

## Supporting Information

# Synthesis, Crystal Structure and White Luminescence of Zero-Dimensional Organic-Inorganic Zinc Halides

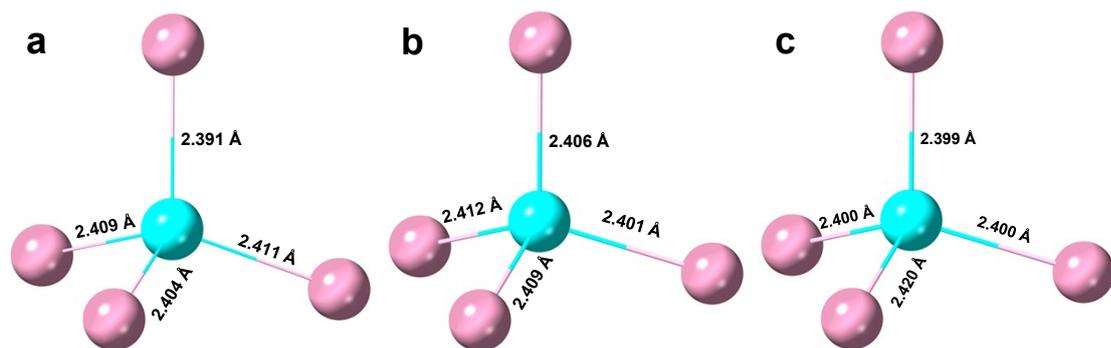
Qian Chen<sup>1</sup>, Fangxu Dai<sup>1</sup>, Kai Zhang<sup>1</sup>, Hong Zhou<sup>1</sup>, Mingming Zhang<sup>1\*</sup>, Dong Quan<sup>2</sup>, Lei Wang<sup>1,3</sup>, Jun Xing<sup>1\*</sup>

<sup>1</sup>Key Laboratory of Eco-chemical Engineering, Ministry of Education, College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, P. R. China.

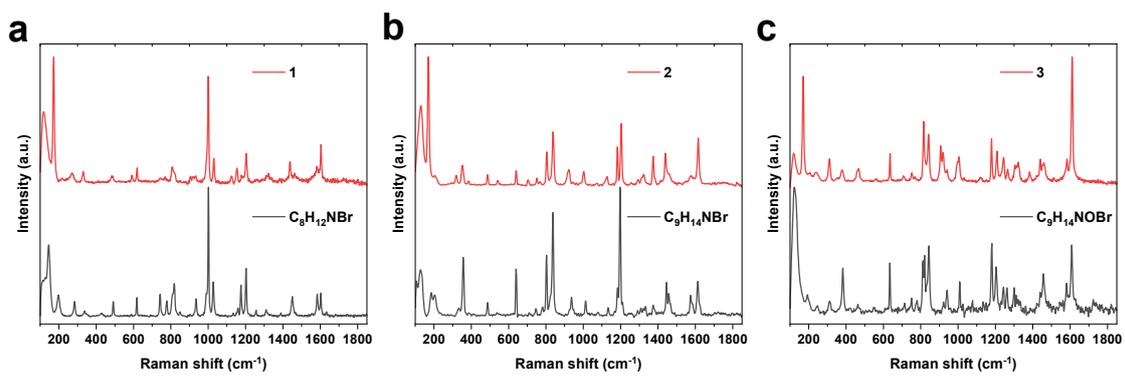
<sup>2</sup>School of Materials Science and Engineering, Shandong University, Jinan 250100, P. R. China.

<sup>3</sup>College of Environment and Safety Engineering, Qingdao University of Science and Technology, Shandong Engineering Research Center for Marine Environment Corrosion and Safety Protection, Qingdao 266042, P. R. China.

