Supporting Information (SI)

Photodimerization behaviour of 1D–3D Zn(II) coordination polymers with tetrazoyl styrylpyridine

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Materials and Instruments

All reagents and solvents were purchased from commercial sources and used without further purification. The 4-(4-cyanostyryl)pyridine precursor was synthesized according to a literature method.[S1] Infrared spectra (KBr pellet) were recorded on a Nicolet Avatar 360 spectrophotometer in the range of 4000–400 cm^{-1}. Thermal analyses were conducted using a PYRIS Diamond TG/DTA instrument. Powder X-ray diffraction (PXRD) patterns were measured on a Bruker D8 Advance diffractometer (Cu Kα, λ = 1.5418 Å) at room temperature. Luminescence properties were recorded on an Edinburgh Instruments FLS920 spectrofluorometer.

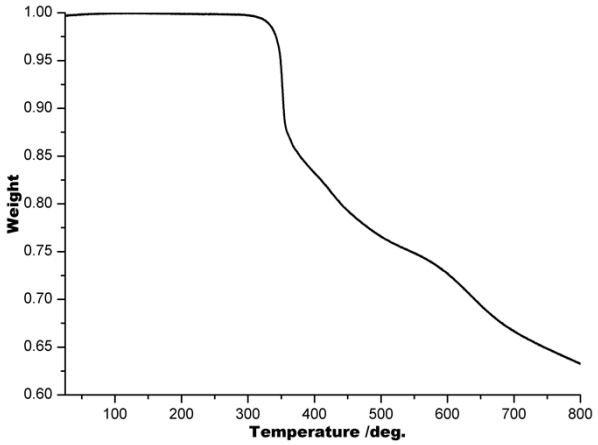

Figure S1. TG curve of **1-Cl**.

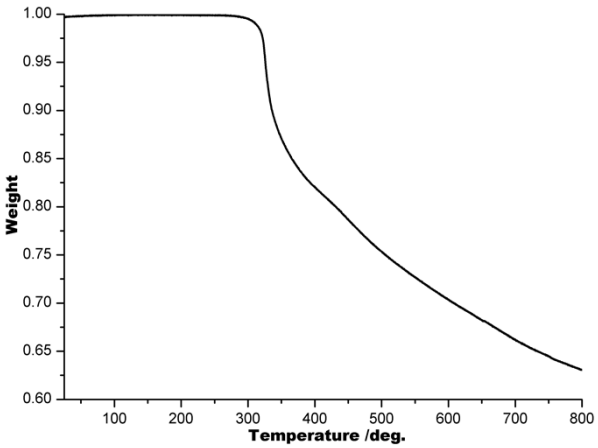

Figure S2. TG curve of **2**.

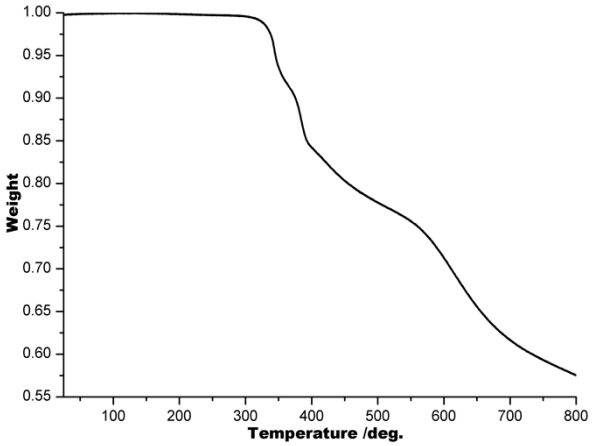

Figure S3. TG curve of **3**.

		CP 1-Br	
Zn(1)-O(1)	1.917(3)	Zn(1)-N(2)	2.056(4)
Zn(1)-N(6)	2.010(4)	Zn(1)-N(8)#1	1.985(4)
Zn(2)-Br(1)	2.3864(13)	Zn(2)-N(4)#2	2.007(4)
Zn(2)-O(1)	1.902(4)	Zn(2)-N(1)#3	2.021(4)
O(1)-Zn(1)-N(6)	107.64(17)	N(6)-Zn(1)-N(2)	101.57(17)
O(1)-Zn(1)-N(2)	107.21(16)	N(8)#1-Zn(1)-N(6)	120.56(18)
O(1)-Zn(1)-N(8)#1	109.69(17)	N(8)#1-Zn(1)-N(2)	109.26(18)
O(1)-Zn(2)-Br(1)	110.89(10)	N(4)#2-Zn(2)-Br(1)	111.03(13)
O(1)-Zn(2)-N(4)#2	108.17(17)	N(4)#2-Zn(2)-N(1)#3	110.11(18)
O(1)-Zn(2)-N(1)#3	109.35(17)	N(1)#3-Zn(2)-Br(1)	107.29(14)
Zn(2)-O(1)-Zn(1)	133.25(18)		
		CP 1-Br′	
Zn(1)-Br(1)	2.3789(10)	Zn(1)-N(8)#1	2.027(5)
Zn(1)-N(6)	2.025(5)	Zn(1)-O(1)	1.918(4)
Zn(2)-N(10)	2.063(5)	Zn(2)-O(1)	1.914(4)
Zn(2)-N(3)	1.986(5)	Zn(2)-N(1)#2	2.028(5)
C(21)-C(20)	1.658(11)	Zn(2)-O(1)-Zn(1)	133.8(2)
N(6)-Zn(1)-Br(1)	105.98(15)	O(1)-Zn(1)-Br(1)	109.83(13)
N(6)-Zn(1)-N(8)#1	108.8(2)	O(1)-Zn(1)-N(6)	109.4(2)
N(8)#1-Zn(1)-Br(1)	114.51(16)	O(1)-Zn(1)-N(8)#1	108.2(2)
N(3)-Zn(2)-N(10)	107.8(2)	O(1)-Zn(2)-N(3)	113.8(2)
N(3)-Zn(2)-N(1)#2	115.5(2)	O(1)-Zn(2)-N(1)#2	105.4(2)
O(1)-Zn(2)-N(10)	110.1(2)	N(1)#2-Zn(2)-N(10)	103.8(2)

