

Supporting Information for:

Narrowing the band of green emission in manganese hybrid by reducing the hydrogen bond strength and structural distortion

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Table S1. Crystal data and structure refinement of (MDPA)₂MnBr₄ and (MTPP)₂MnBr₄.

Empirical formula	(C ₁₃ H ₁₄ N) ₂ MnBr ₄	(C ₁₉ H ₁₈ N) ₂ MnBr ₄
Formula weight	743.08	929.19
Temperature	150.0 K	
Wavelength	0.71073 Å	
Crystal system	triclinic	monoclinic
Space group	<i>P</i> 1	<i>P</i> 2 ₁
Unit cell dimensions	<i>a</i> = 8.3674(4) Å, <i>α</i> = 87.103(2)° <i>b</i> = 8.5704(4) Å, <i>β</i> = 67.081(2)° <i>c</i> = 10.6100(5) Å, <i>γ</i> = 86.628(2)°	<i>a</i> = 9.7629(6) Å, <i>α</i> = 90° <i>b</i> = 12.4204(6) Å, <i>β</i> = 105.027(2)° <i>c</i> = 16.5351(10) Å, <i>γ</i> = 90°
Volume	699.27(6) Å ³	1936.47(19) Å ³
<i>Z</i>	1	2
Density (calculated)	1.765 g/cm ³	1.594 g/cm ³
Absorption coefficient	6.203 mm ⁻¹	4.575 mm ⁻¹
<i>F</i> (000)	363	918
Crystal size	0.22×0.18×0.18 mm ³	0.15×0.15×0.12 mm ³
<i>θ</i> range for data collection	3.213 to 26.426°	2.077 to 26.394°
Index ranges	-10 ≤ <i>h</i> ≤ 10 -10 ≤ <i>k</i> ≤ 10 -13 ≤ <i>l</i> ≤ 13	-12 ≤ <i>h</i> ≤ 12 -15 ≤ <i>k</i> ≤ 15 -20 ≤ <i>l</i> ≤ 20
Reflections collected	16228	22338
Independent reflections	5619 [Rint = 0.0261]	7870 [Rint = 0.0402]
Completeness	98.1%	99.9%
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	5619/3/289	7870/1/408
Goodness-of-fit	1.054	0.910
Flack factor	0.043(13)	0.013(6)
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> _{obs} = 0.0302, <i>wR</i> _{obs} = 0.0727	<i>R</i> _{obs} = 0.0320, <i>wR</i> _{obs} = 0.0517
<i>R</i> indices [all data]	<i>R</i> _{all} = 0.0341, <i>wR</i> _{all} = 0.0740	<i>R</i> _{all} = 0.0507, <i>wR</i> _{all} = 0.0563
Largest diff. peak and hole	0.708 and -0.413 e·Å ⁻³	0.320 and -0.267 e·Å ⁻³

