Supplementary information

Tuning of net architectures of Ni(II) and Zn(II) coordination polymers using isomeric organic linkers

*Shuang-De Liu, Bing-Chiuan Kuo, Yen-Wen Liu, Jing-Yi Lee, Kwun Yip Wong and Hon Man Lee**

Department of Chemistry, National Changhua University of Education, Changhua 50058, Taiwan, R.O.C.

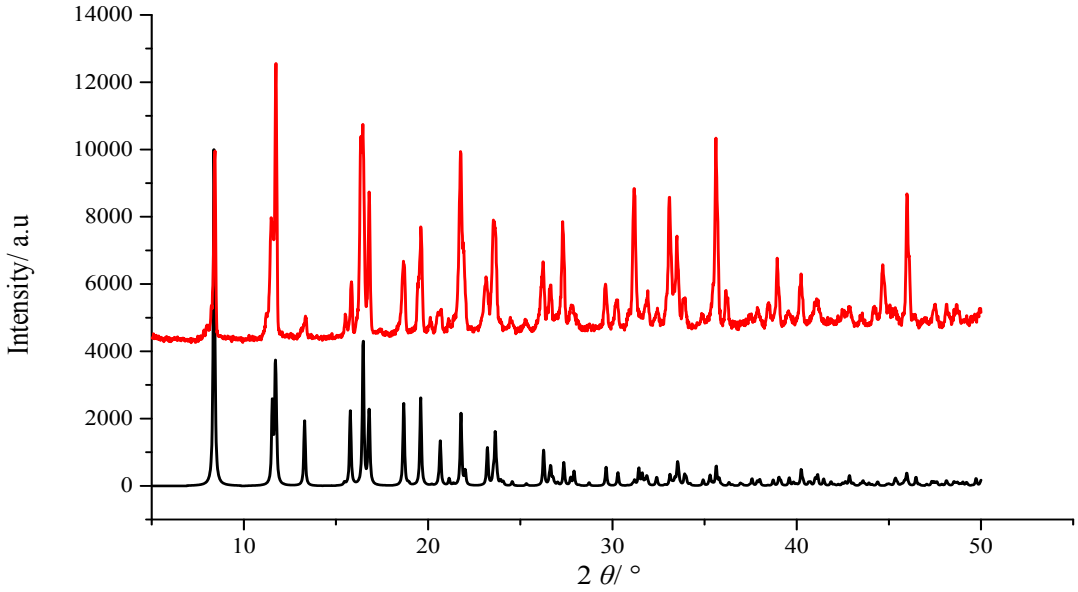

Figure S1. Comparison of the experimental PXRD patterns for as-asynthesized **1** (upper trace) and the simulated pattern from single-crystal X-ray diffraction data (lower trace).

