Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

A smart sensing Zn (Ⅱ) coordination polymer based on a new viologen ligand exhibiting photochromic and thermochromic and multiple solid detection properties

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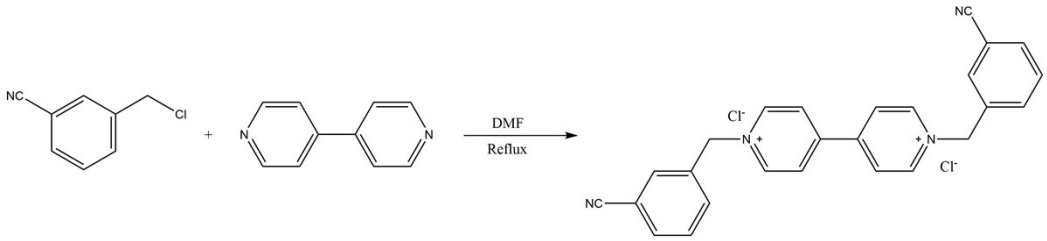

Scheme 1 Synthesis of viologen ligand 1,1'-bis(3-cyanobenzyl)-[4,4'-bipyridine] dichloride.

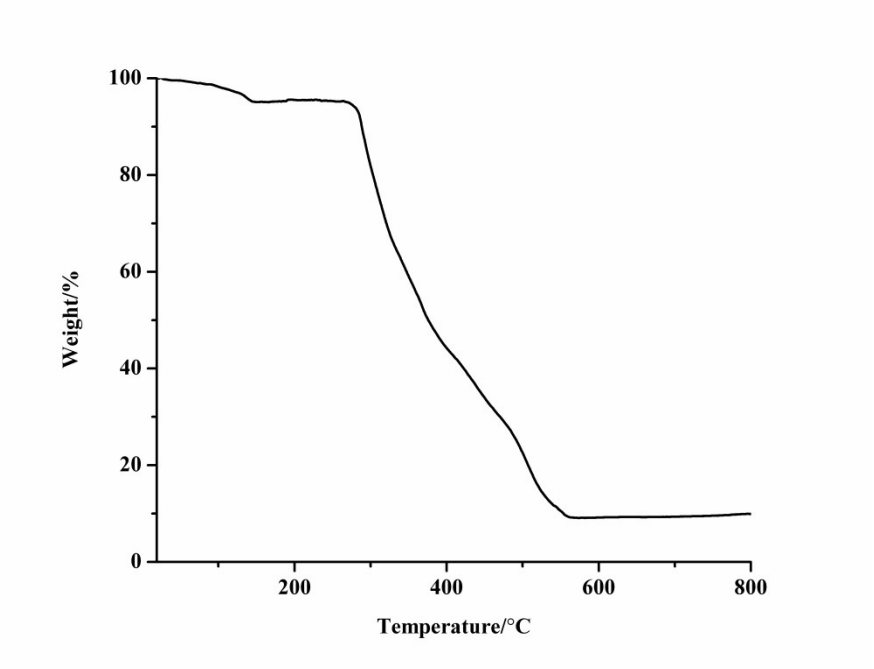

Figure S1 The TGA date of the compound 1.

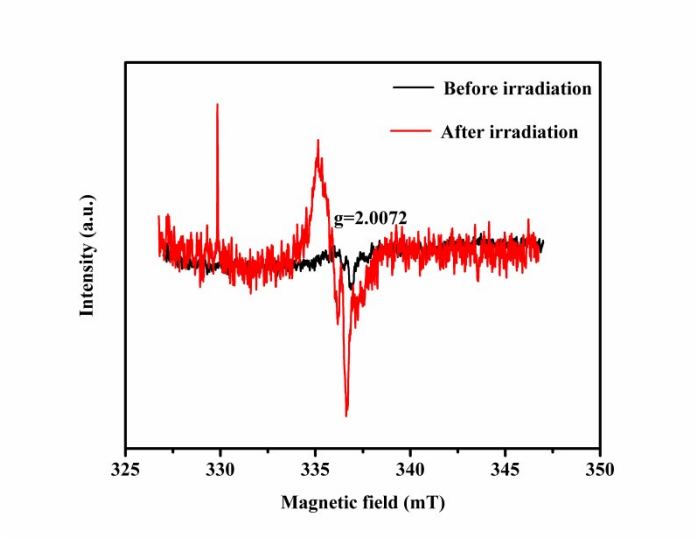

Figure S2 EPR spectral changes of the compound 1 before and after irradiation with Xe lamp.