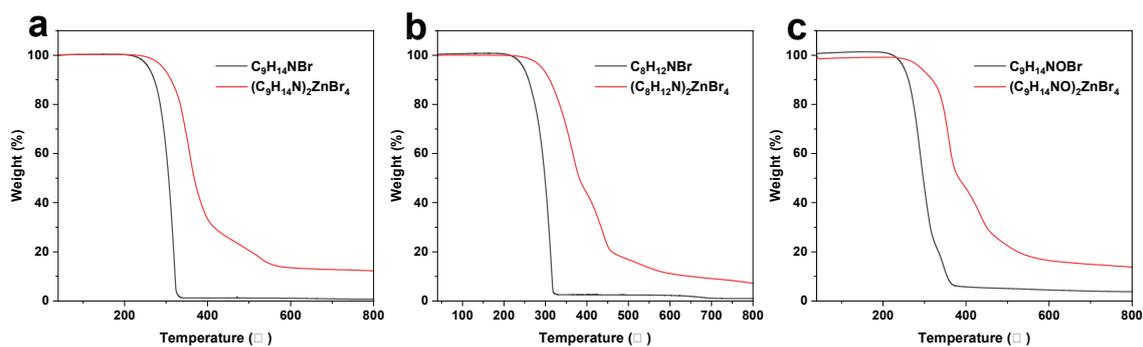
\*Correspondence: [zmm@qust.edu.cn](mailto:zmm@qust.edu.cn) (M.Z.) and [xingjun@qust.edu.cn](mailto:xingjun@qust.edu.cn) (J.X.)



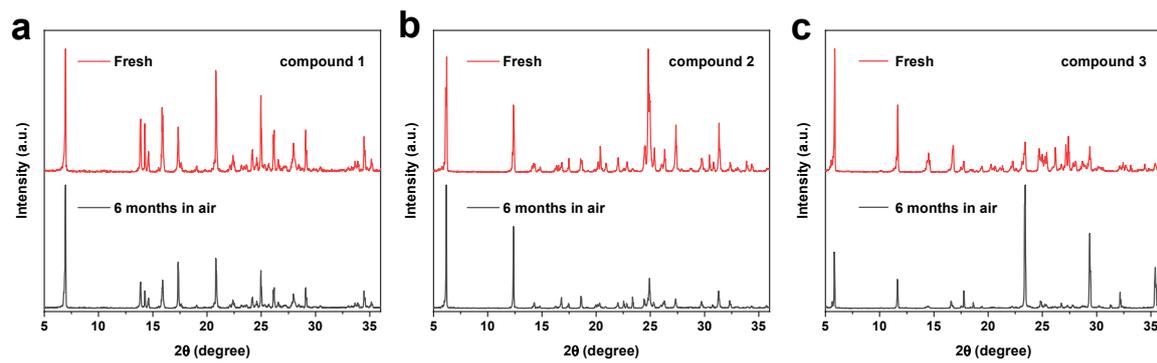
**Figure S1.** The Zn-Br bond length in crystals **1** (a), **2** (b), and **3** (c).



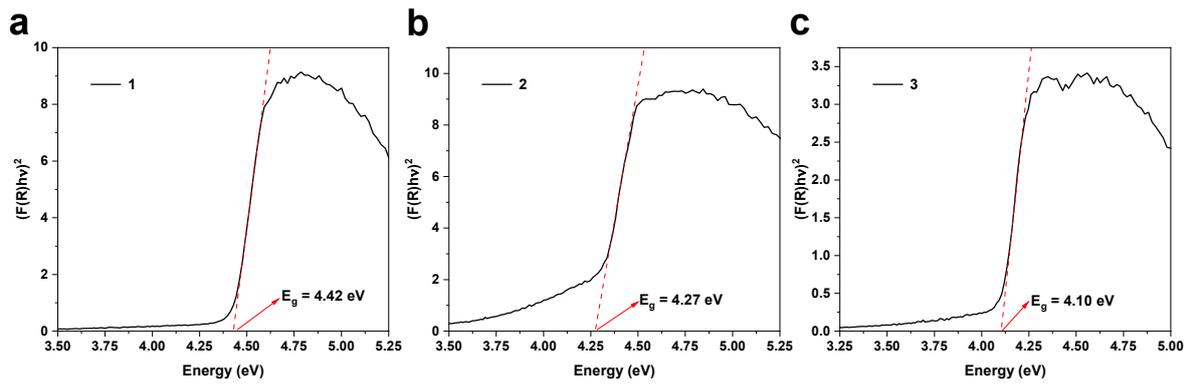
**Figure S2.** The Raman spectra of **1** and  $\text{C}_8\text{H}_{12}\text{NBr}$  (a), **2** and  $\text{C}_9\text{H}_{14}\text{NBr}$  (b), and **3** and  $\text{C}_9\text{H}_{14}\text{NOBr}$  (c).