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for **1-Br** and **1-Br'**.

		*CP **2***	
Zn(1)-N(10)#1	2.0458(18)	Zn(1)-N(1)	1.955(2)
Zn(1)-N(9)#2	2.0026(18)	Zn(1)-O(1)	1.9323(16)
Zn(2)-N(11)#3	2.0151(18)	Zn(2)-N(4)	2.0324(17)
Zn(2)-N(5)	2.0228(17)	Zn(2)-O(1)	1.9008(15)
N(9)#1-Zn(1)-N(10)#2	106.24(7)	O(1)-Zn(1)-N(10)#2	106.83(7)
N(1)-Zn(1)-N(10)#2	113.81(8)	O(1)-Zn(1)-N(9)#1	112.55(7)
N(1)-Zn(1)-N(9)#1	108.85(9)	O(1)-Zn(1)-N(1)	108.64(9)
N(11)#3-Zn(2)-N(5)	106.30(7)	O(1)-Zn(2)-N(11)#3	118.49(7)
N(11)#3-Zn(2)-N(4)	105.74(7)	O(1)-Zn(2)-N(5)	105.87(7)
N(5)-Zn(2)-N(4)	106.28(8)	O(1)-Zn(2)-N(4)	113.36(7)
Zn(2)-O(1)-Zn(1)	133.08(9)		
		*CP **2′***	
Zn(1)-O(1)	1.898(3)	Zn(1)-N(10)	2.034(4)
Zn(1)-N(6)	2.039(3)	Zn(1)-N(1)	2.032(3)
Zn(2)-O(1)	1.932(3)	Zn(2)-N(11)	1.950(4)
Zn(2)-N(7)#1	2.046(3)	Zn(2)-N(2)#2	1.997(3)
C(20)-C(21)	1.623(6)	Zn(1)-O(1)-Zn(2)	135.40(18)
O(1)-Zn(1)-N(6)	106.04(14)	N(10)-Zn(1)-N(6)	108.05(14)
O(1)-Zn(1)-N(10)	117.95(13)	N(1)-Zn(1)-N(6)	105.28(13)
O(1)-Zn(1)-N(1)	114.05(15)	N(1)-Zn(1)-N(10)	104.69(14)
O(1)-Zn(2)-N(7)#1	108.26(13)	N(11)-Zn(2)-N(7)#1	111.24(16)
O(1)-Zn(2)-N(11)	109.35(16)	N(11)-Zn(2)-N(2)#2	109.41(15)
O(1)-Zn(2)-N(2)#2	112.47(14)	N(2)#2-Zn(2)-N(7)#1	106.09(14)

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) for **2** and **2'**.

		CP 3	
Zn(2)-O(1)	1.905(4)	Zn(1)-Br(1)	2.3512(9)
Zn(2)-O(2)	1.940(4)	Zn(1)-N(2)	2.046(4)
Zn(2)-N(4)#1	2.053(4)	Zn(1)-O(1)	1.924(4)
Zn(2)-N(1)#2	2.022(4)	Zn(1)-O(2)#3	1.984(4)
O(1)-Zn(2)-O(2)	116.3(2)	N(2)-Zn(1)-Br(1)	112.83(13)
O(1)-Zn(2)-N(4)#1	106.74(18)	O(1)-Zn(1)-Br(1)	116.87(15)
O(1)-Zn(2)-N(1)#2	110.02(19)	O(1)-Zn(1)-N(2)	103.98(17)
O(2)-Zn(2)-N(4)#1	107.33(18)	O(1)-Zn(1)-O(2)#3	106.4(2)
O(2)-Zn(2)-N(1)#2	112.3(2)	O(2)#3-Zn(1)-Br(1)	109.68(16)
N(1)#2-Zn(2)-N(4)#1	103.17(18)	O(2)#3-Zn(1)-N(2)	106.34(17)
Zn(2)-O(1)-Zn(1)	136.8(2)	Zn(2)-O(2)-Zn(1)#4	129.0(2)
		CP 3'	
Zn(2)-N(4)	2.025(11)	Zn(2)-O(2)	1.983(9)
Zn(2)-O(1)#1	1.897(8)	Zn(2)-N(1)#2	2.019(12)
Zn(1)-N(2)	2.044(10)	Zn(1)-O(2)3	1.987(9)
Zn(1)-O(1)	1.921(8)	Zn(1)-Br(1A)	2.344(7)
Zn(1)-Br(1B)	2.32(2)	C(6)-C(7)#4	1.63(2)
O(1)#1-Zn(2)-N(4)	107.2(4)	O(2)-Zn(2)-N(4)	109.4(4)
O(1)#1-Zn(2)-O(2)	112.5(4)	O(2)-Zn(2)-N(1)#2	118.0(5)
O(1)#1-Zn(2)-N(1)#2	104.9(5)	N(1)#2-Zn(2)-N(4)	104.1(5)
O(1)-Zn(1)-N(2)	104.1(4)	N(2)-Zn(1)-Br(1A)	106.5(4)
O(1)-Zn(1)-O(2)#3	102.8(4)	N(2)-Zn(1)-Br(1B)	114.4(7)
O(2)#3-Zn(1)-N(2)	111.6(4)	O(2)#3-Zn(1)-Br(1A)	108.9(4)
O(2)#3-Zn(1)-Br(1B)	113.6(9)	Zn(2)-O(2)-Zn(1)#6	123.5(5)
Zn(2)#5-O(1)-Zn(1)	134.3(5)		

