Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

A Reversible Thermo-Responsive 2D Zn(II) coordination Polymer as a Potential Self-referenced Luminescent Thermometer

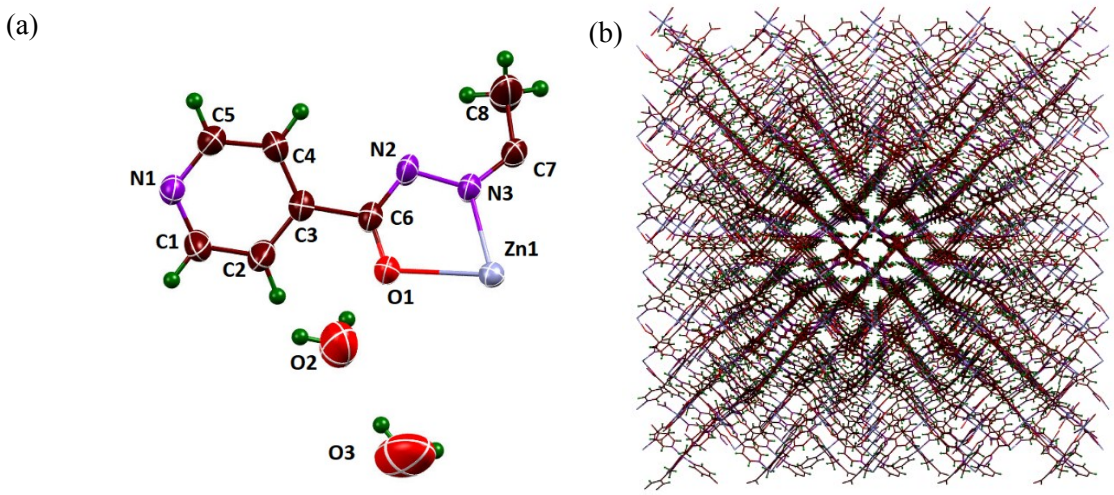

Fig. S1. (a) View (at the 50% probability level) of the building unit of CP-Zn with the atom numbering scheme. (b) Perspective image showing the 3D structure along 'c' axis.

Table S1. Crystal refinement parameters

Empirical formula	$C_{16}H_{20}ZnN_6O_5$
Formula weight	441.77
Temperature	296(2) K
Wavelength	0.71073 Å
Space group	P*bcn*
Unit cell dimensions	a = 12.90(13) Å α= 90°. b = 12.08(2) Å β= 90°. c = 12.44(7) Å γ= 90°.
Volume	1941.3(19) $Å^3$
Z	4
Density (calculated)	1.511 Mg/m^3
Absorption coefficient	1.306 mm^{-1}
F(000)	912
Reflections collected	21393
Independent reflections	2056 [R(int) = 0.0490]
Goodness-of-fit on F2	1.043
Data / restraints / parameters	2048 / 5 / 145
Final R indices [I>2sigma(I)]	R_1 = 0.0314, wR_2 = 0.0812

Bond lengths		Bond angles	
Zn(1)–N(1)	2.0691(18)	N(1)[a]–Zn(1)–N(3)	109.89(7)
Zn(1)–N(3)	2.1053(18)	N(1)–Zn(1)–O(1)	82.94(7)
Zn(1)–O(1)	2.2589(3)	N(3)–Zn(1)–O(1)	71.40(6)
C(6)–O(1)	1.261(3)	N(1)[a]–Zn(1)–N(1)[b]	138.77(11)
N(2)–C(6)	1.329(3)	N(1)[b]–Zn(1)–N(3)	102.75(7)
N(2)–N(3)	1.393(2)	N(3)–Zn(1)–N(3)[c]	74.36(10)

Symmetry transformations used to generate equivalent atoms: a = x+1/2,-y+1/2,-z+1; b = -x+1/2,-y+1/2,z-1/2; c= -x+1,y,-z+1/2

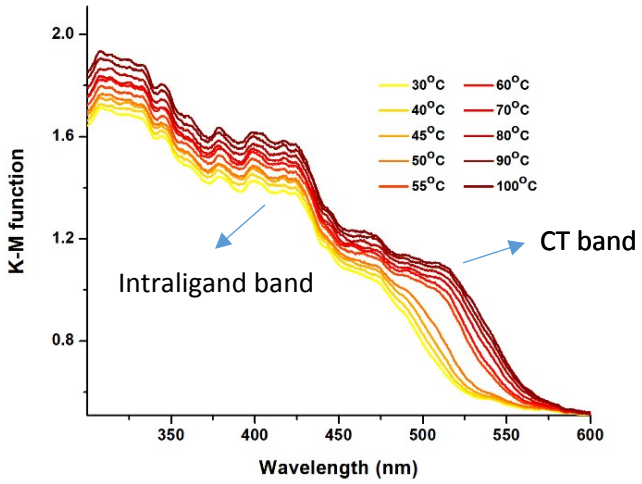

Fig. S2. UV-Vis Kubelka-Munk transformed spectra of CP-Zn showing three band regions.