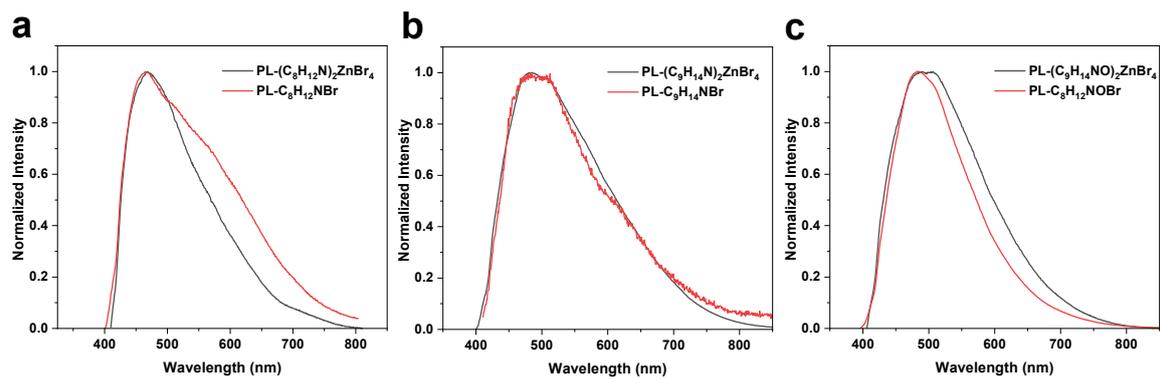
**Figure S3.** TG curves of compounds **1** (a), **2** (b), and **3** (c) with the corresponding organic ammonium.



**Figure S4.** PXRD patterns of **1** (a), **2** (b), and **3** (c) stored 6 months in air.



**Figure S5.** Tauc plots of **1** (a), **2** (b), and **3** (c) for the case of direct bandgaps.



**Figure S6.** PL spectra of **1** and C<sub>8</sub>H<sub>12</sub>NBr (a), **2** and C<sub>9</sub>H<sub>14</sub>NBr (b), and **3** and C<sub>9</sub>H<sub>14</sub>NOBr (c).

**Table S1.** Fitting parameters for the PL decay curves using a two-exponential decay model of  $(\text{C}_8\text{H}_{12}\text{N})_2\text{ZnBr}_4$  at different emission wavelengths.

Wavelength (nm)	$\tau_1$ (ns)	$A_1$	$\tau_2$ (ns)	$A_2$
440	2.90	0.34	0.31	4488.63
460	3.16	0.36	0.35	1703.58
500	3.51	0.25	0.31	5391.08

**Table S2.** Fitting parameters for the PL decay curves using a two-exponential decay model of  $(\text{C}_9\text{H}_{14}\text{N})_2\text{ZnBr}_4$  at different emission wavelengths.

Wavelength (nm)	$\tau_1$ (ns)	$A_1$	$\tau_2$ (ns)	$A_2$
440	0.37	1401.98	3.16	0.32
460	0.50	180.92	3.47	0.50
500	0.39	898.32	3.54	0.36

**Table S3.** Fitting parameters for the PL decay curves using a two-exponential decay model of  $(\text{C}_9\text{H}_{14}\text{NO})_2\text{ZnBr}_4$  at different emission wavelengths.

Wavelength (nm)	$\tau_1$ (ns)	$A_1$	$\tau_2$ (ns)	$A_2$
440	0.30	6888.29	3.11	0.26
460	0.33	2772.65	3.27	0.32
500	0.29	8260.31	3.34	0.28