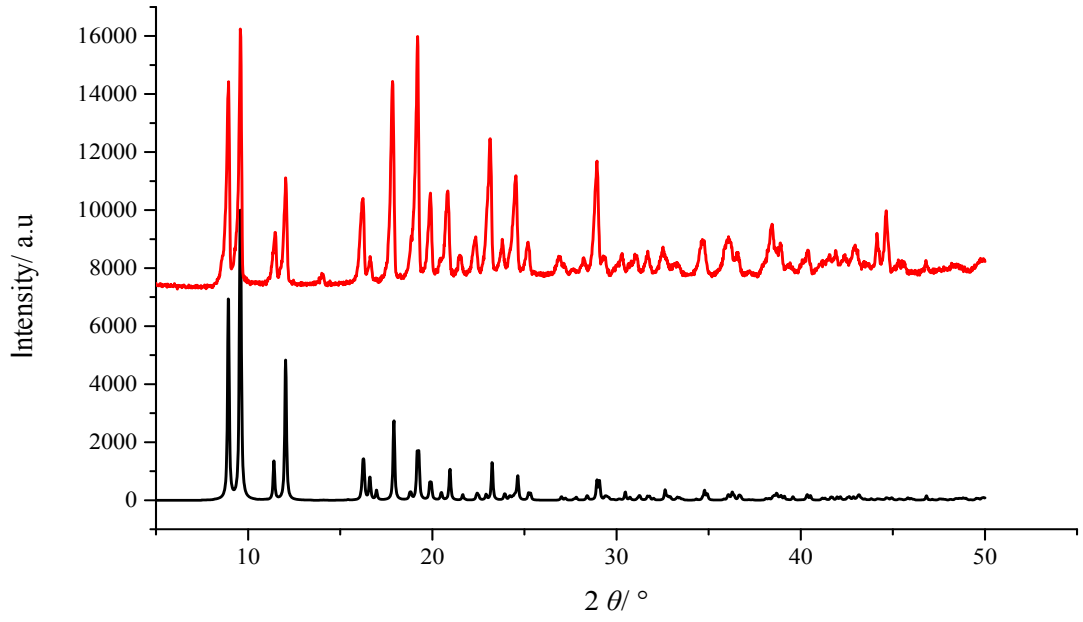

Figure S2. Comparison of the experimental PXRD patterns for as-asynthesized **2** (upper trace) and the simulated pattern from single-crystal X-ray diffraction data (lower trace).

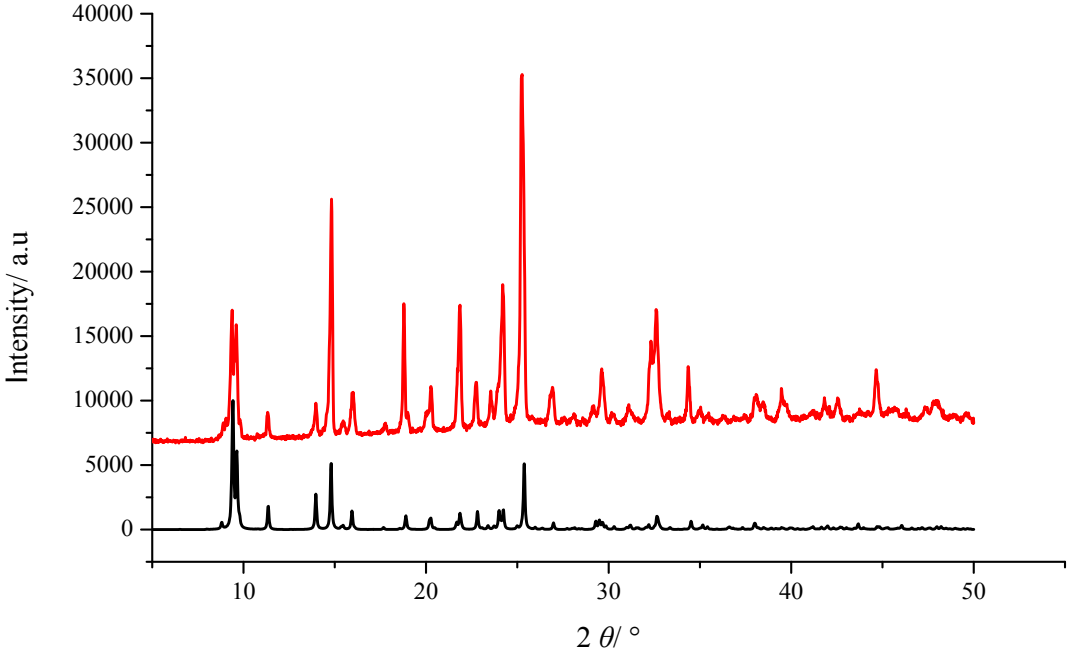

Figure S3. Comparison of the experimental PXRD patterns for as-asynthesized **3** (upper trace) and the simulated pattern from single-crystal X-ray diffraction data (lower trace).

