Ultra Broadband Yellow Emitting Lead-Free Metal Halide Perovskite like Compound with Near-Unity Emission Quantum Yield

Sayed Ali Khan[1,2*], Noor Zamin Khan[3], Jahangeer Ahmed[4], Marcin Runowski[6], Saad M Alshehri[4], Simeon Agathopoulos[5], Simon J. Teat[7], Jing Li[2,1*]

[1]Hoffmann Institute of Advanced Materials, Shenzhen Polytechnic University, Liuxian Blvd, Nanshan District, Shenzhen, 5018055, P.R. China

[2]Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, New Jersey 08854, United States

[3]School of Physics and Material Sciences, Guangzhou University, Guangzhou 510006, China

[4]Department of Chemistry, Collage of Science, King Saud University, Riyadh 11451, Saudi Arabia

[5]Department of Materials Science and Engineering, University of Ioannina, GR-451 10 Ioannina, Greece

[6]Adam Mickiewicz University, Faculty of Chemistry, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland

[7]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

*Corresponding author: Jing Li

Email: jingli@rutgers.edu

**Corresponding author: Sayed Ali Khan

Email: sayedali@szu.edu.cn

Table S1: The fundamental bond length (Å) of BCNCI single crystals

Cu1-I1	2.5285	Na1-C15	3.1266
Cu1-I2	2.5810	Na1-C24	3.040
Cu1-I3	2.5344	Na1-C25	3.080
Cu2-I1	2.5884	Na1-C28	3.113
Cu2-I2	2.5178	O1-C6	1.361
Cu2-I3	2.5738	O1-C7	1.431
Cu3-I1	2.5650	O2-C8	1.405
Cu3-I2	2.5786	O2-C9	1.432
Cu3-I3	2.6162	O3-C10	1.418
Cu4-I1	2.5599	O3-C11	1.426
Cu4-I2	2.5933	O4-C12	1.415
Cu4-I3	2.5443	O4-C13	1.411
Na1-O6	2.2097	O5-C1	1.3682
Na1-O7	2.3549	O5-C14	1.423
Na1-O8	2.3406	O7-C24	1.430
Na1-O9	2.333	C7-C25	1.428
Na1-O10	2.3845	O8-C26	1.423
Na1-O11	2.3188	O8-C27	1.422
		O9-C28	1.434
		O10-C20	1.3664
		O10-C21	1.432
		O11-C22	1.438
		O11-C23	1.415

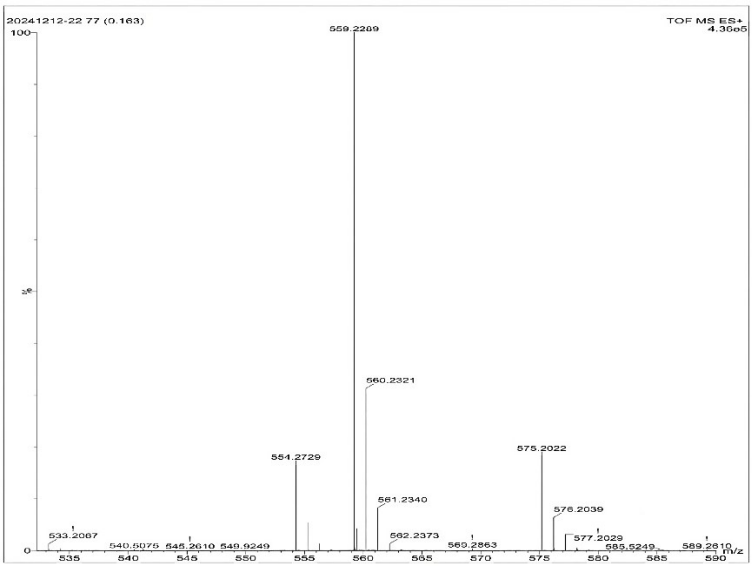

Figure S1: The measure of mass of the synthesized compound which confirms the peak of the legends Benzo-15-crown-5 or $[C_{14}H_{20}O_5)_2]$ mass.