Table S3. Selected Bond Lengths (Å) and Bond Angles (°) for **3** and **3'**.

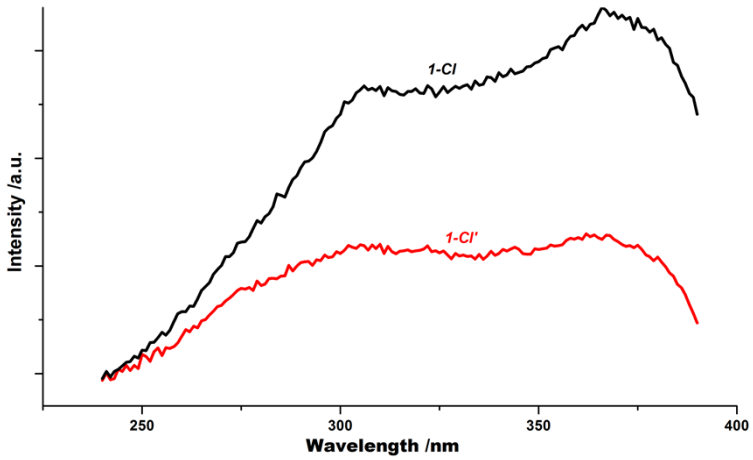

Figure S4. Excitation spectra of **1-Cl** and **1-Cl'**.

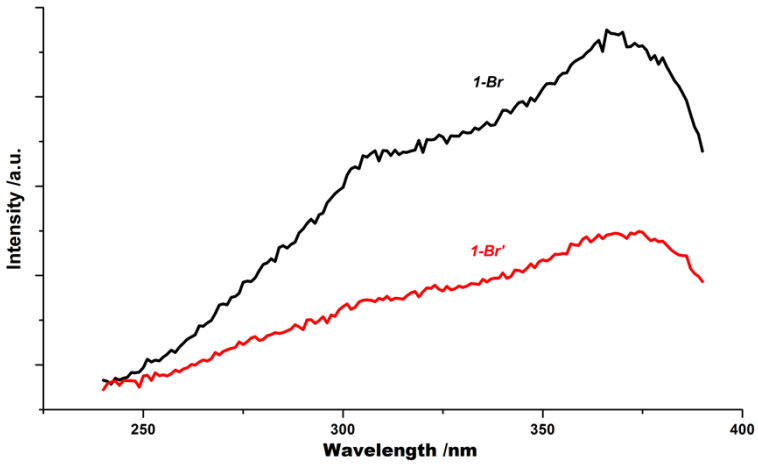

Figure S5. Excitation spectra of **1-Br** and **1-Br'**.

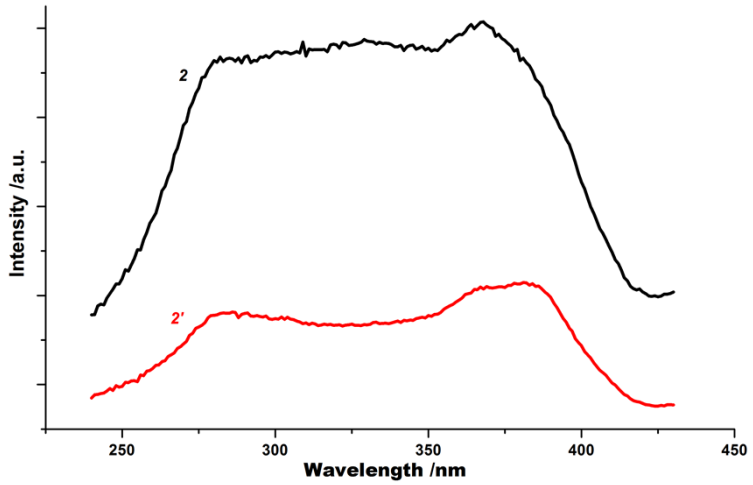

Figure S6. Excitation spectra of **2** and **2'**.