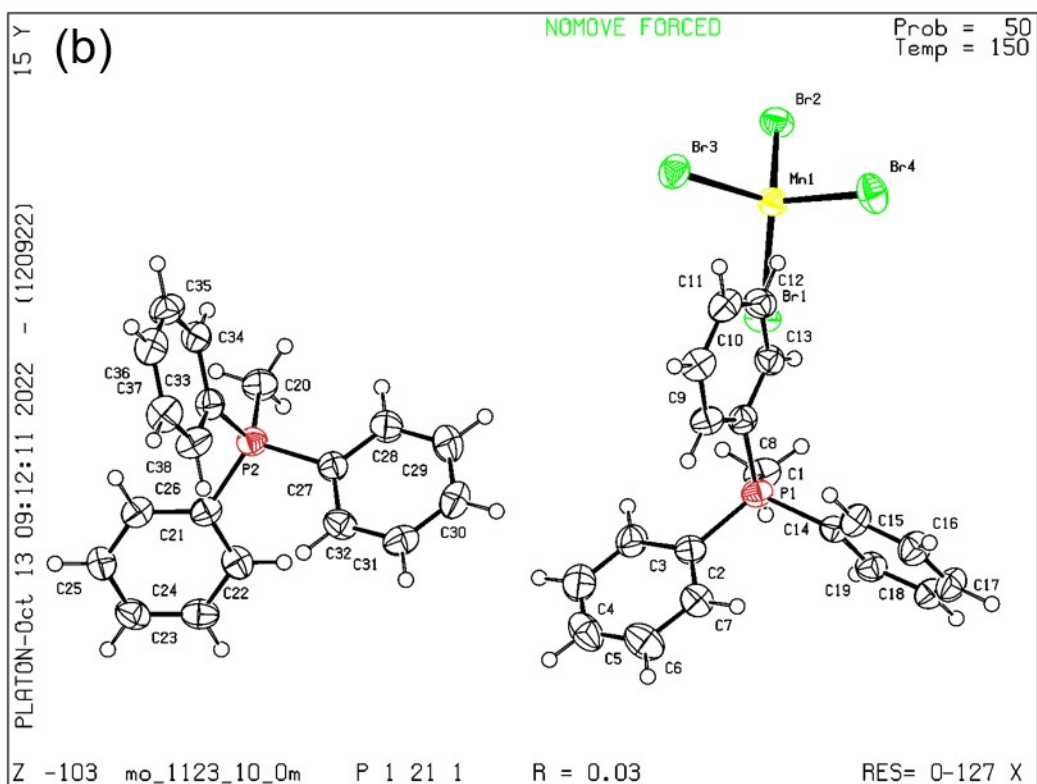
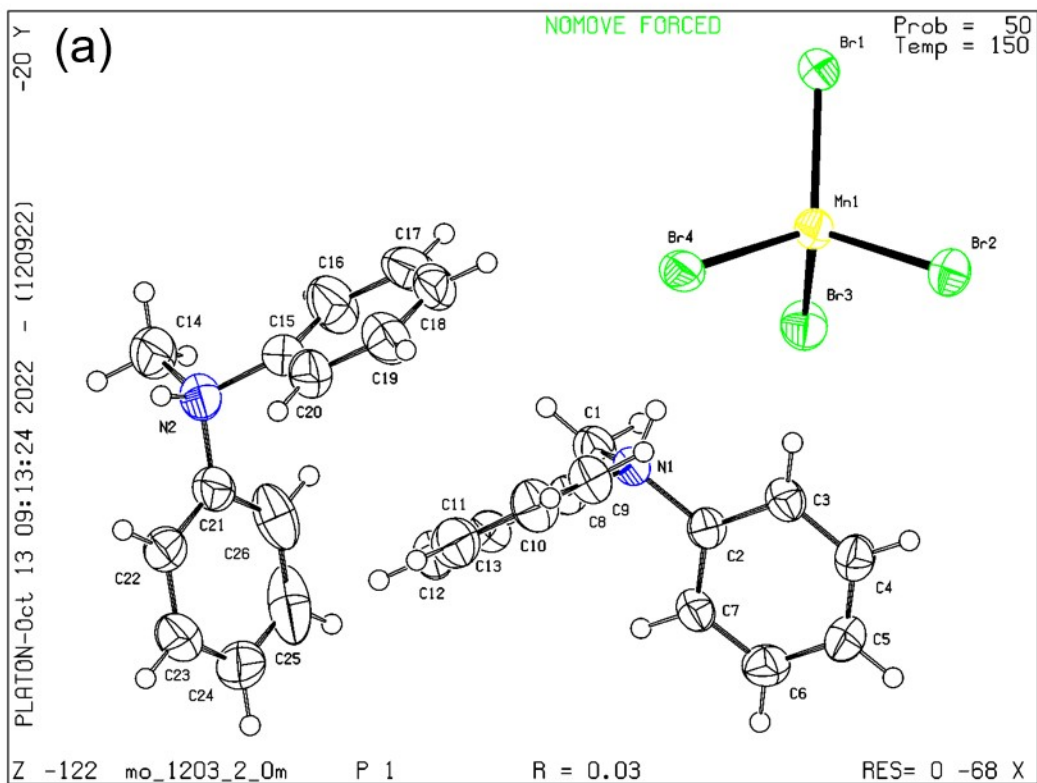