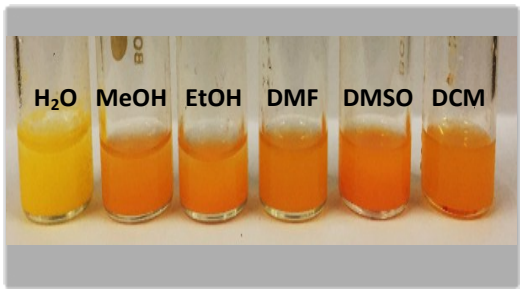

Fig. S3. Solvatochromism of CP-Zn in various solvents.

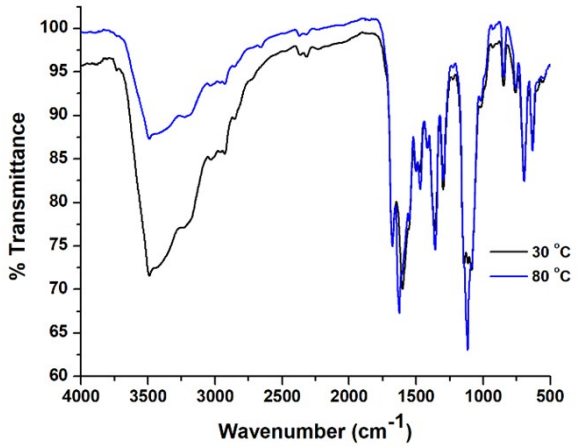

Fig. S4. Infrared spectrum of CP-Zn at room temperature and thermochromic temperature.

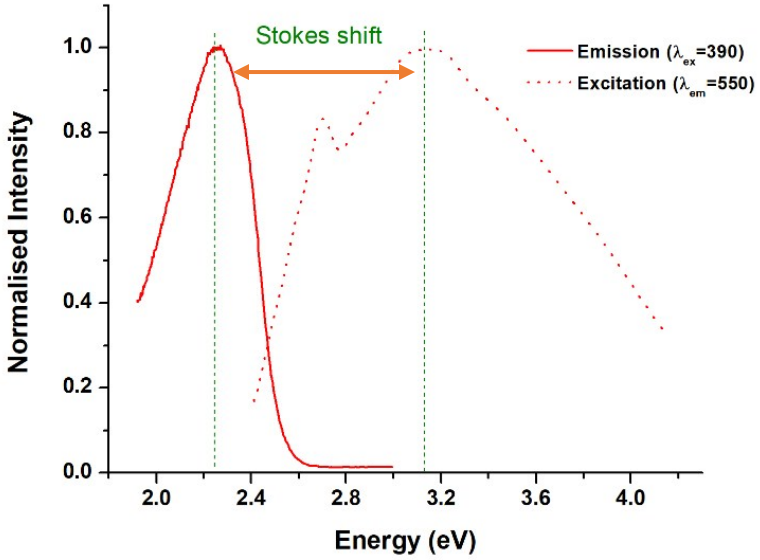

Fig S5. Ensemble excitation and emission spectra CP-Zn. The excitation and emission spectra show characteristic peaks.

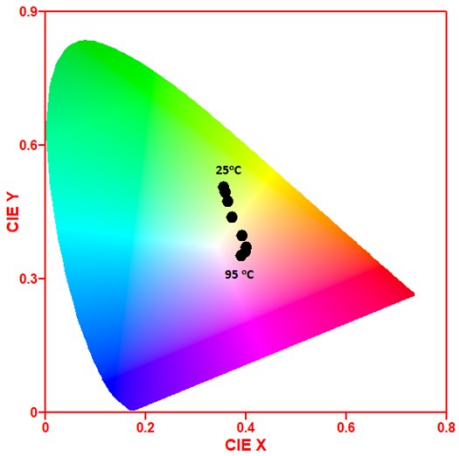

Fig. S6. CIE chromaticity diagram showing the temperature dependence of the (x,y) color coordinates of CP-Zn

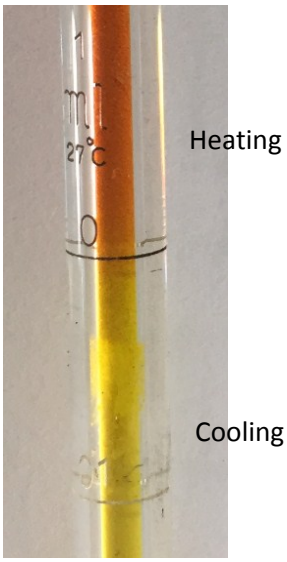

Fig. S7. Photograph showing gradient color change of CP-Zn with gradient temperature (Gradient region was zoomed for clarity).