Counter cations effect on the photochromic behaviors of three Zn-viologen complexes

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Table S1. Selected bond lengths (Å) and bond angles (°) for **1**–**3**.

Compound **1**			
Zn(1)–O(2)	2.082(2)	Zn(1)–O(9)	2.046(2)
Zn(1)–O(10)	2.128(2)	Zn(1)–O(8)	2.124(3)
Zn(1)–O(11)	2.121(2)	Zn(1)–O(7)	2.085(2)
O(2)–Zn(1) –O(10)	175.74(10)	O(2)–Zn(1) –O(8)	91.43(11)
O(2)–Zn(1) –O(11)	94.83(9)	O(2)–Zn(1) –O(7)	87.71(10)
O(9)–Zn(1) –O(2)	86.88(10)	O(9)–Zn(1) –O(10)	92.27(9)
O(9)–Zn(1) –O(8)	86.54(11)	O(9)–Zn(1) –O(11)	176.77(10)
O(9)–Zn(1) –O(7)	91.56(11)	O(8)–Zn(1) –O(10)	92.68(10)
O(11)–Zn(1) –O(10)	86.22(9)	O(11)–Zn(1) –O(8)	90.67(10)
O(7)–Zn(1) –O(10)	88.14(10)	O(7)–Zn(1) –O(8)	177.96(10)
O(7)–Zn(1) –O(11)	91.25(10)		
Compound **2**			
Zn(1)–O(2)	2.1221(19)	Zn(1)–O(7)	2.043(2)
Zn(1)–O(8)	2.069(2)	Zn(1)–O(10)	2.130(2)
Zn(1)–O(9)	2.1199(19)	Zn(1)–O(11)	2.099(2)
O(2)–Zn(1) –O(10)	91.32(9)	O(7)–Zn(1) –O(2)	87.00(8)
O(7)–Zn(1) –O(8)	92.75(10)	O(7)–Zn(1) –O(10)	85.97(10)
O(7)–Zn(1) –O(9)	90.71(8)	O(7)–Zn(1) –O(11)	177.28(9)
O(8)–Zn(1) –O(2)	88.14(9)	O(8)–Zn(1) –O(10)	178.63(9)
O(8)–Zn(1) –O(9)	89.69(8)	O(8)–Zn(1) –O(11)	89.97(9)
O(9)–Zn(1) –O(2)	176.77(8)	O(9)–Zn(1) –O(10)	90.80(8)
O(11)–Zn(1) –O(2)	93.21(8)	O(11)–Zn(1) –O(10)	91.31(9)
O(11)–Zn(1) –O(9)	89.18(8)		
Compound **3**			

Zn(1)–O(6)	2.1095(2)	Zn(1)–O(10)	2.0542(18)
Zn(1)–O(7	2.0988(18)	Zn(1)–O(9)	2.1291(17)
Zn(1)–O(11)	2.1378(19)	Zn(1)–O(8)	2.0745(19)
O(6)–Zn(1) –O(9)	177.30(7)	O(6)–Zn(1) –O(11)	92.50(8)
O(10)–Zn(1) –O(6)	87.15(7)	O(10)–Zn(1) –O(7)	176.34(8)
O(10)–Zn(1) –O(9)	91.35(7)	O(10)–Zn(1) –O(11)	85.15(8)
O(10)–Zn(1) –O(8)	93.08(8)	O(7)–Zn(1) –O(6)	93.38(7)
O(7)–Zn(1) –O(9)	88.25(7)	O(7)–Zn(1) –O(11)	91.21(8)
O(9)–Zn(1) –O(11)	89.61(7)	O(8)–Zn(1) –O(6)	88.96(8)
O(8)–Zn(1) –O(7)	90.55(8)	O(8)–Zn(1) –O(9)	88.87(7)
O(8)–Zn(1) –O(11)	177.64(8)		

Table S2. The hydrogen bond lengths (Å) in **1**–**3**.

