Supporting Information

The Red Light Emission in 2D (C₄SH₃CH₂NH₃)₂SnI₄ and (C₄OH₇CH₂NH₃)₂SnI₄ Perovskites

Mi-Hee Jung*,[†]

Department of Nanotechnology and Advanced Materials Engineering, Sejong University, 209, Neungdong-ro, Gwangjin-gu, Seoul 05006, Republic of Korea; Fax: +82-2-3408-4342; Tel: +82-2-6935-2597

*To whom correspondence should be addressed.

E-mail: mhjung@sejong.ac.kr

No.	Component	Result	Unit	Detection limit	Elemental line	Intensity
1	С	11.8588	mass%	0.10757	C-KA	19.6850
2	S	9.2842	mass%	0.00368	S-KA	144.2332
3	Cl	0.4592	mass%	0.00909	Cl-KA	1.5698
4	Sn	13.3760	mass%	0.06005	Sn-KA	23.6686
5	Ι	65.0218	mass%	0.22799	I-KB1	84.3837

Table S1. Elemental analysis of the (TPM)2SnI4 perovskite performed by X-ray fluorescence spectroscopy

No.	Component	Result	Unit	Detection limit	Elemental line	Intensity
1	С	7.4117	mass%	0.05228	C-KA	25.1218
2	Cl	0.0683	mass%	0.00856	Cl-KA	0.2706
3	Sn	11.2432	mass%	0.06599	Sn-KA	19.8557
4	Ι	81.2768	mass%	0.25079	I -KB1	105.8344

Table S2. Elemental analysis of the $(TFF)_2SnI_4$ perovskite performed by X-ray fluorescence spectroscopy

Empirical formula	(TPM) ₂ SnI ₄	(TFF) ₂ SnI ₄		
Formula weight	854.66	830.60		
Temperature (K)	298	298		
Wavelength (Å)	0.700	0.700		
Crystal system	Orthorhombic	Monoclinic		
Space group	Pbca	$P2_1/c$		
Unit cell dimensions				
a, A b Å	8.7730(18)	16.341(5) 8.8044(17)		
c. Å	28 961(6)	8.7912(17)		
α, deg	90°	90°		
β, deg	90°	91.19(2)°		
γ, deg	90°	90°		
Volume(Å ³)	2199.8(8)	1264.6(5)		
Z	4	2		
Density (calculated)(Mg/m ³)	2.581	2.181		
Absorption coefficient(mm ⁻¹)	6.589	5.894		
F(000)	1536	752		
Crystal size(mm ³)	$0.570 \times 0.073 \times 0.033$	$0.670\times0.047\times0.036$		
Theta range for data collection	2.674 to 33.555°	2.628 to 30.550°		
Index ranges	$-12 \le h \le 12,$ $-11 \le k \le 11,$ $-42 \le 1 \le 42$	$-22 \le h \le 22$ $-12 \le k \le 11$ $-11 \le l \le 12$		
Reflections collected	22122	15559		
Independent reflections	3767 [R(int) = 0.1093]	3368 [R(int) = 0.1213]		
Completeness to theta = 25.242°	97.3 %	99.9 %		
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²		
Data/restraints/ parameters	3767 / 6 / 89	3368 / 45 / 88		
Goodness-of-fit on F ²	1.208	1.159		
Final R indices	R1 = 0.1587,	R1 = 0.1630,		
[I > 2sigma(I)]	wR2 = 0.2828	wR2 = 0.3832		
R indices (all data)	R1 = 0.1694, wR2 = 0.2910	R1 = 0.1/44, wR2 = 0.3905		
Absolute structure parameter				
Extinction coefficient	0.175(11)			
Largest diff. peak and hole (e Å ⁻³)	4.710 and -9.534	12.193 and -3.889		

Table S3. Crystallographic data for (TPM)₂SnI₄ and (TFF)₂SnI₄ perovskites prepared from SnO



Figure S1. Photoluminescence spectra for the crystals of $(TPM)_2SnI_4$ and $(TFF)_2SnI_4$ perovskites prepared from SnO. The excitation wavelength is 514 nm.



Figure S2. Configuration coordinate diagram for free excition and bound exciton state for the compound $(TPM)_2SnI_4$



Figure S3. Comparison of the PXRD patterns for the as made $(TPM)_2SnI_4$ and $(TFF)_2SnI_4$ perovskites crystals and the ones after storage in air for 4 days.