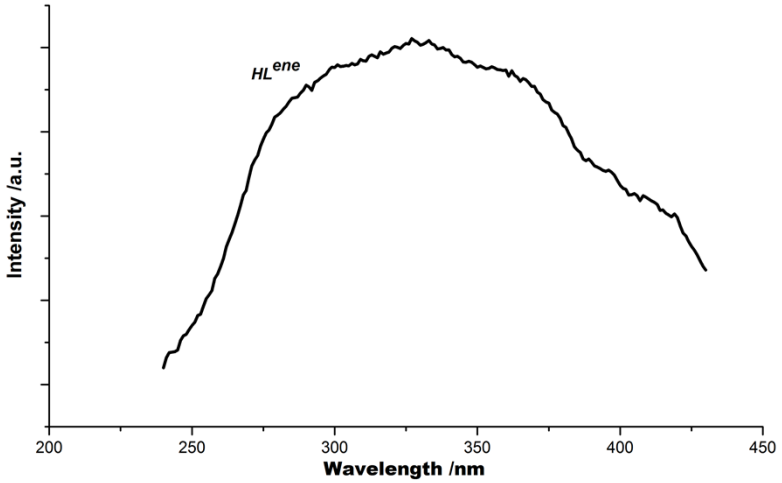

Figure S7. Excitation spectra of **HL^{ene}**.

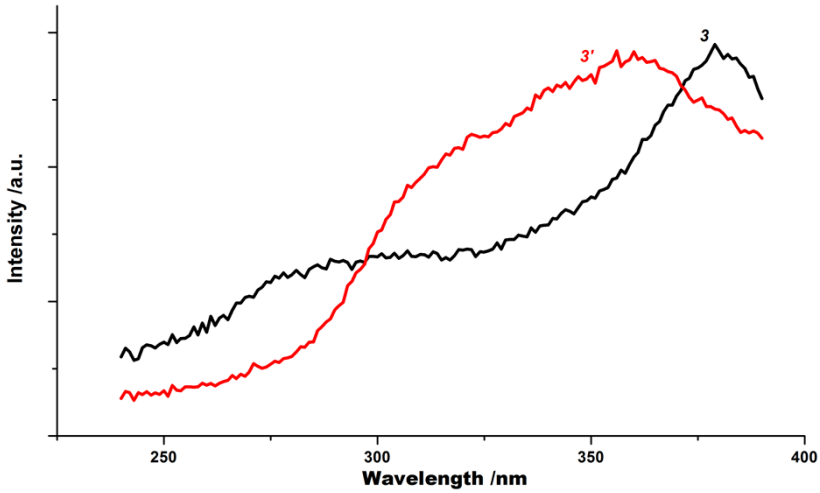

Figure S8. Excitation spectra of **3** and **3**'.

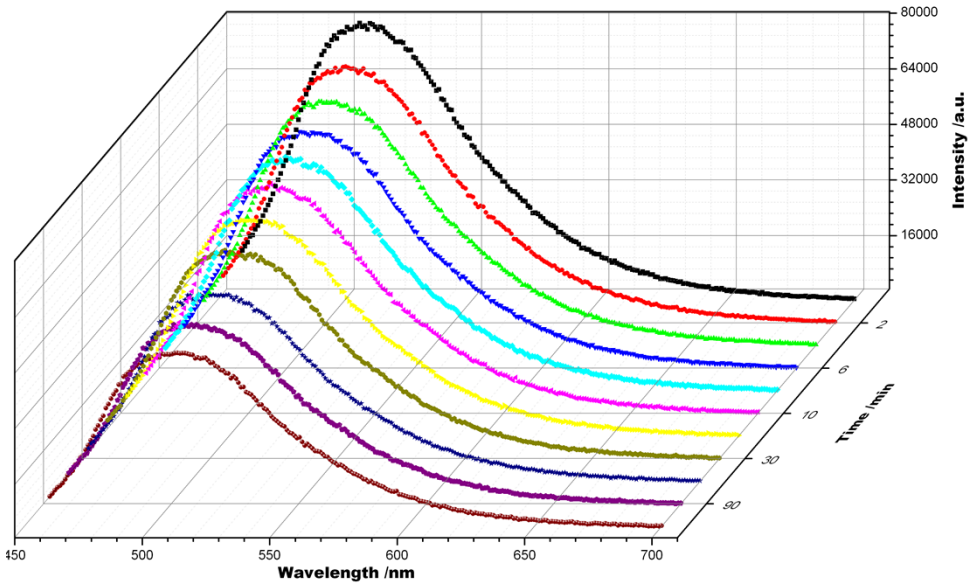

Figure S9. Time-dependent fluorescence of **2**.

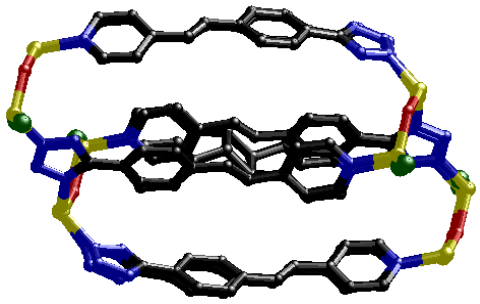

Figure S10. The overlay of structures of **1** and **1'** to show their bulk similarity.