Compound **1**			
O(12)–H ··O(1)	1.899	C(2)–H ··O(1)	2.467
O(13)–H ··O(3)	1.939	O(7)–H ··O(4)	1.874
O(9)–H ··O(4)	2.521	O(7)–H ··O(5)	1.794
O(9)–H ··O(5)	1.852	O(10)–H ··O(6)	1.911
O(8)–H ··O(6)	2.015	C(1)–H ··O(7)	2.710
O(8)–H ··O(12)	1.785	O(12)–H ··O(8)	2.616
C(4)–H ··O(8)	2.432	O(10)–H ··O(11)	1.984
O(11)–H ··O(10)	1.983	C(2)–H ··O(11)	2.593
O(12)–H ··O(13)	2.304	O(12)–H ··O(13)	2.698
C(3)–H ··O(13)	2.579	O(13)–H ··O(12)	2.480
C(9)–H ··O(13)	2.649	C(10)–H ··O(1)	2.559
O(11)–H ··O(1)	1.899	C(9)–H ··O(2)	2.531
C(9)–H ··O(3)	2.528	C(13) –H ··O(4)	2.531
C(13) –H ··O(5)	2.545	C(10)–H ··O(6)	2.534
O(9)–H ··O(8)	2.624	O(7)–H ··O(2)	2.656
Compound **2**			
O(12)–H ··O(1)	1.891	C(3)–H ··O(1)	2.393
O(12)–H ··O(2)	2.140	O(9)–H ··O(3)	2.694
O(7)–H ··O(4)	1.881	O(8)–H ··O(4)	1.794
O(7)–H ··O(5)	1.941	O(9)–H ··O(6)	1.831
O(10)–H ··O(6)	1.852	C(1)–H ··O(6)	2.574
O(8)–H ··N(1)	2.508	C(2)–H ··O(8)	2.631
O(11)–H ··O(9)	1.945	O(9)–H ··O(11)	1.934
C(5)–H ··O(10)	2.399	O(10)–H ··O(12)	1.786
C(2)–H ··O(11)	2.664	C(4)–H ··O(12)	2.495
Compound **3**			
O(9)–H ··O(1)	1.839	O(8)–H ··O(2)	1.911
O(10)–H ··O(2)	1.920	O(8)–H ··O(3)	1.858
O(10)–H ··O(3)	1.948	O(9)–H ··O(4)	1.859
O(11)–H ··O(5)	2.018	O(12)–H ··O(5)	1.797
C(5)–H ··O(5)	2.434	O(12)–H ··O(6)	2.101
O(7)–H ··O(9)	1.950	C(5)–H ··O(7)	2.603

C(4)–H ··O(10)	2.613	C(7)–H ··O(11)	2.407
O(11)–H ··O(12)	1.839	C(1)–H ··O(12)	2.699

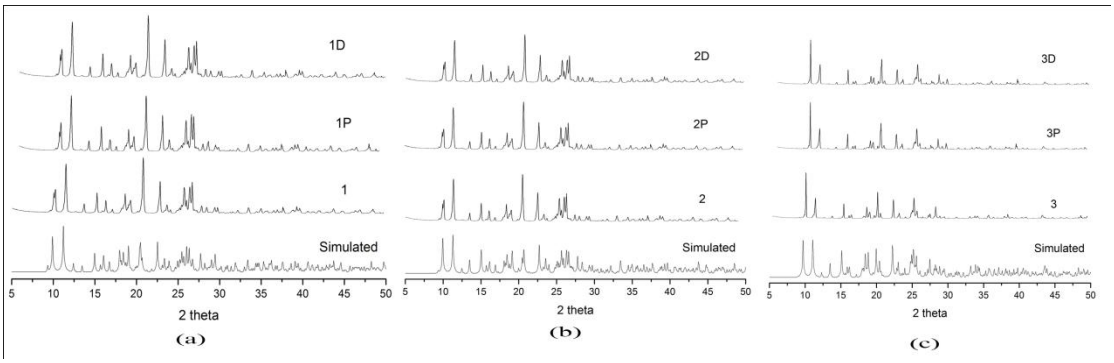

Fig. S1. The PXRD spectra before and after irradiation for **1-3** (**1P**, **2P**, **3P**, photoproducts for three compounds; **1D**, **2D**, **3D**, decolored samples for three compounds).

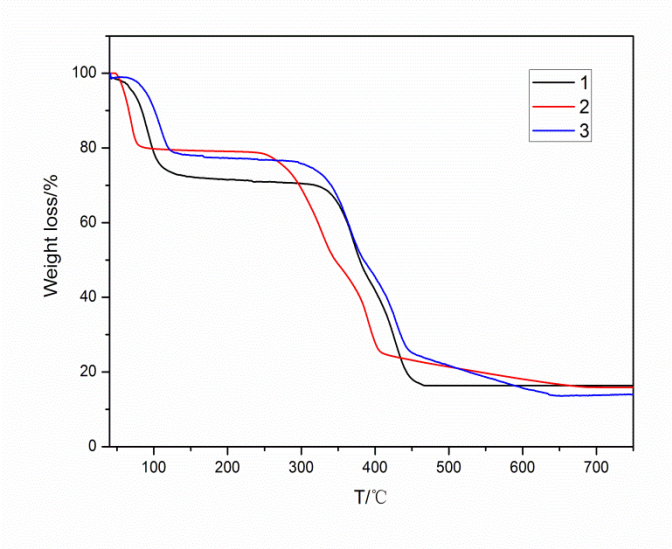

Fig. S2. TG tests of compounds **1-3**.