Figure S1. Oak Ridge thermal ellipsoid plots (ORTEP) for (a) $(\text{MDPA})_2\text{MnBr}_4$ and (b) $(\text{MTPP})_2\text{MnBr}_4$.

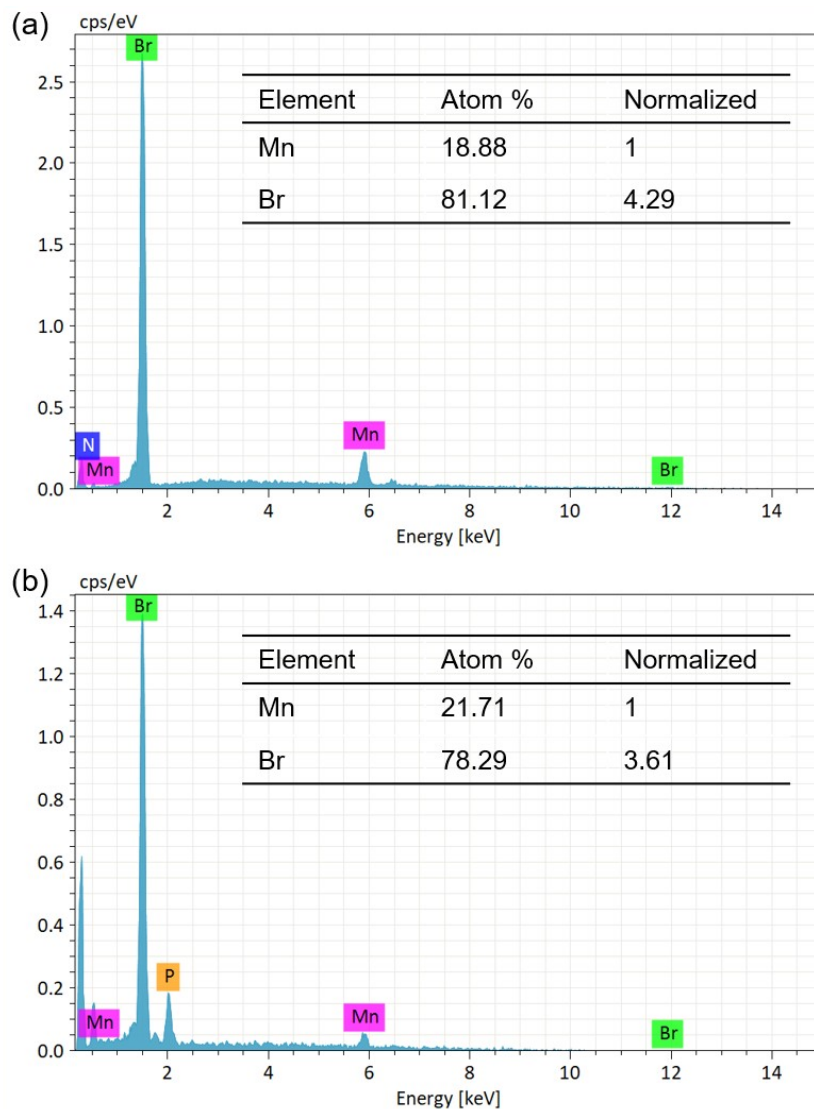


Figure S2. Element analysis results via EDS for (a) $(\text{MDPA})_2\text{MnBr}_4$ and (b) $(\text{MTPP})_2\text{MnBr}_4$.

