}	**2.0860(19)**	**Zn1—O3^{iii}**	**2.2451(19)**
Zn1—N1	**2.126(2)**	**Zn1—O4^{iii}**	**2.2471(19)**
O1—Zn1—O2^{i}	**119.41(8)**	**N1—Zn1—O3^{iii}**	**95.71(9)**
O1—Zn1—N1	**94.41(9)**	**N4^{ii}—Zn1—O3^{iii}**	**86.35(8)**
O2^{i}—Zn1—N1	**87.43(8)**	**O1—Zn1—O4^{iii}**	**148.90(8)**
O1—Zn1—N4^{ii}	**90.49(9)**	**O2^{i}—Zn1—O4^{iii}**	**91.53(7)**
O2^{i}—Zn1—N4^{ii}	**88.32(8)**	**N1—Zn1—O4^{iii}**	**89.84(9)**
N1—Zn1—N4^{ii}	**174.66(9)**	**N4^{ii}—Zn1—O4^{iii}**	**87.05(9)**
O1—Zn1—O3^{iii}	**90.48(7)**	**O3^{iii}—Zn1—O4^{iii}**	**58.42(7)**
O2^{i}—Zn1—O3^{iii}	**149.68(7)**		

Symmetry transformations used to generate equivalent atoms:

(i)-*x, 1-y, 1-z; (ii) -1+x, -1+y, z; (iii) x, 0.5-y, 0.5+z*..

Table S5. Bond lengths [Å] and angles [°] for complex **4**.

Zn1—O4^{i}	**1.944(4)**	**Zn2—O5^{ii}**	**1.957(4)**
Zn1—O1	**1.971(4)**	**Zn2—O7**	**1.975(4)**
Zn1—N1	**1.999(6)**	**Zn2—N7**	**2.011(5)**
Zn1—N3	**2.032(5)**	**Zn2—N5**	**2.018(6)**
O4^{i}—Zn1—O1	**114.67(17)**	**O5^{ii}—Zn2—O7**	**113.11(18)**
O4^{i}—Zn1—N1	**116.8(2)**	**O5^{ii}—Zn2—N7**	**116.2(2)**

O1—Zn1—N1	**102.5(2)**	**O7—Zn2—N7**	**103.3(2)**
O4^{i}—Zn1—N3	**109.95(19)**	**O5^{ii}—Zn2—N5**	**113.1(2)**
O1—Zn1—N3	**104.86(18)**	**O7—Zn2—N5**	**101.4(2)**
N1—Zn1—N3	**107.1(2)**	**N7—Zn2—N5**	**108.3(2)**

Symmetry transformations used to generate equivalent atoms:

(i) *x, 1+y, z; (ii) x, -1+y, z.*

7. Fluorescent Emission and Excitation Data

Table S6. The emission and excitation data for H_4bptc, 4,4'-bpy, bpe, bpmp, biim-4, $\{[Zn_2(bptc)(4,4'\text{-bpy})(H_2O)_2]\cdot 2H_2O\}_n$ (**1**), $\{[Zn(H_2bptc)(bpe)]\cdot 2H_2O\}_n$ (**2**), $\{[Zn_2(bptc)(bpmp)_2]\cdot 2H_2O\}_n$ (**3**) and $\{[Zn_2(bptc)(biim\text{-}4)_2]\cdot H_2O\}_n$ (**4**)

Compound	λ_{em}/nm	λ_{ex}/nm
H_4bptc	385	326
4,4'-bpy	421	348
bpe	456	360
bpmp	391	341
biim-4	423	360
1	456	366
2	378	335
3	428	340
4	438	347