

# A dual-functional 2D coordination polymer exhibiting photomechanical and electrically conductive behaviours

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## Supporting Information

**Table S1.** Crystal data and refinement parameters for compound **1**

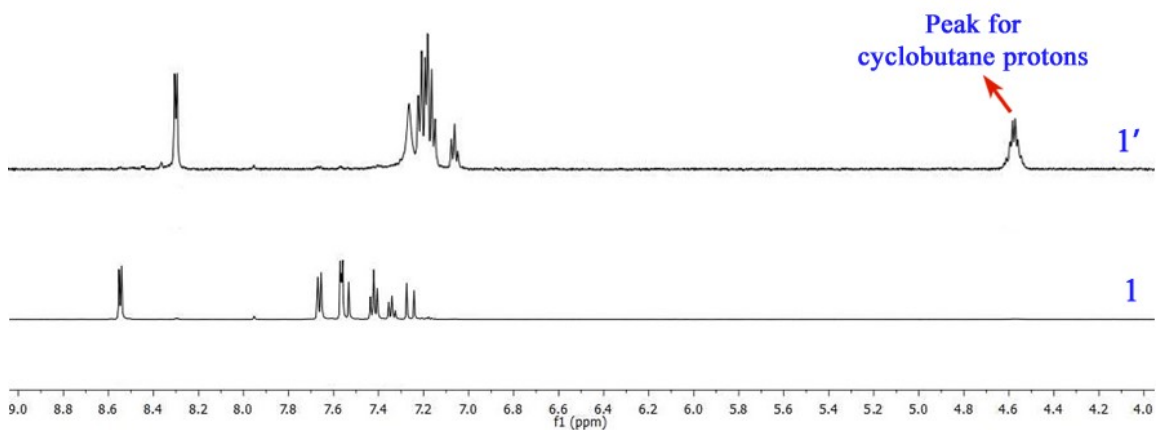
Formula	C <sub>42</sub> H <sub>26</sub> N <sub>2</sub> O <sub>8</sub> Zn <sub>2</sub> ( <b>1</b> )
fw	817.43
cryst syst	Triclinic
space group	<i>P</i> $\bar{1}$
<i>a</i> (Å)	10.1102(10)
<i>b</i> (Å)	12.4476(11)
<i>c</i> (Å)	15.9753(16)
$\alpha$ (deg)	107.400
$\beta$ (deg)	90.586
$\gamma$ (deg)	106.080
<i>V</i> (Å <sup>3</sup> )	1833.9(3)
<i>Z</i>	2
<i>D</i> <sub>calcd</sub> (g/cm <sup>3</sup> )	1.480
$\mu$ (mm <sup>-1</sup> )	1.365
$\lambda$ (Å)	0.71073
GOF on <i>F</i> <sup>2</sup>	1.043
Final <i>R</i> indices [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] <sup>a,b</sup>	<i>R</i> 1 = 0.0273 <i>wR</i> 2 = 0.0747

$${}^a R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, {}^b wR2 = [\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}]^{1/2}$$

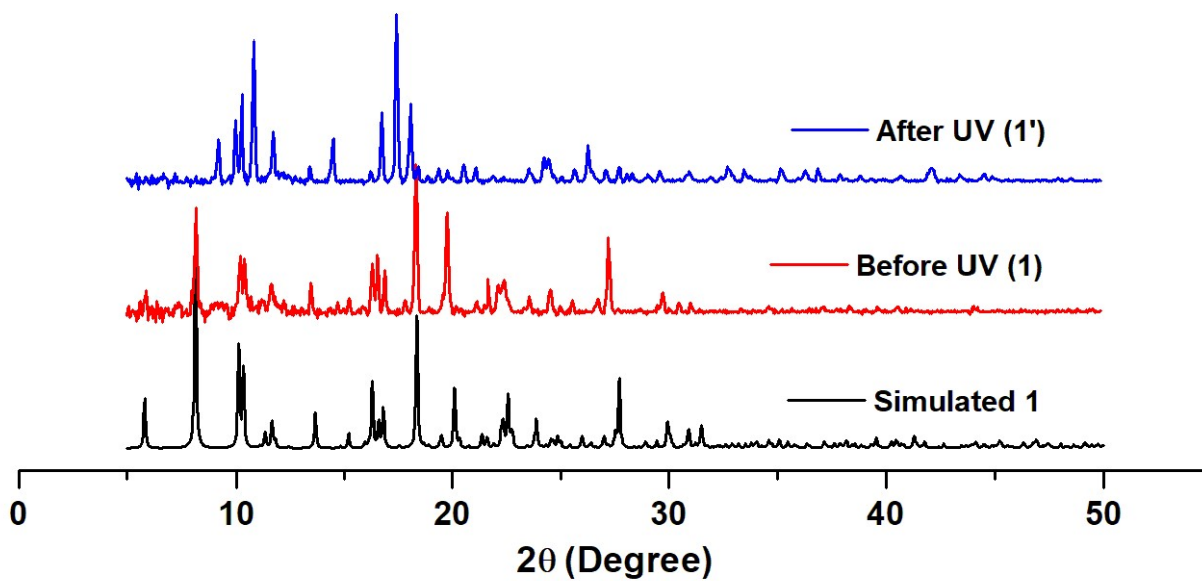
**Table S2.** Selected bond lengths and bond angles in **1**