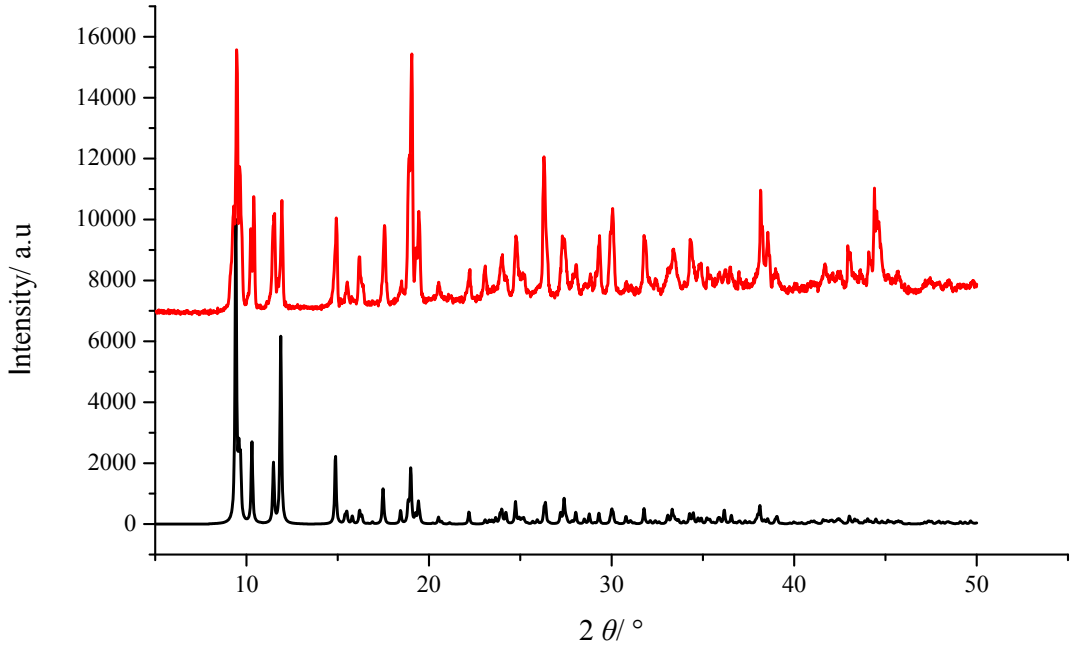

Figure S4. Comparison of the experimental PXRD patterns for as-asynthesized **4** (upper trace) and the simulated pattern from single-crystal X-ray diffraction data (lower trace).

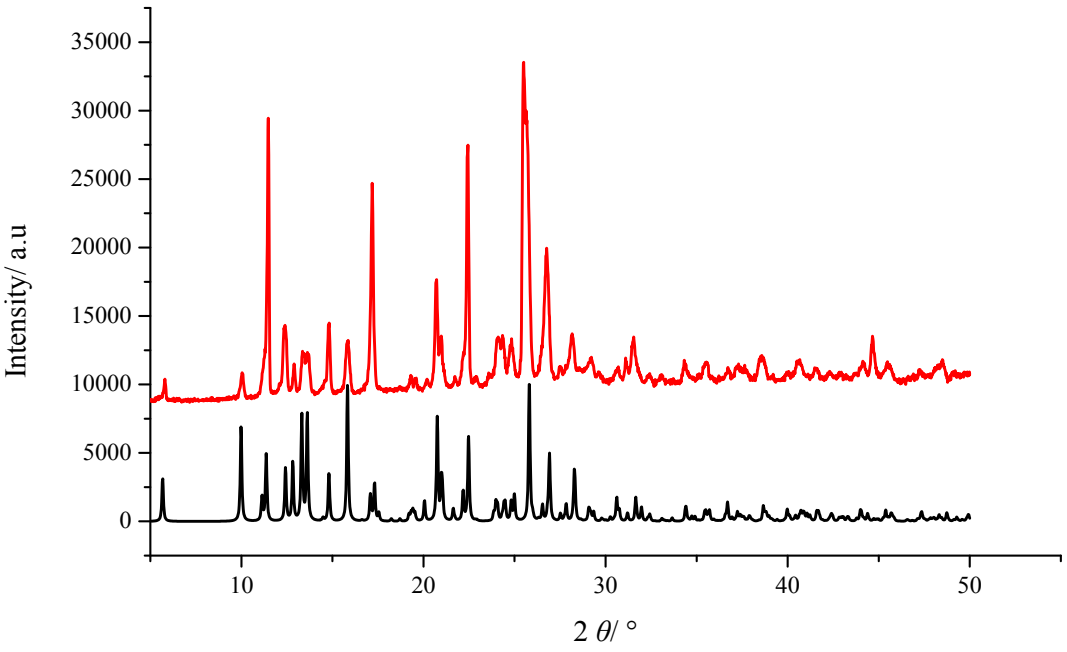

Figure S5. Comparison of the experimental PXRD patterns for as-asynthesized **5** (upper trace) and the simulated pattern from single-crystal X-ray diffraction data (lower trace).