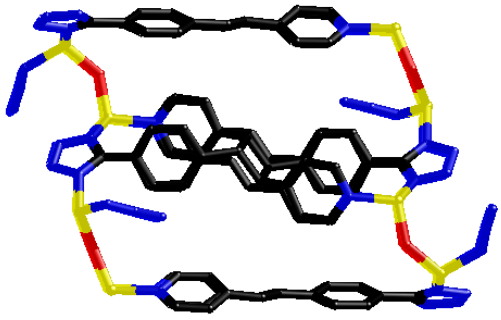

Figure S11. The overlay of structures of **2** and **2'**.

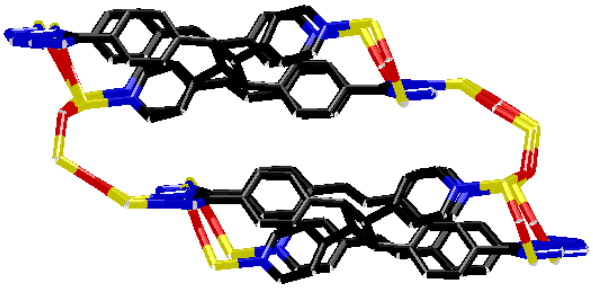

Figure S12. The overlay of structures of **3** and **3'.**

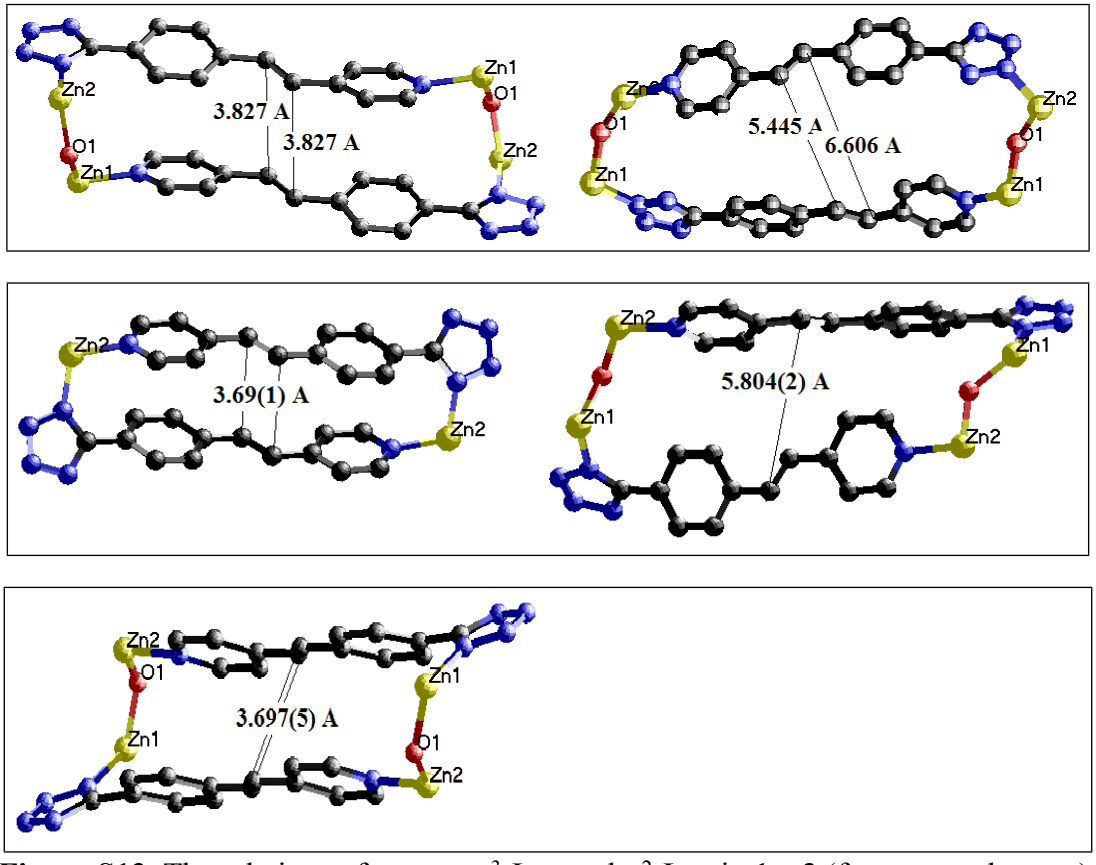

Figure S13. The relations of nearest μ^3-L^{ene} and μ^2-L^{ene} in **1**—**3** (from top to bottom).