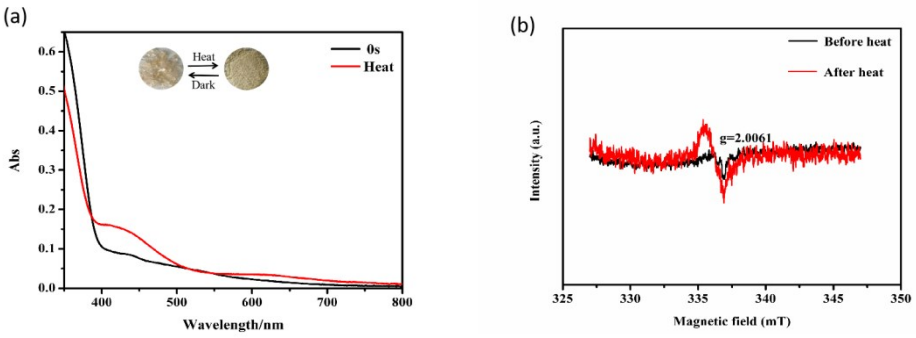

Figure S3 (a) Uv-vis diffuse-reflectance spectral changes of compound 1 by heat at about 98 ℃for 6min; (b) EPR spectral changes of compound 1 by heat at about 98 ℃ for 6min.

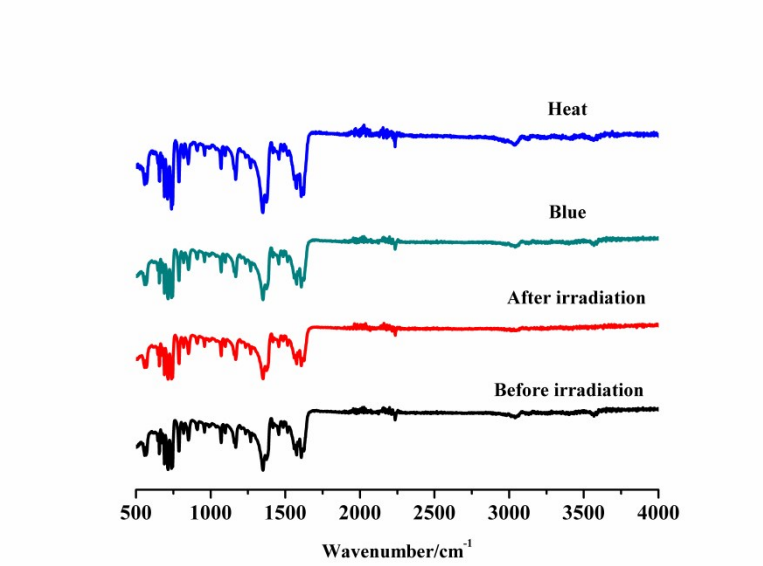

Figure S4 FTIR spectra of compound 1before irradiation (black), after irradiation (red), blue ray (green) and heat (blue).

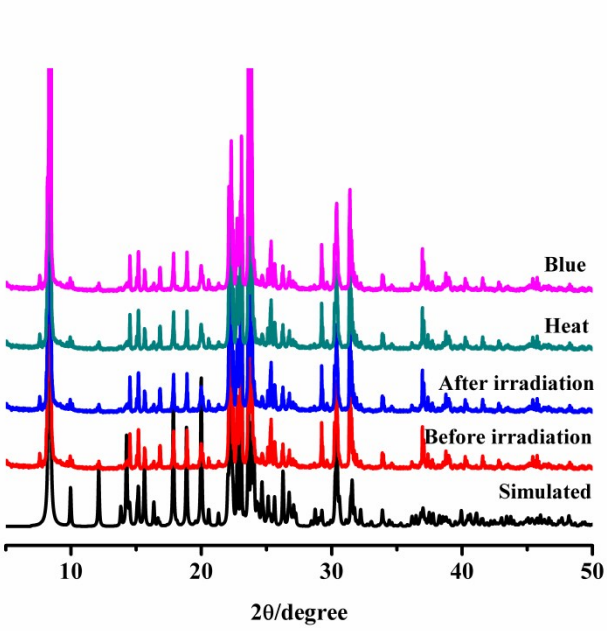

Figure S5 Powder XRD patterns of compound 1 before irradiation (red), after irradiation (blue), heat (green), blue ray(pink). The black line is simulated curve.