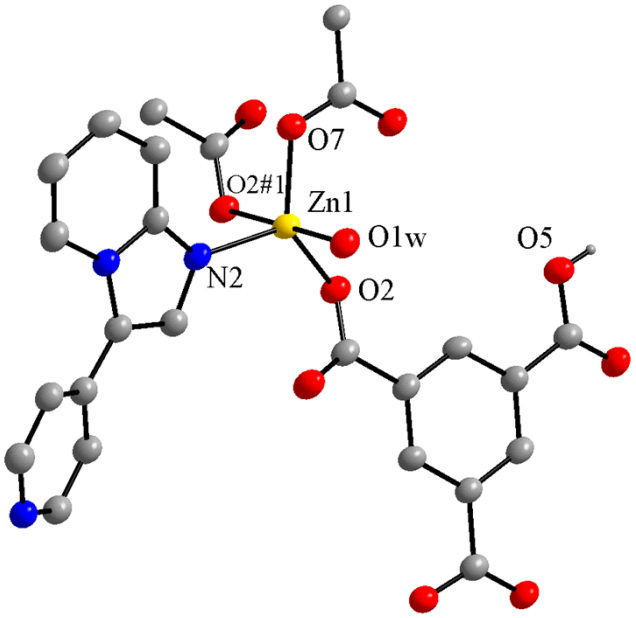

Figure S6. Coordination environment of the Zn atoms in **6** with thermal ellipsoids shown at 50 % probability.

The hydrogen atoms, except that on O5, are omitted for clarity. Symmetry code: #1 = –x + 1,-y, –z + 2

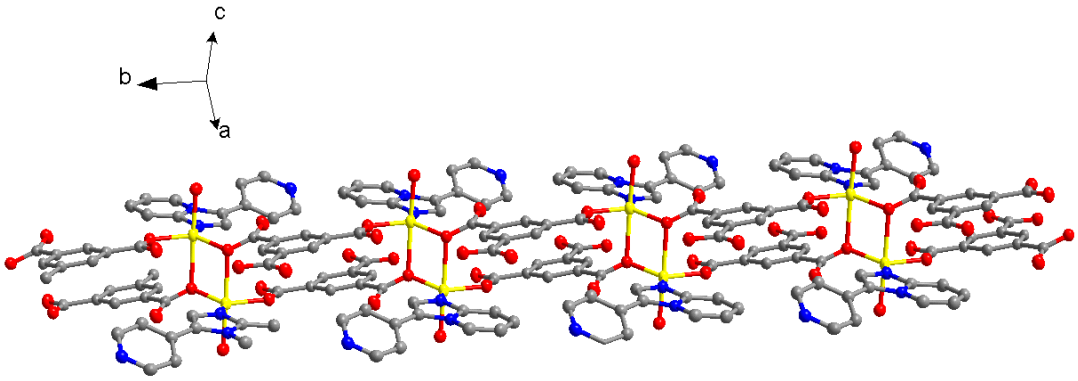

Figure S7. Schematic view of the 1D chain in **6**.