<b>Bond length (Å)</b>	
Zn(1)-O(1)	1.9337(16)
Zn(1)-N(1)	2.0088(16)
Zn(1)-O(6)a	1.9722(14)
Zn(1)-O(8)b	1.9666(15)
Zn(2)-O(3)	1.9375(15)
Zn(2)-O(5)	1.9672(15)
Zn(2)-N(2)	2.0053(16)
Zn(2)-O(7)c	1.9783(14)
<b>Bond angle (°)</b>	
O(1)-Zn(1)-N(1)	123.64(7)
O(1)-Zn(1)-O(6)a	105.12(6)
O(1)-Zn(1)-O(8)b	111.77(6)
O(6)a-Zn(1)-N(1)	101.03(7)
O(8)b-Zn(1)-N(1)	101.34(7)
O(6)a-Zn(1)-O(8)b	113.83(6)
O(3)-Zn(2)-O(5)	111.00(6)
O(3)-Zn(2)-N(2)	126.55(6)
O(3)-Zn(2)-O(7)c	105.23(6)
O(5)-Zn(2)-N(2)	102.16(6)
O(5)-Zn(2)-O(7)c	112.47(6)
O(7)c-Zn(2)-N(2)	98.89(6)

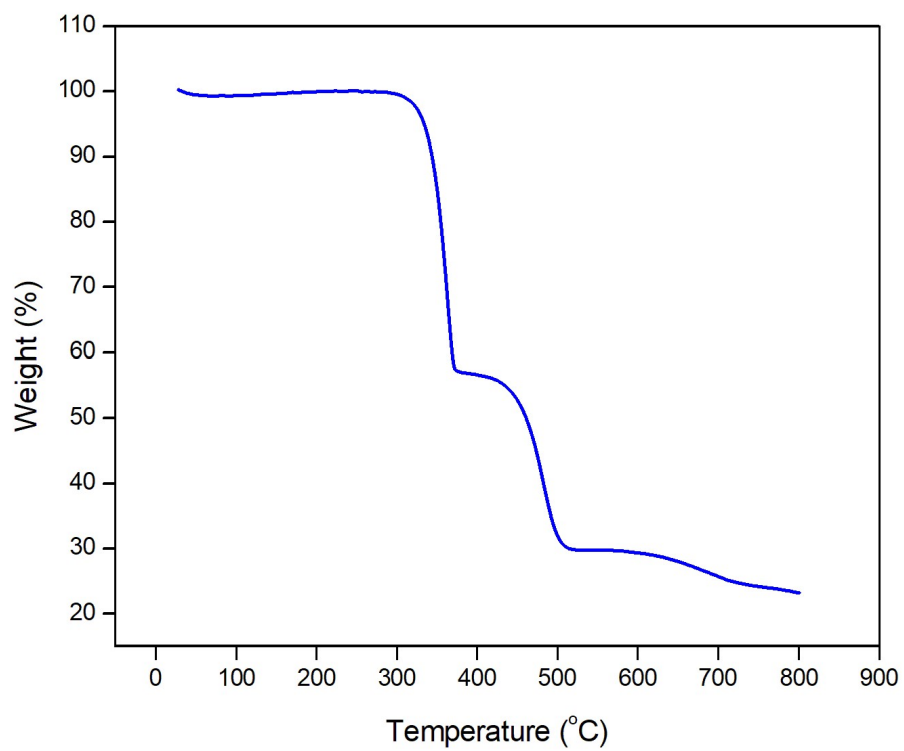
Symmetric transformation: a = x, 1+y, z; b = 1+x, 1+y, z; c = 1+x, y, z