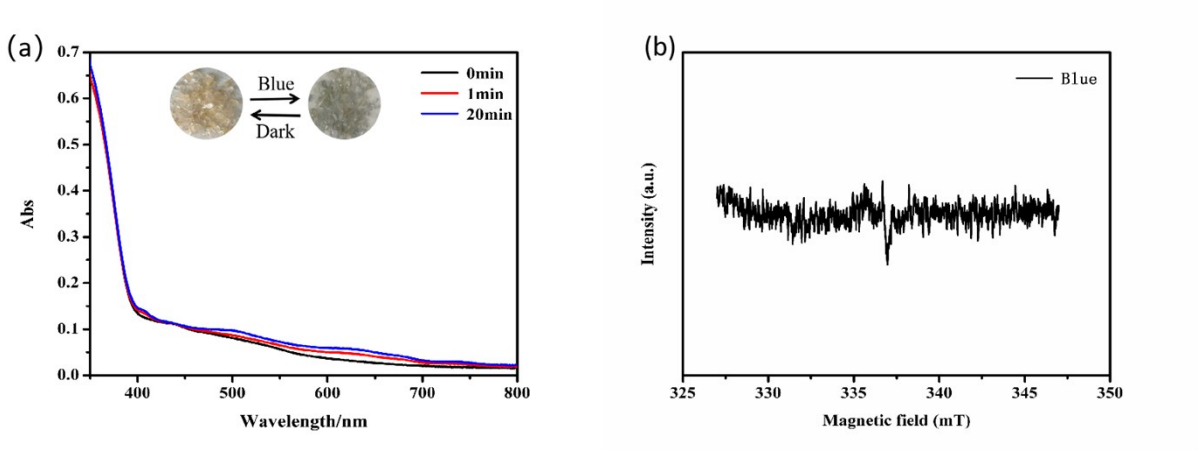

Figure S6 (a) UV-vis spectra and photographs of compound 1 before and after irradiation with blue ray; (b) EPR spectral changes of the compound 1 before and after irradiation with blue ray.

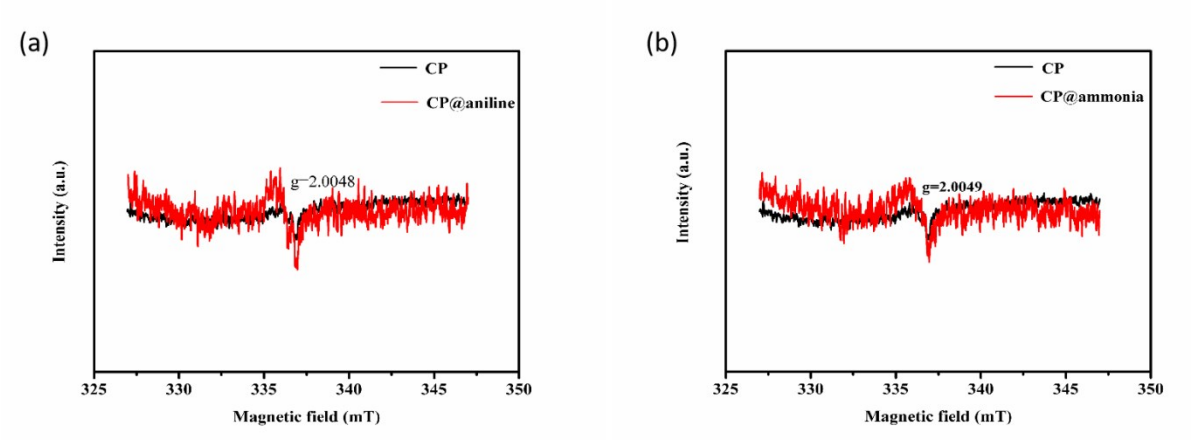

Figure S7 (a) EPR spectral changes of CP@aniline; (b) EPR spectral changes of CP@ ammonia.

