

Supporting Information for

Methylviologen-templated layered bimetal phosphate: a multifunctional X-ray-induced photochromic material

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Table S1. Crystal data and structure refinement for JU99 ^[a]

Empirical formula	C ₆ H ₁₂ NO ₁₄ P ₃ Zn ₃ Mn _{0.5}
Formula weight	638.66
Temperature	296(2) K
Wavelength (Å)	0.71073
Crystal system, space group	Triclinic, <i>P</i> -1
Unit cell dimensions	
<i>a</i> (Å)	9.4416(9)
<i>b</i> (Å)	9.5014(9)
<i>c</i> (Å)	9.8153(9)
<i>α</i> (deg)	107.922(2)
<i>β</i> (deg)	91.314(2)
<i>γ</i> (deg)	92.350(2)
Volume (Å ³)	836.50(14)
<i>Z</i> , calculated density (mg m ⁻³)	2, 2.536
Absorption coefficient (mm ⁻¹)	4.990
<i>F</i> (000)	629
Crystal size (mm ³)	0.250 × 0.240 × 0.220
<i>θ</i> range (°) for data collection	2.160–26.371
Limiting indices	-11 ≤ <i>h</i> ≤ 11, -11 ≤ <i>k</i> ≤ 10, -12 ≤ <i>l</i> ≤ 10
Reflections collected/unique	5367/3406, [<i>R</i> (int) = 0.0238]
Completeness to <i>θ</i> (%)	25.242, 99.8
Absorption correction	semi-empirical from equivalents
Refinement method	full-matrix least-squares on <i>F</i> ²
Data/restraints/parameters	3406/47/254
Goodness-of-fit on <i>F</i> ²	1.049
Final <i>R</i> indices [<i>I</i> > 2 <i>σ</i> (<i>I</i>)]	<i>R</i> ₁ = 0.0434, <i>wR</i> ₂ = 0.1129
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0556, <i>wR</i> ₂ = 0.1207
Largest diff. peak and hole (eÅ ⁻³)	1.189 and -0.840

^a*R*₁ = $\sum(\Delta F/\sum(F_o))$, *wR*₂ = $(\sum[w(F_o^2 - F_c^2)])/\sum[w(F_o^2)]^{1/2}$ and $w=1/[\sigma^2(F_o^2)+(0.0595P)^2+2.8937P]$ where $P=(F_o^2+2F_c^2)/3$

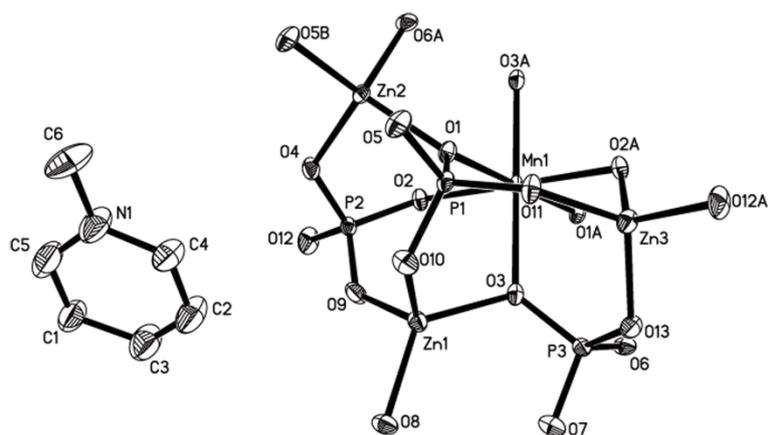


Fig. S1 Thermal ellipsoids of JU99 given at 50% probability, showing the atomic labelling scheme.

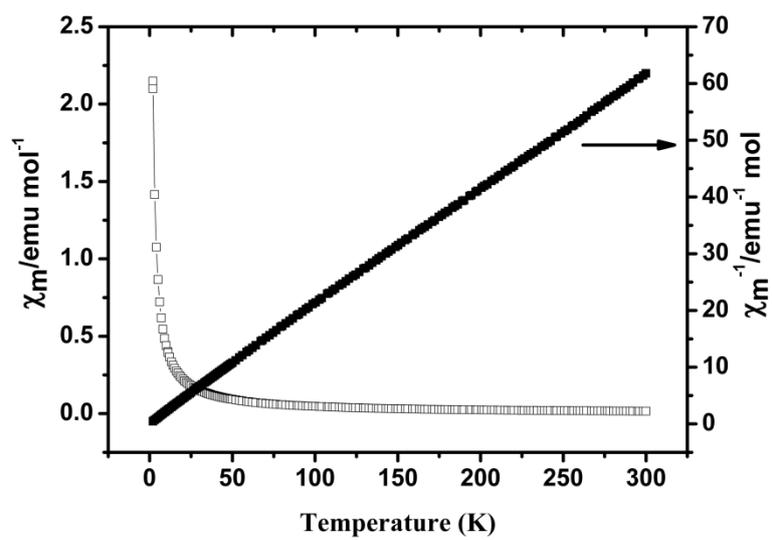


Fig. S2 Temperature dependence of χ_m and χ_m^{-1} for JU99 at 1000 Oe, suggesting that JU99 possesses paramagnetic property.