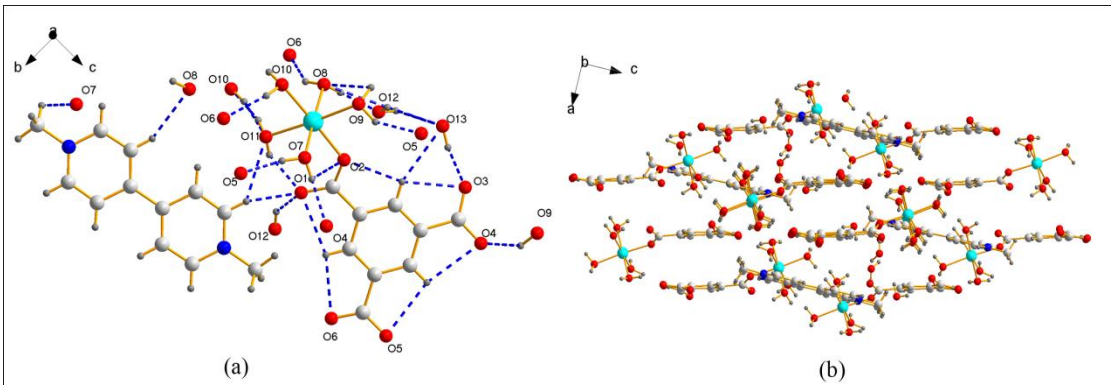

Fig. S3. For compound **1**: (a) Hydrogen bonding interactions; (b) Packing diagram.

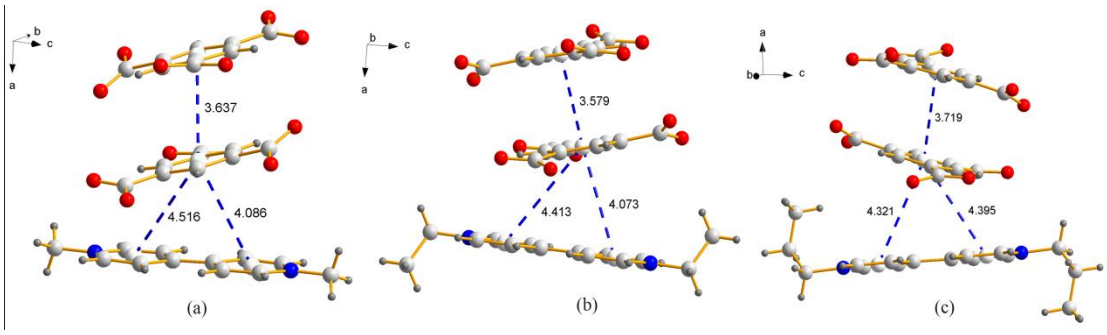

Fig. S4. The intermolecular π···π interactions for **1** (a) and **2** (b) and **3** (c).

Section S1. Kinetic rate calculations

The photochemical reactions of compounds **1**-**3** all exhibit first order kinetics which can be analyzed with eq[1]:

$$\ln\left(\frac{R_0 - R_\infty}{R_t - R_\infty}\right) = kt$$

where k is the first-order rate constant, R_0, R_t, R_∞ refer to the UV−vis diffuse reflectance intensity values (405 nm for compound **1**, 404 nm for compound **2**, 394 nm for compound **3**) at the beginning, versus time, and at the end of the reaction, respectively.

Reference

[1] J. Sworakowski, K. Janus and S. Nešpůrek, *Adv. Colloid Interface Sci.*, 2005, **116**, 97.

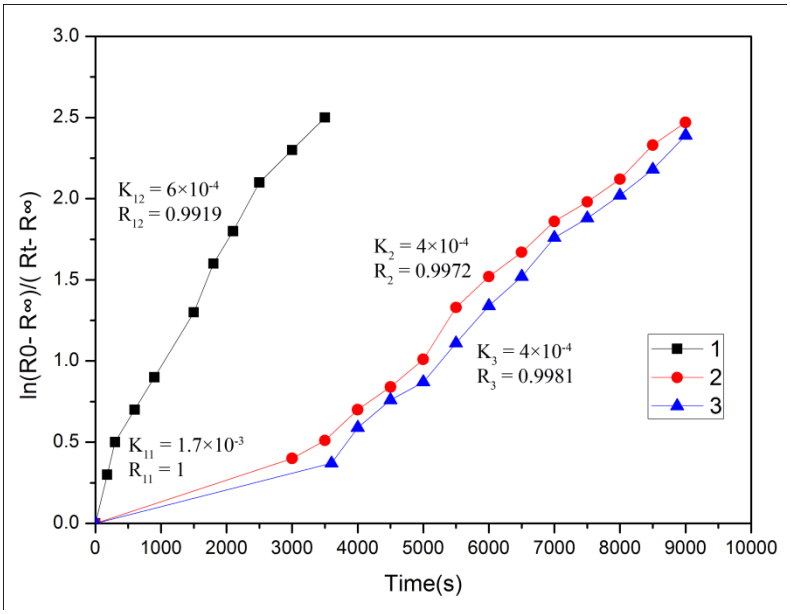

Fig. S5. Solid-state first-order photoresponsive rate plot for compounds **1**-**3**.