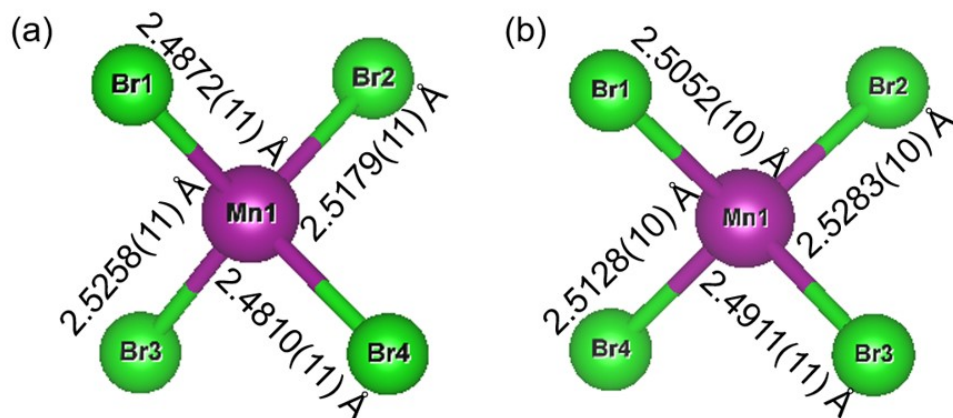


Figure S3. Mn-Br bond lengths of $[\text{MnBr}_4]^{2-}$ in (a) $(\text{MDPA})_2\text{MnBr}_4$ and (b) $(\text{MTPP})_2\text{MnBr}_4$.

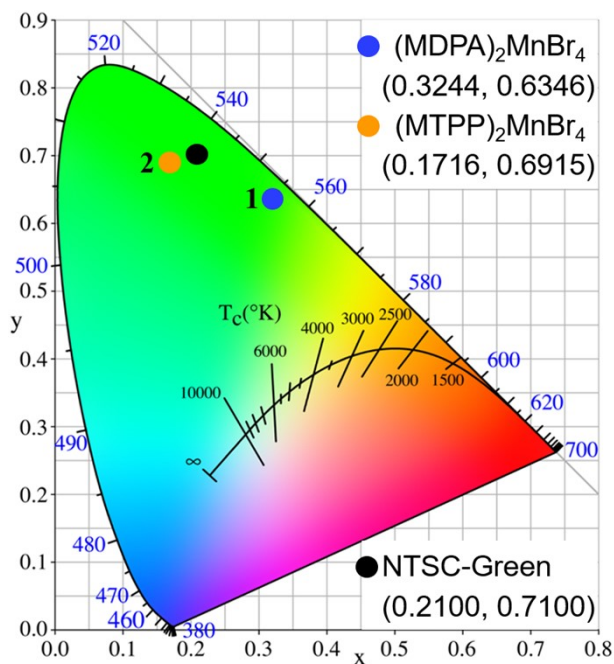


Figure S4. The coordinates of $(\text{MDPA})_2\text{MnBr}_4$, $(\text{MTPP})_2\text{MnBr}_4$ and NTSC-green standard in CIE 1931 system.