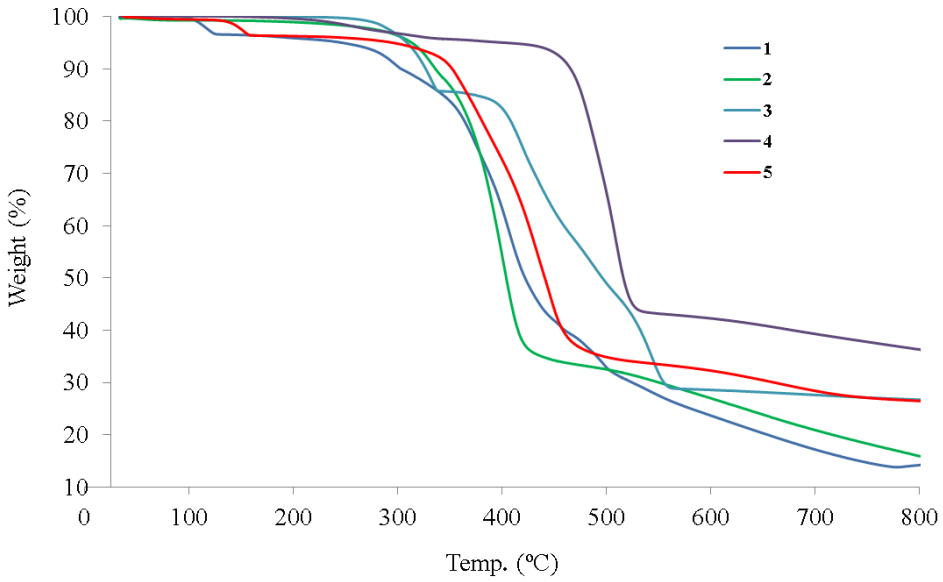

Figure S8. TG curves of **1**–**5**

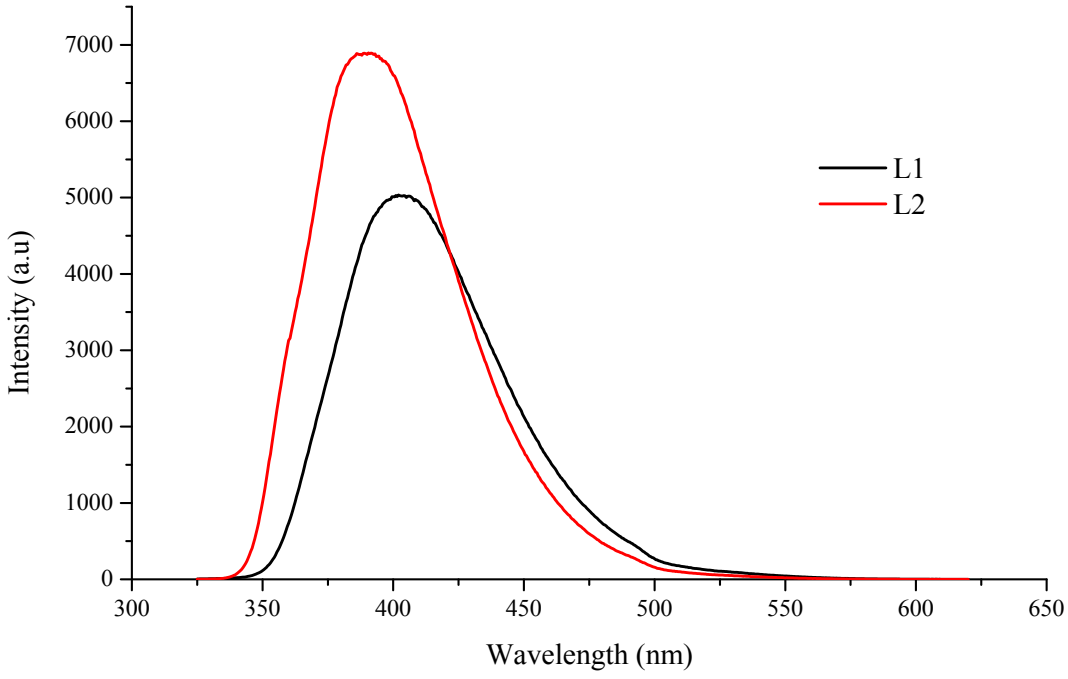

Figure S9. Fluorescence spectra of L1 and L2 (6 x 10^{-5} M in DCM; L1: λ_{ex} = 308 nm, λ_{max} = 401 nm. L2: λ_{ex} = 318 nm, λ_{max} = 391 nm)

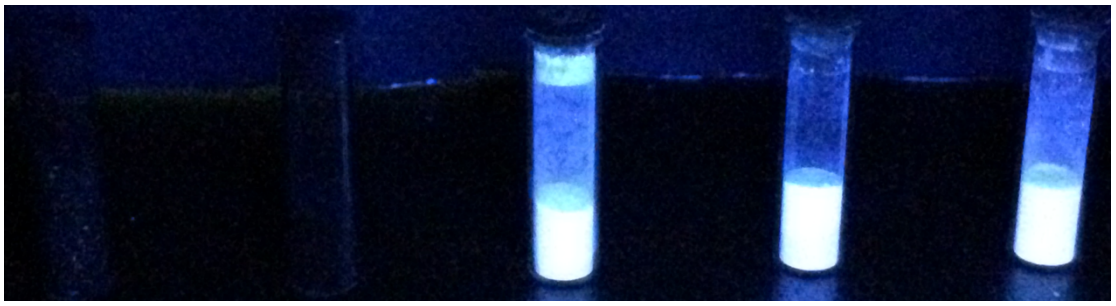

Figure S10. Irradiation of **1**–**5** (from left to right) under UV light (325 nm)