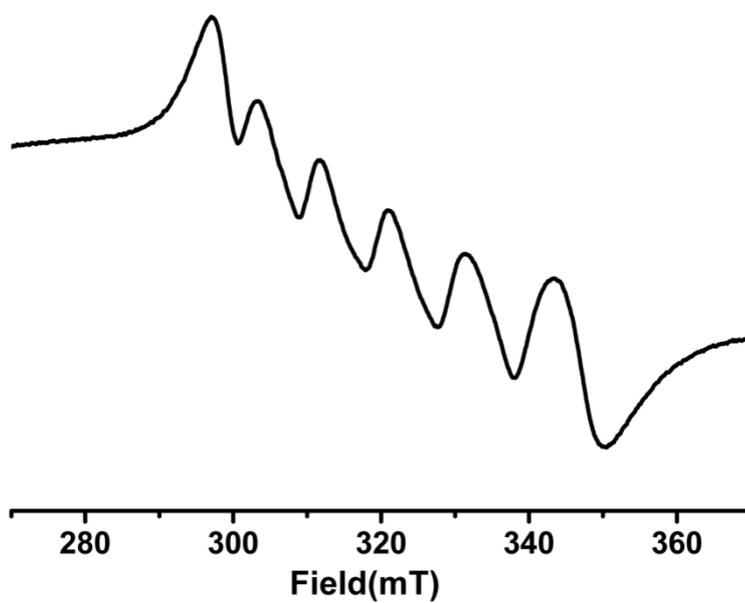


Fig. S3 EPR spectrum of JU99 at 123K, showing the characteristic six hyperfine lines with high resolution of Mn²⁺ ions.

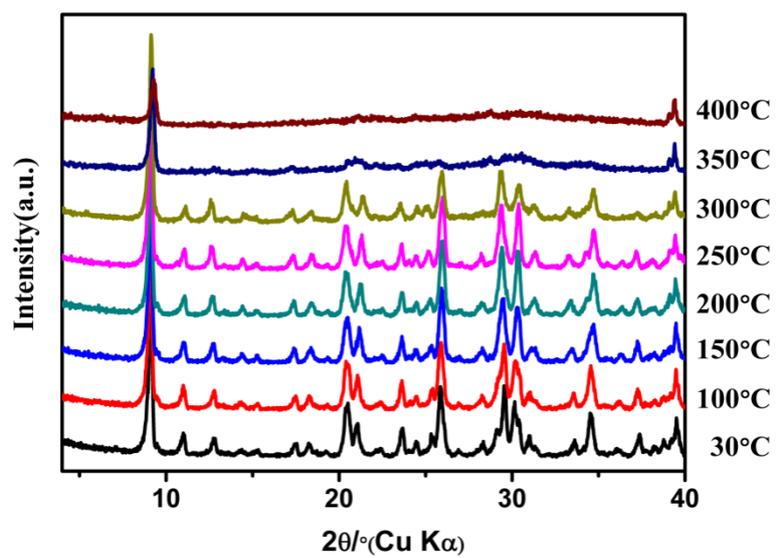


Fig. S4 HT-PXRD patterns of JU99 recorded from room temperature to 400 °C with a heating rate of 10°C min⁻¹.