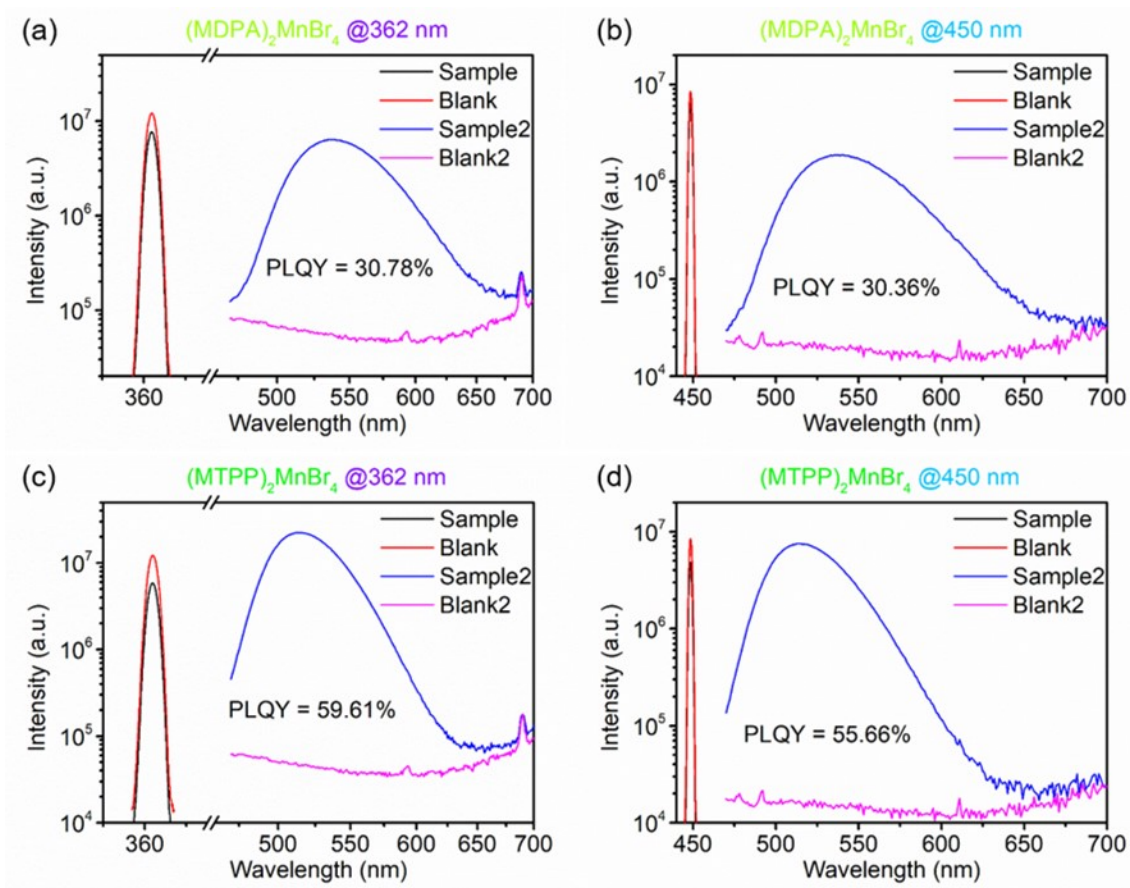


Figure S5. PLQY experimental data of (a) (b) $(\text{MDPA})_2\text{MnBr}_4$, and (c) (d) $(\text{MTPP})_2\text{MnBr}_4$.

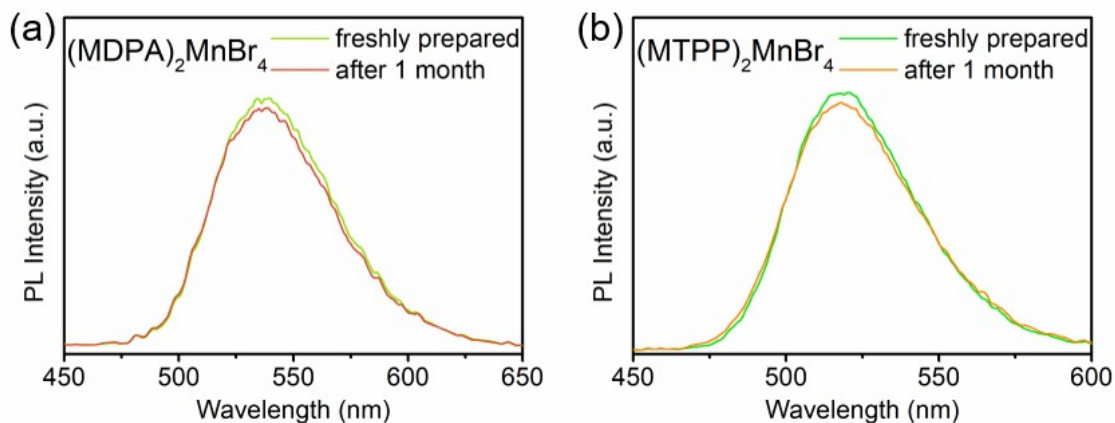


Figure S6. Comparison of the PL spectra of the as-prepared **1** (a) and **2** (b) and the ones of samples exposed in the air for 1 month.