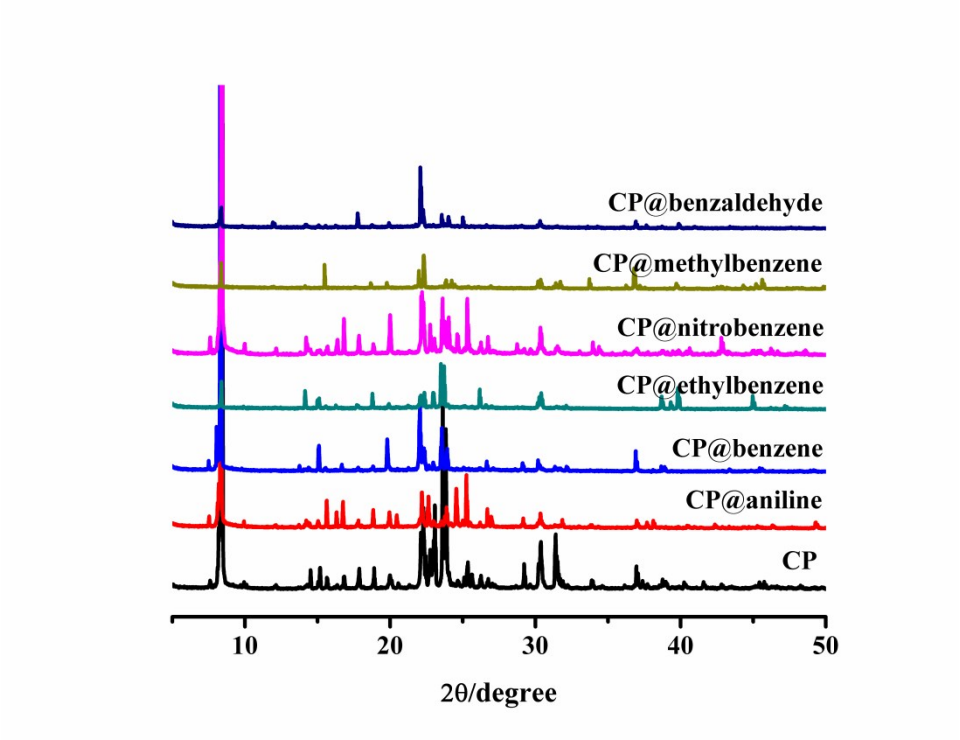

Figure S8 PXRD patterns of CP@ different benzenes. The black line is simulated curve.

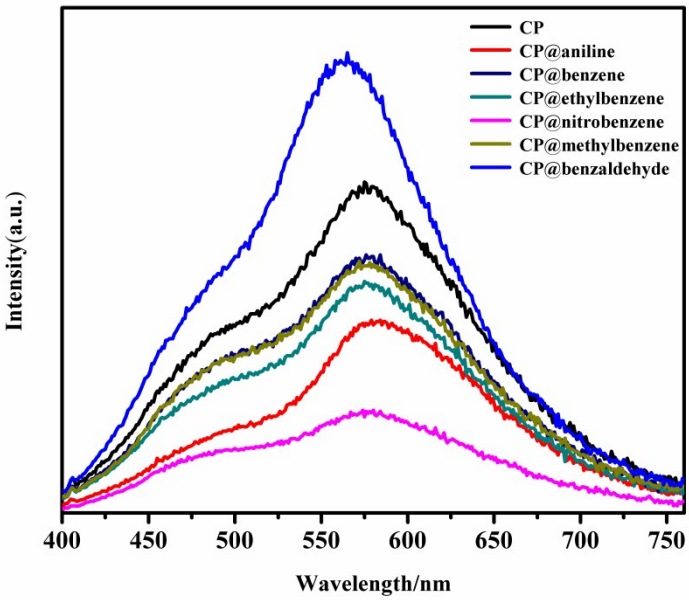

Figure S9 The luminescence emission spectral changes (λex = 380 nm), when detected different benzenes in solid state.