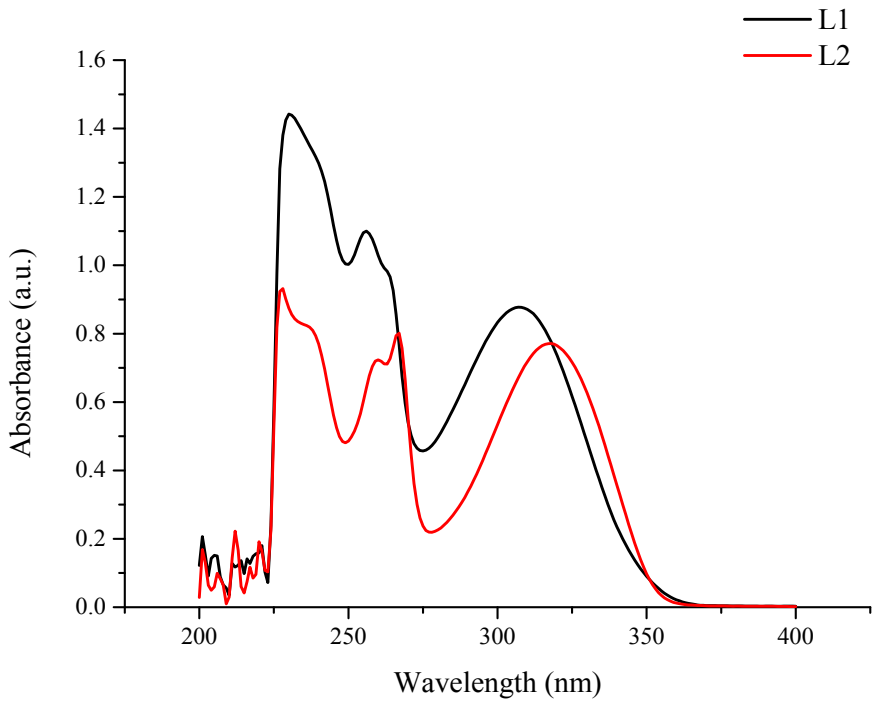

Figure S11. Absorption spectrum of L1 and L2 (6 x 10^{-5} M in DCM)