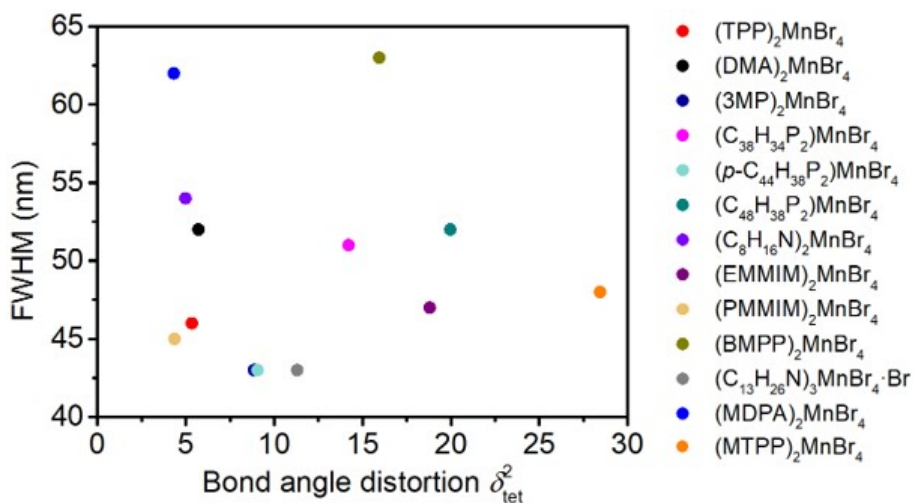


Figure S7. Relationship between the fwhm values and the bond angle distortion degree (δ_{tet}^2) in 0D Mn(II) tetrabromide hybrids.

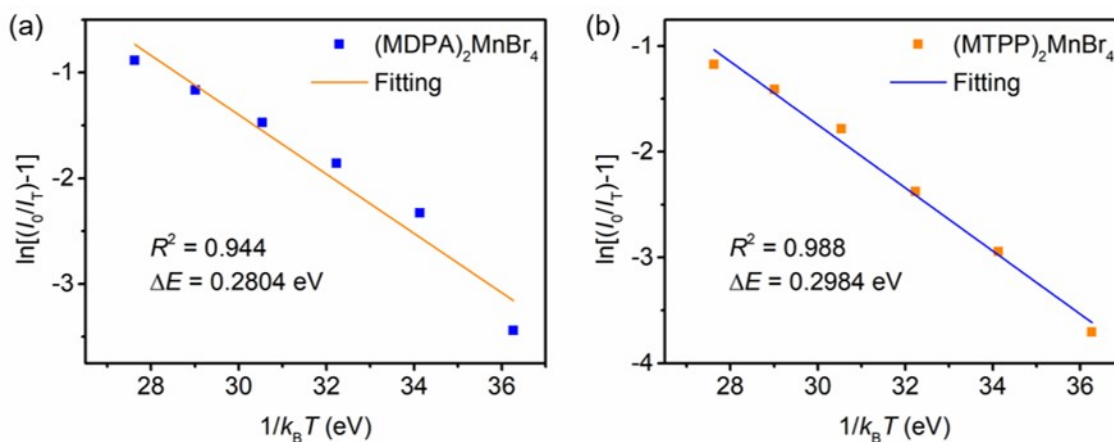


Figure S8. The thermal activation energy ΔE of (a) $(\text{MDPA})_2\text{MnBr}_4$ and (b) $(\text{MTPP})_2\text{MnBr}_4$ analyzed by using the Arrhenius equation.