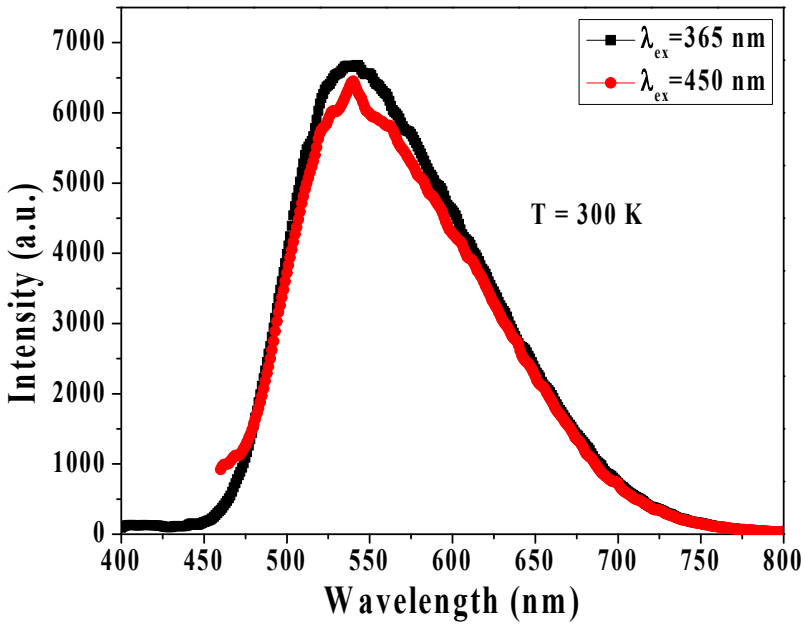

Figure S2: Room temperature (RT) photoluminescence emission of the synthesized (benzo-15-crown-5)$_2$NaH$_2$OCu$_4$I$_6$ crystals under 365 nm (UV) and 450 nm (blue) light irradiation.

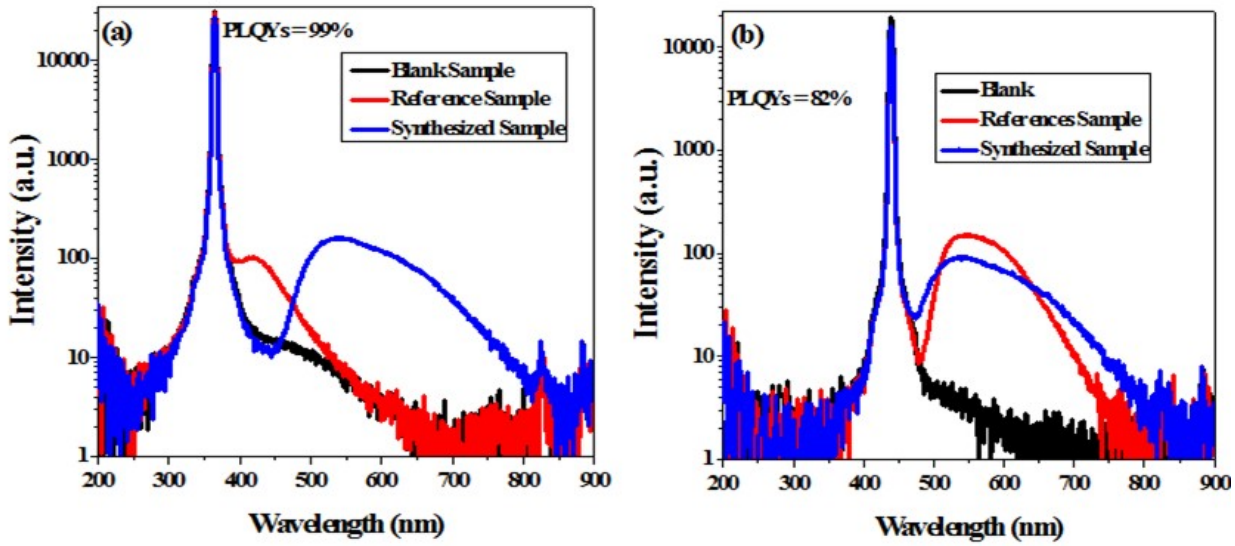

Figure S3: Emission spectra used to calculate the PLQYs of the synthesized (benzo-15-crown-5)$_2$NaH$_2$OCu$_4$I$_6$ halides (a) under 365 nm excitation, and (b) under 450 nm excitation respectively.

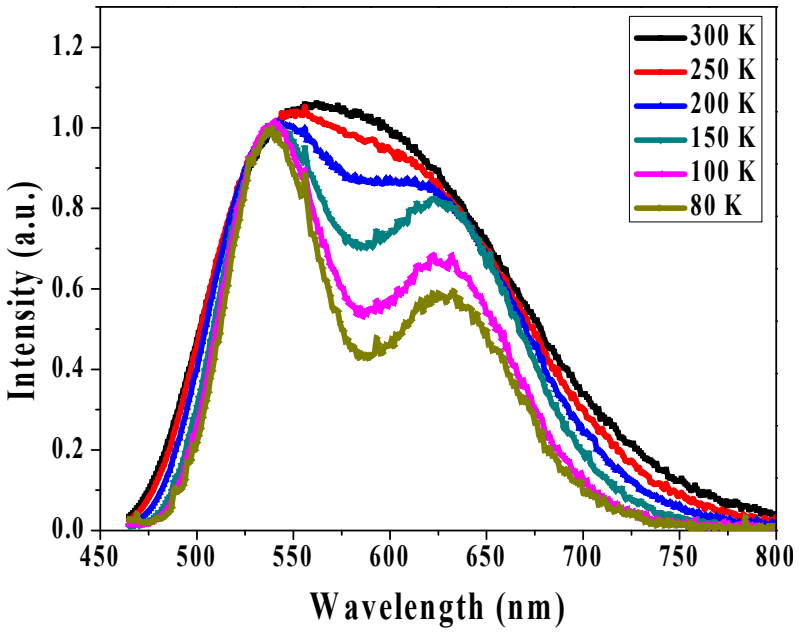

Figure S4: Temperature dependent photoluminescence (300 K, 250, 200, 150, 100 and 80K) under 450 nm blue light irradiation.