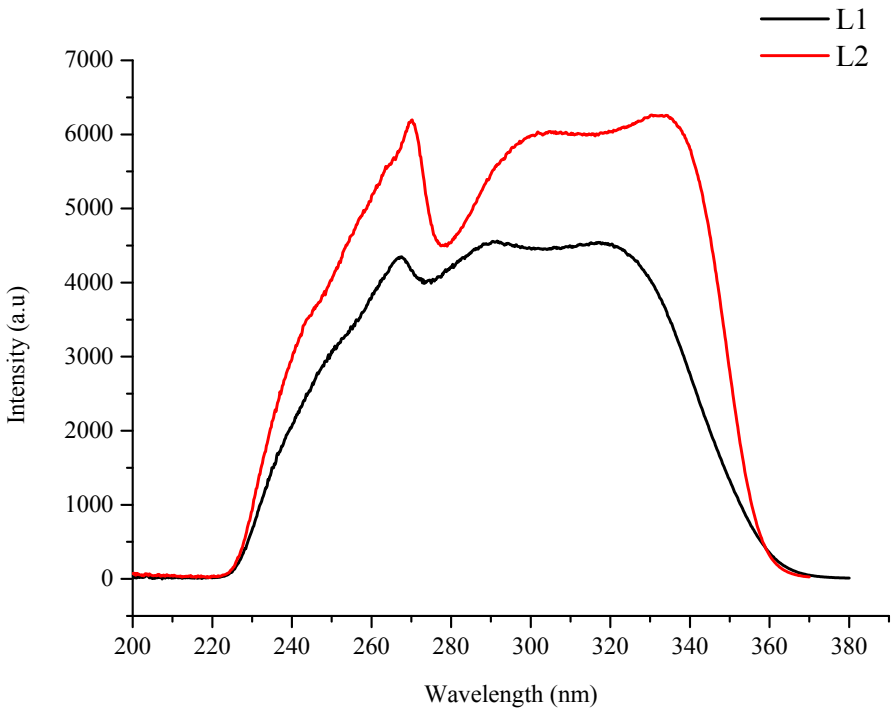

Figure S12. Excitation spectrum of L1 and L2 (6 x 10^{-5} M in DCM)