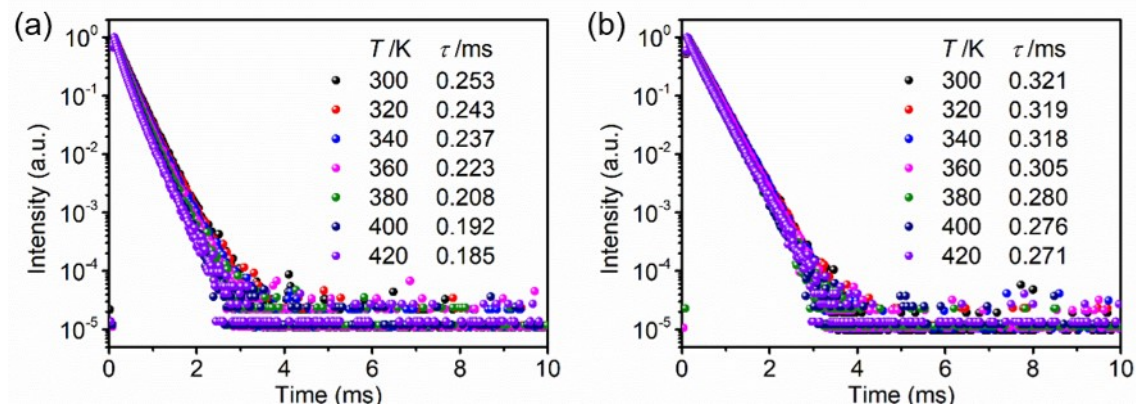


Figure S9. Temperature-dependent PL decay curves and lifetimes of (a) $(\text{MDPA})_2\text{MnBr}_4$ and (b) $(\text{MTPP})_2\text{MnBr}_4$.

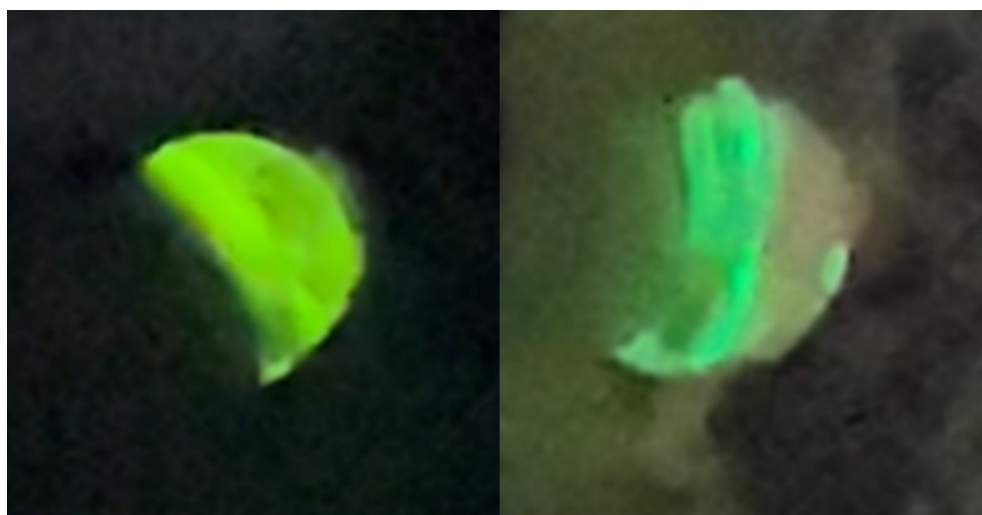


Figure S10. Photographs of the TL light captured from crystals of $(\text{MDPA})_2\text{MnBr}_4$ (left) and $(\text{MTPP})_2\text{MnBr}_4$ (right) upon grinding with a glass rod at ambient conditions.