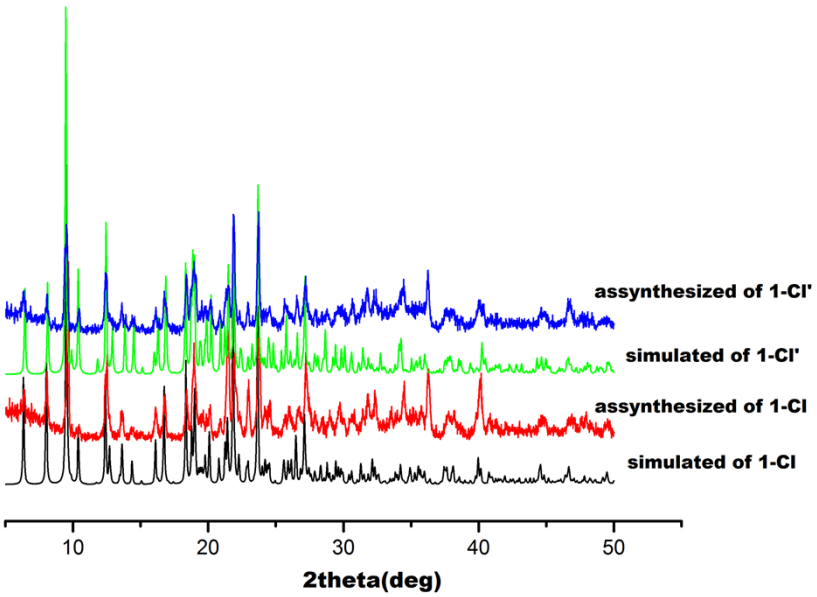

Figure S14. Powder X-ray diffraction patterns of **1-Cl** and **1-Cl'**.

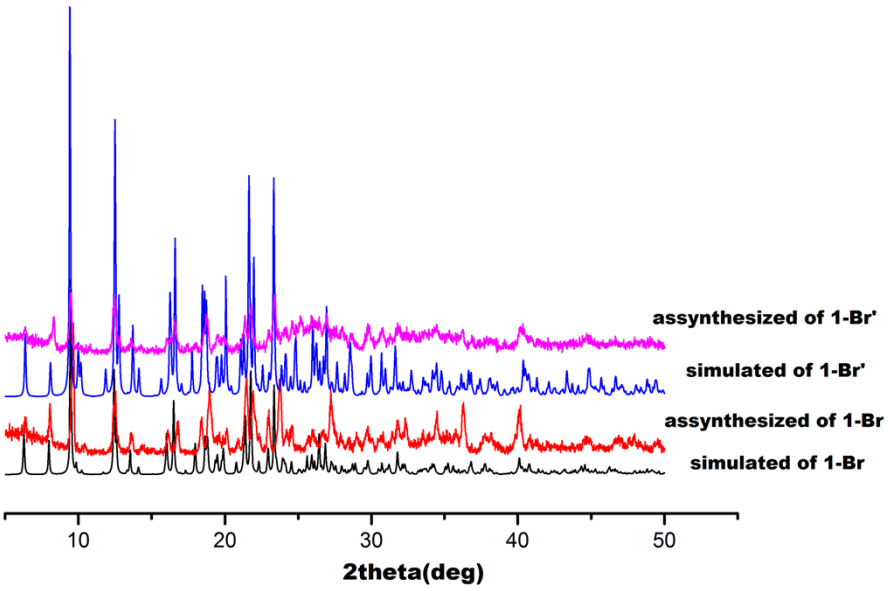

Figure S15. Powder X-ray diffraction patterns of **1-Br** and **1-Br'**.

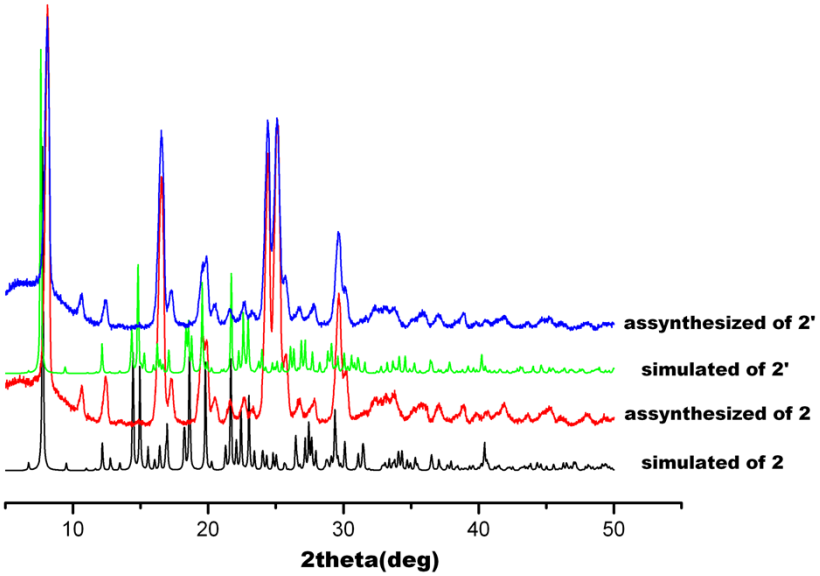

Figure S16. Powder X-ray diffraction patterns of **2** and **2'**.