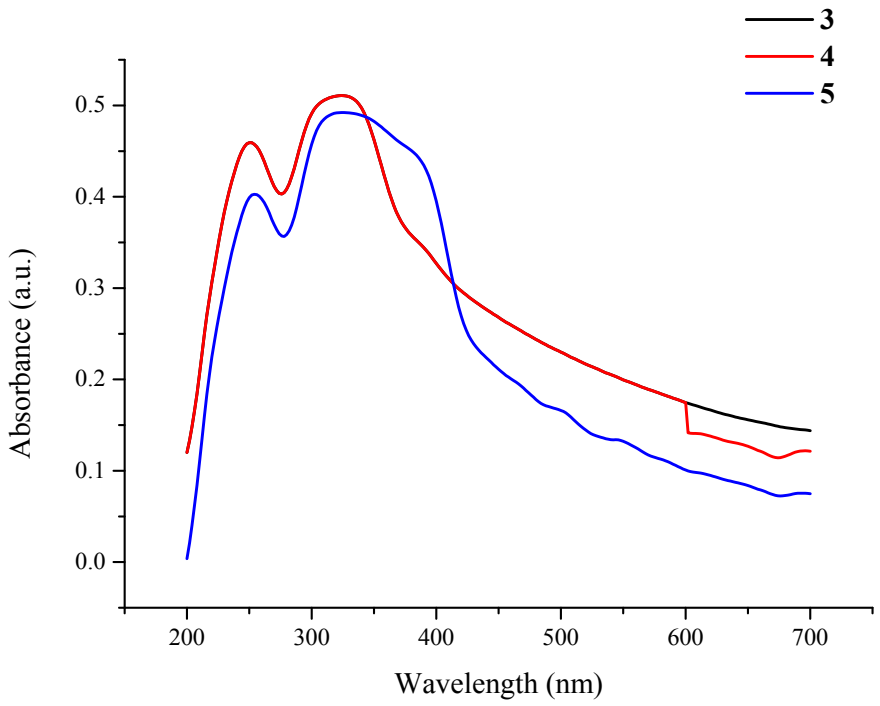

Figure S13. Solid-state Absorption spectrum of Zn **3**–**5**

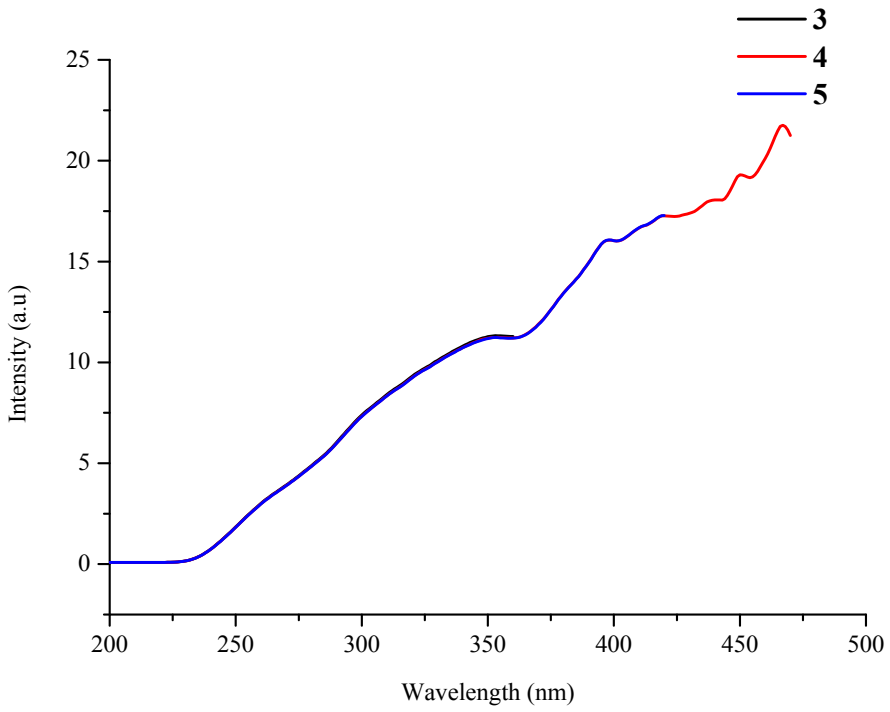

Figure S14. Solid-state excitation spectrum of Zn **3**–**5**

Table S1. Crystallographic data

	1	2	3	4	5	6
empirical formula	$C_{20}H_{17}N_3NiO_6$	$C_{40}H_{28}N_6Ni_2O_9$	$C_{24}H_{16}N_3O_7Zn_2$	$C_{21}H_{13}N_3O_7Zn_2 \cdot 0.5H_2O$	$C_{22}H_{15}N_3O_9Zn_2$	$C_{21}H_{15}N_3O_7Zn \cdot H_2O$
formula weight	454.08	854.10	589.14	558.09	596.11	504.75
crystal system	orthorhombic	orthorhombic	triclinic	monoclinic	monoclinic	triclinic
space group	F*dd*2	F*dd*2	$P\bar{1}$	$C2/c$	$P2_1/c$	$P\bar{1}$
a, Å	17.297(2)	11.723(2)	10.4229(5)	20.233(4)	7.5106(2)	7.2889(4)
b, Å	30.446(4)	22.957(6)	10.5611(6)	10.901(2)	31.1959(7)	9.7098(5)
c, Å	14.7303(19)	31.011(11)	12.2119(6)	20.355(4)	10.5537(3)	13.6547(7)
α, deg	90	90	114.782(3)	90	90	95.558(1)
β, deg	90	90	109.889(4)	115.467(10)	118.658	90.979(1)
γ, deg	90	90	96.087(3)	90	90	93.688(1)
V, Å^3	7757.3(17)	8346(4)	1097.91(10)	4053.3(13)	2169.82(10)	959.59(9)
T, K	150(2)	150(2)	150(2)	150(2)	150(2)	150(2)
Z	16	8	2	8	4	2
no. of unique data	5007	4545	4795	4202	4716	3957
no. of params refined	281	263	326	315	325	298
R_1[a] [$I > 2\sigma I$]	0.0684	0.0432	0.0537	0.0842	0.0774	0.0788
wR_2[b] (all data)	0.1824	0.1076	0.1533	0.2432	0.2229	0.2498

[a] $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$. [b] $wR_2 = [\Sigma(|F_o|^2 - |F_c|^2)^2/\Sigma(F_o^2)]^{1/2}$

Table S2. Classical hydrogen bonds linking the 2D layers into a 3D net in **1** [Å and °]

D–H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
O3–H3B···O5#1	0.84	1.96	2.789(6)	167
O4–H4A···O2#2	0.82	2.00	2.805(4)	167

Symmetry transformations used to generate equivalent atoms: #1: 1/4 + x, 1/4 – y, –3/4 + z; #2: 1/4 + x, 1/4 – y, 1/4 + z

Table S3. Important Bond Distances (Å) and Angles (°) of **6**.

Zn1–N2	2.019(5)
Zn1–O1w	2.125(4)
Zn1–O2	1.950(4)
Zn1–O7	1.950(4)
Zn1–O2#1	2.433(4)
O1w–Zn1–O2	97.11(16)
O1w–Zn1–O7	95.57(16)
O2–Zn1–O7	128.96(17)
O1w–Zn1–N2	93.94(17)
O2–Zn1–N2	119.22(18)
O7–Zn1–N2	108.89(18)
O7–Zn1–O2#1	85.57(15)
O2–Zn1–O2#1	79.71(15)
N2–Zn1–O2#1	88.72(16)
O1w–Zn1–O2#1	176.59(14)

Symmetry code: #1 = –x + 1,–y, –z + 2