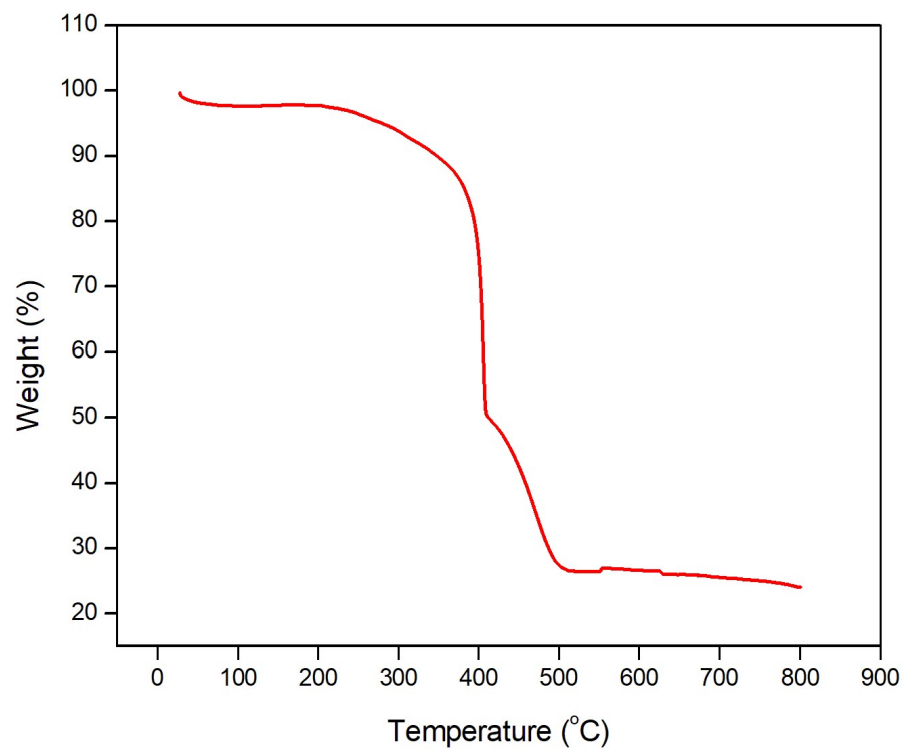
**Fig. S1** Partial <sup>1</sup>H NMR spectra (400 MHz, DMSO-d<sub>6</sub>) of compounds **1** and **1'**.



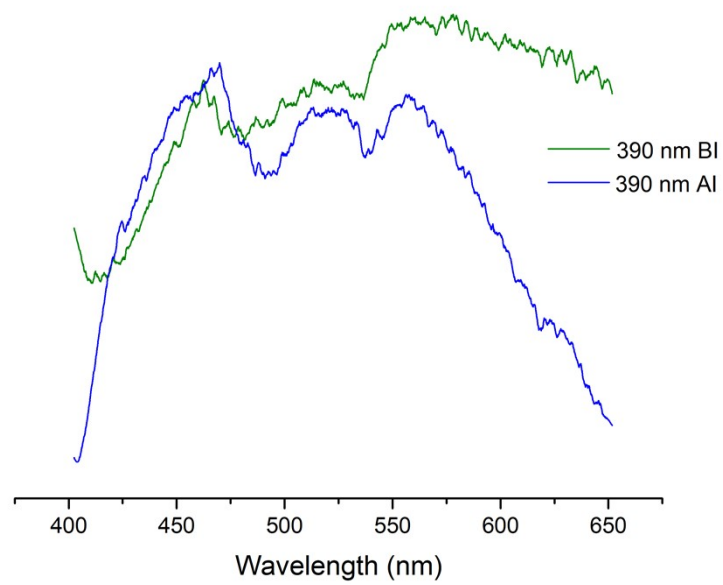
**Fig. S2** PXRD patterns of simulated **1** (black), before (red) and after UV irradiation (blue).



**Fig. S3** TGA plot of compound 1.



**Fig. S4** TGA of compound 1'.



**Fig. S5** Solid-state photoluminescence spectra of **1** and **1'**.