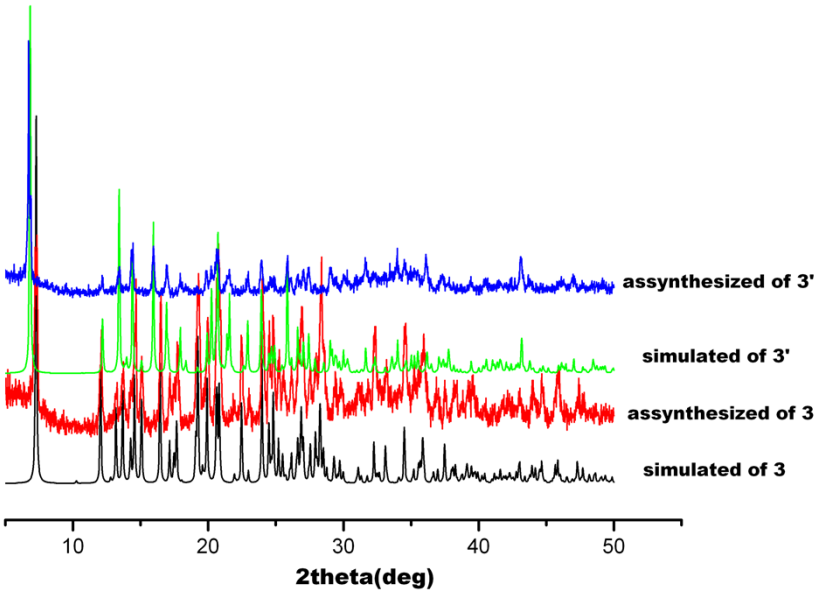

Figure S17. Powder X-ray diffraction patterns of **3** and **3'**.

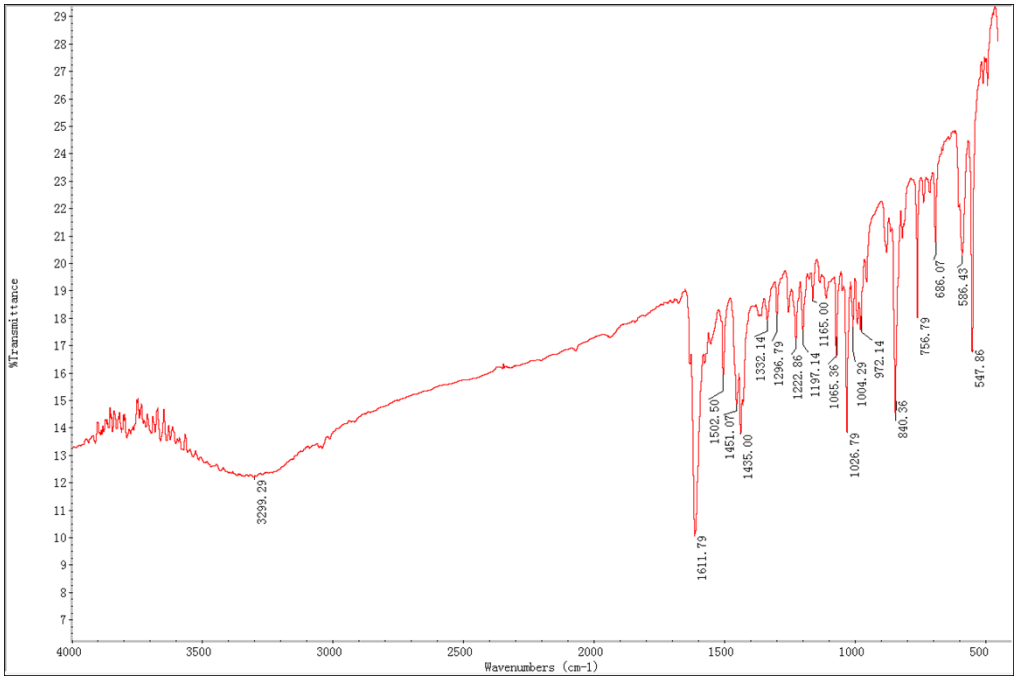

Figure S18. IR spectrum of **1-Cl**.

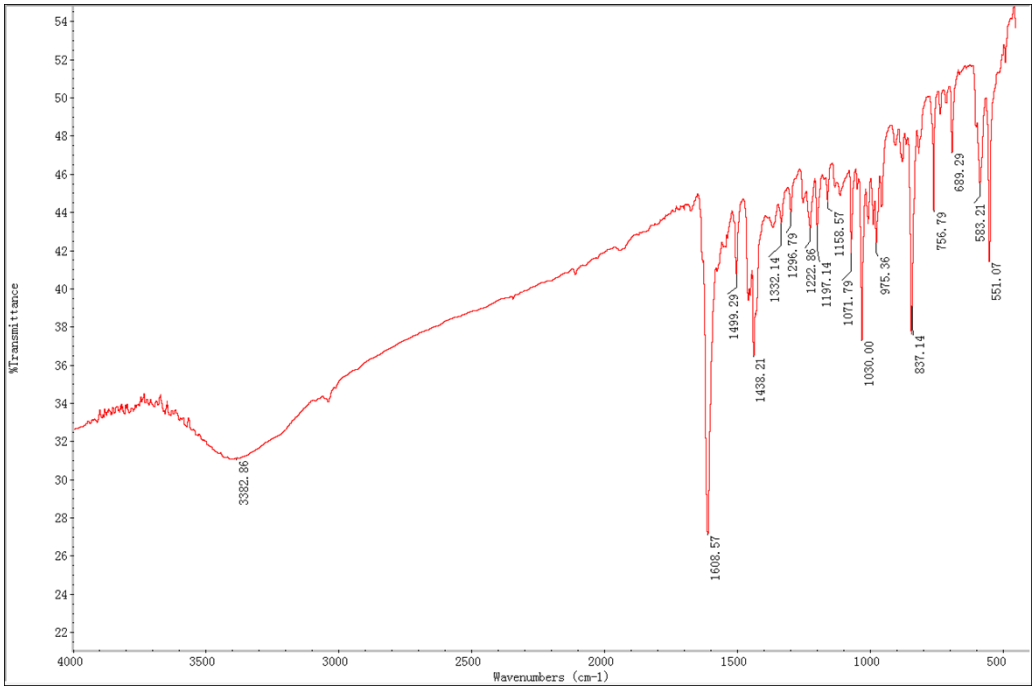

Figure S19. IR spectrum of **1-Br**.