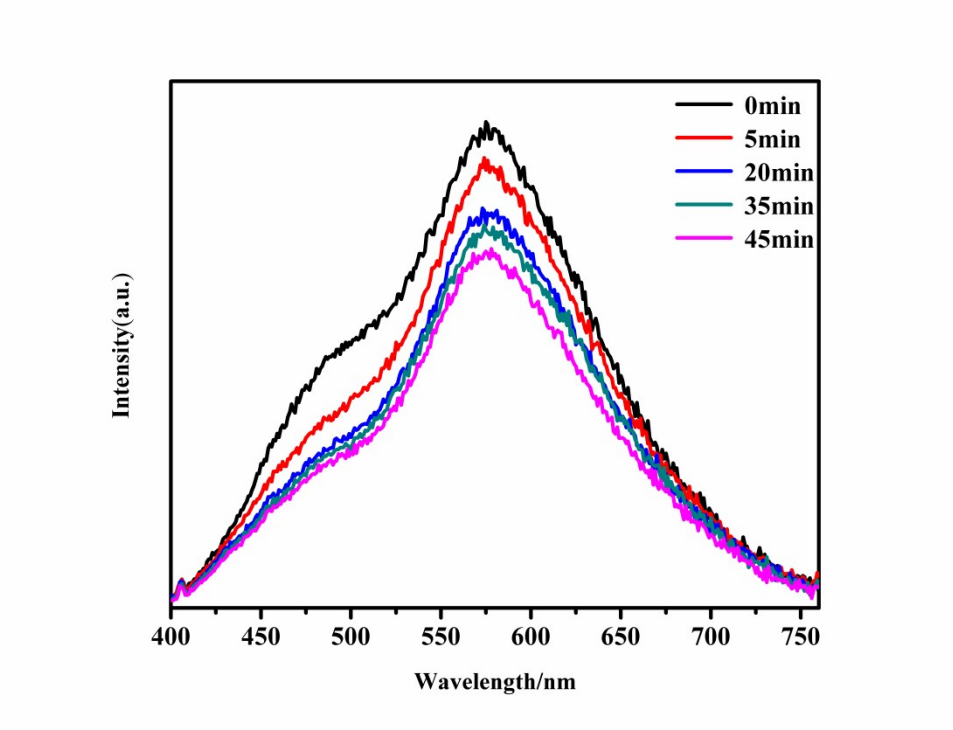

Figure S10 The blue ray luminescence emission spectrum changes of compound 1.

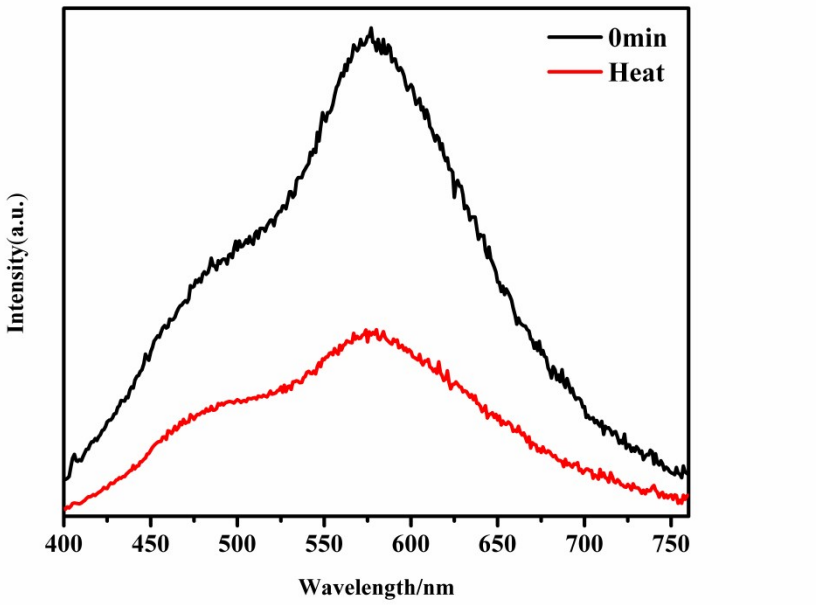

Figure S11 The thermally controlled luminescence emission spectra of the compound 1 heated at about 98℃ for 6 min.