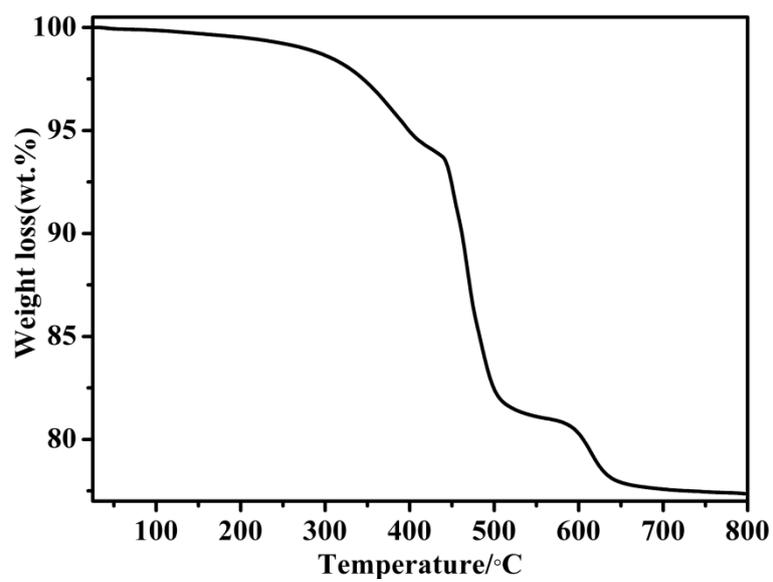


Fig. S5 TGA curve of JU99, showing two stages of weight loss of 21.84% occurring at 200-650°C, corresponding to the loss of the water molecules and the MV^{2+} cations.

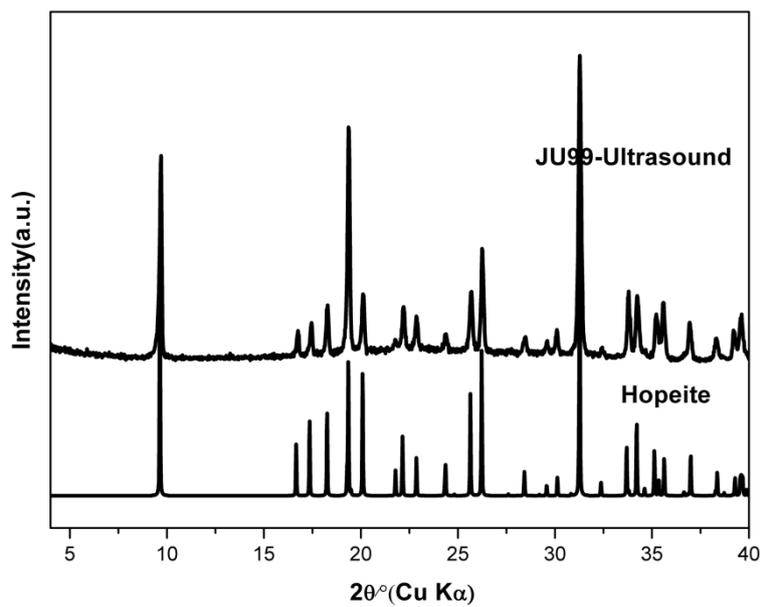


Fig. S6 PXRd pattern of JU99 after ultrasonic treatment compared with the simulated PXRd pattern of mineral Hopeite.

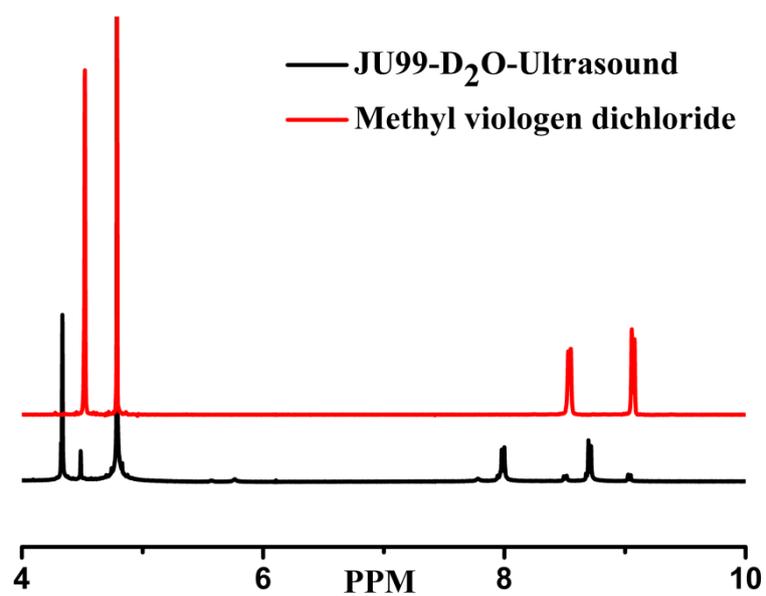


Fig. S7 ¹H MAS NMR of methylviologen dichloride and JU99 after ultrasonic treatment in D₂O.