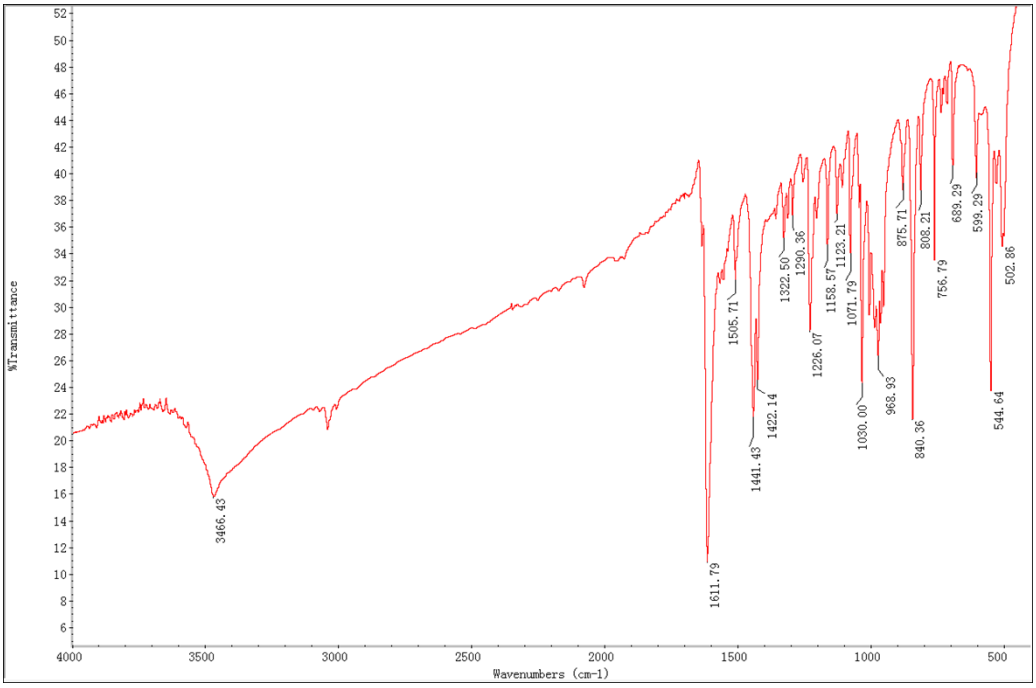

Figure S20. IR spectrum of **2**.

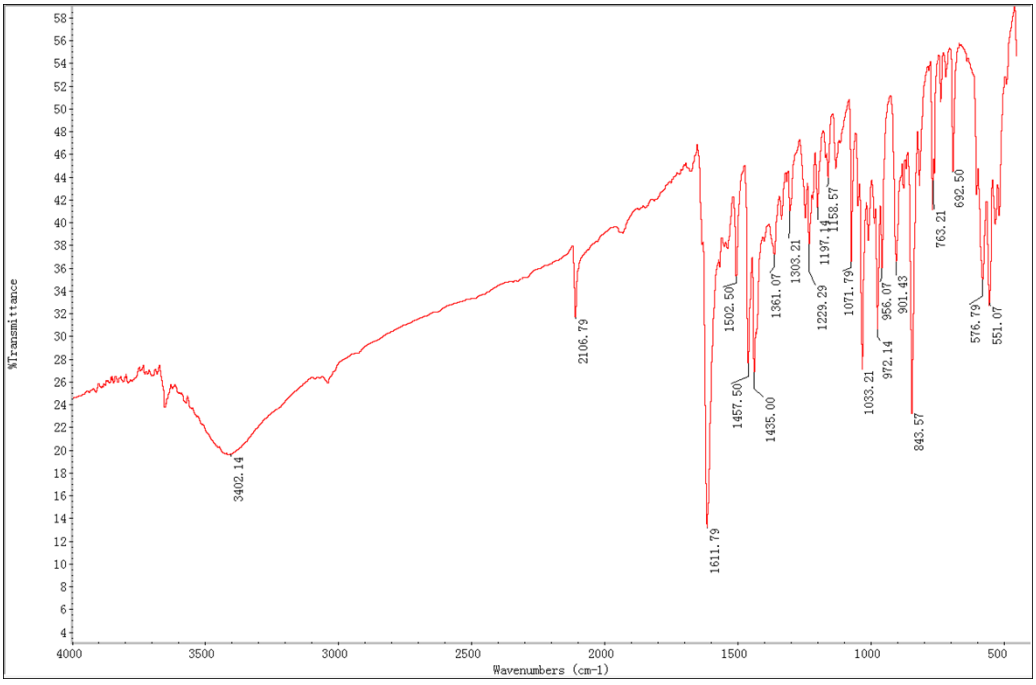

Figure S21. IR spectrum of **3**.

S1 O. R. Evans, W.-B. Lin, *Chem. Mater.*, 2001, **13**, 3009–3017.