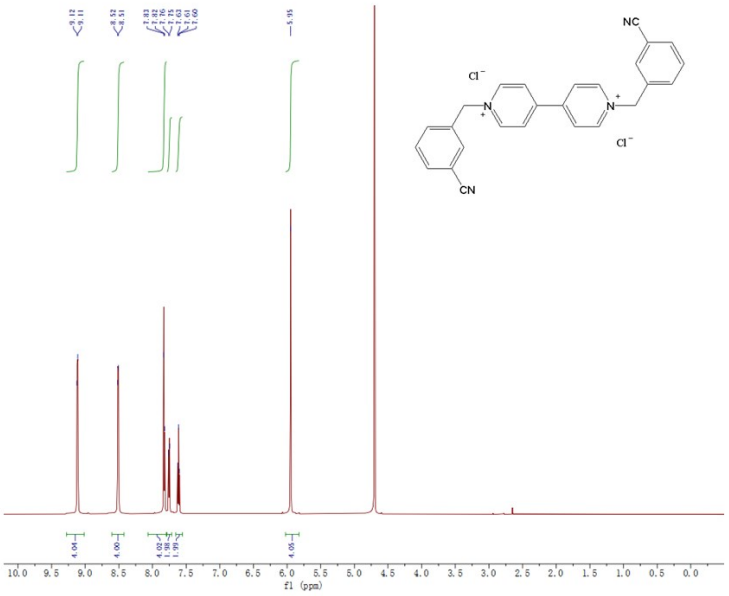

Figure S12 The ^{1}H NMR spectrum of 1,1'-bis(3-cyanobenzyl)-[4,4'-bipyridine] dichloride ligand in D_2O (600 MHz).

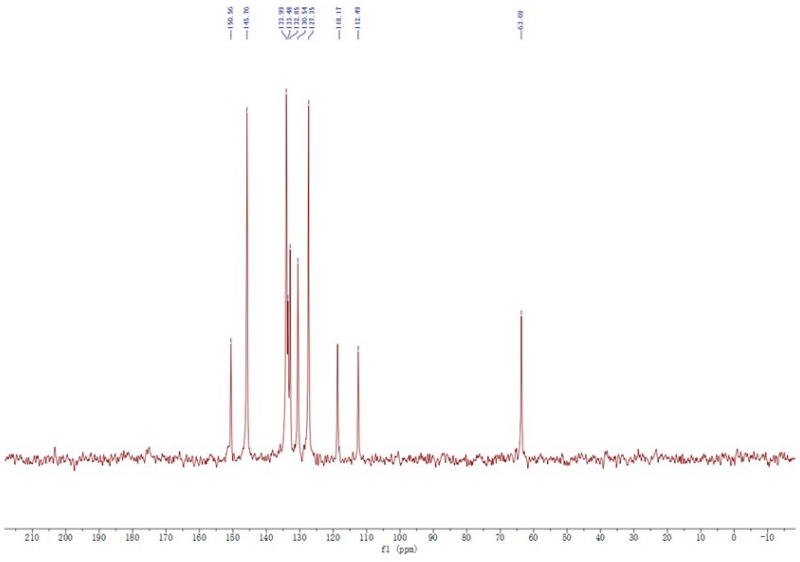

Figure S13 The ^{13}C-NMR spectrum of 1,1'-bis(3-cyanobenzyl)-[4,4'-bipyridine] dichloride ligand in D_2O (151MHz).

Table S1. Crystal Data of the compound 1.

Identification code	1
Empirical formula	$C_{42}H_{32}N_4O_{10}Zn$
Formula weight	818.08
Temperature/K	297.2
Crystal system	monoclinic
Space group	C2/c
a/Å	21.270(2)
b/Å	12.2947(12)
c/Å	14.7085(12)
α/°	90
β/°	97.489(3)
γ/°	90
Volume/Å^3	3813.5(6)
Z	4
ρ_{calc}g/cm^3	1.425
μ/mm^{-1}	0.710
F(000)	1688.0
Crystal size/mm^3	0.3 × 0.26 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.89 to 52.19
Index ranges	-26 ≤ h ≤ 26, -15 ≤ k ≤ 15, -18 ≤ l ≤ 16
Reflections collected	27119
Independent reflections	3775 [R_{int} = 0.0618, R_{sigma} = 0.0342]
Data/restraints/parameters	3775/4/266
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0376, wR_2 = 0.0863
Final R indexes [all data]	R_1 = 0.0541, wR_2 = 0.0938

Table S2. Selected bond length (Å) and angle (°) of the compound 1.

Bonds	Dist. (Å)
Zn1-O4[1]	1.9434(15)
Zn1-O4[2]	1.9434(15)
Zn1-O1	1.9431(16)
Zn1-O1[3]	1.9431(16)
Angle	(°)
O4[1]-Zn1-O4[2]	121.17(10)
O1[3]-Zn1-O4[2]	92.89(7)
O1-Zn1-O4[1]	92.89(7)
O1[3]-Zn1-O4[1]	116.71(8)
O1-Zn1-O4[2]	116.71(8)
O1-Zn1-O1[3]	118.81(11)