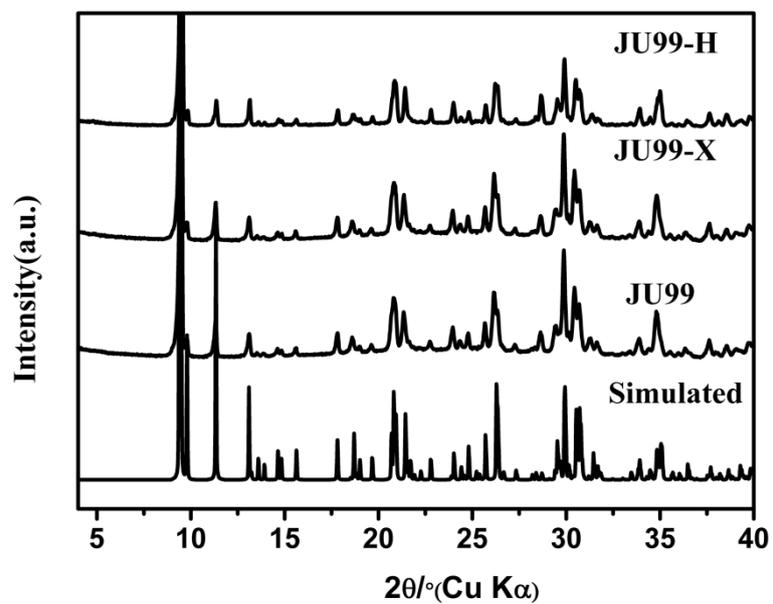


Fig. S8 Experimental and simulated PXRD patterns of JU99, X-ray irradiated JU99-X and heating treated JU99-H.

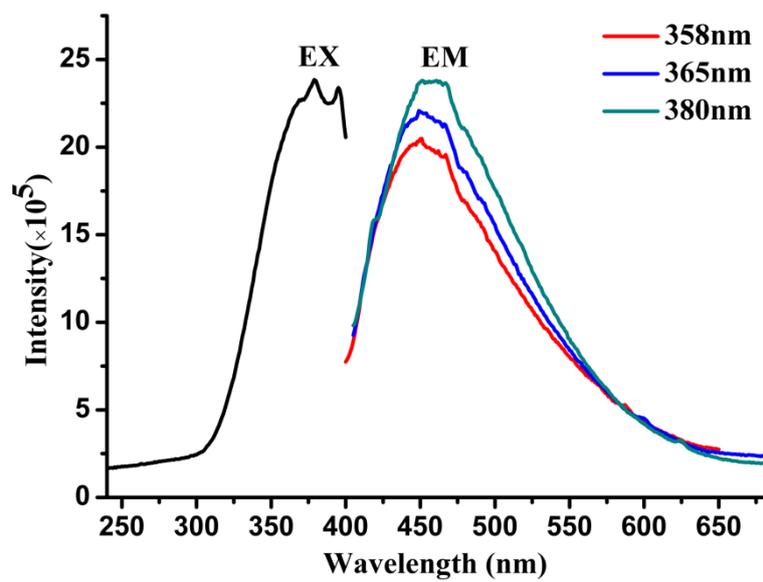


Fig. S9 The emission and excitation spectra of decolorized JU99 upon heating treatment.

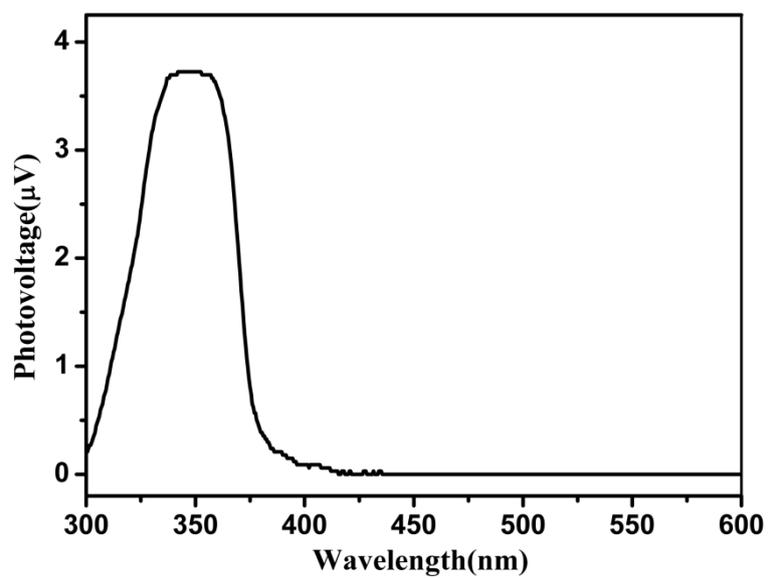


Fig. S10 SPV spectrum of decolored JU99 upon heating treatment in the absence of an external electric field.