

Electronic Supporting Information

**Three-dimensional all-inorganic dual halogen emitter $\text{Cs}_2\text{Cd}_2\text{BrCl}_5$
exhibiting broadband white light emission**

Haiping Xu^{†,a} Xuehua Dong^{†,a} Zhizhuan Zhang,^a Ling Huang,^b Hongmei Zeng,^a Zhien Lin,^a and Guohong Zou^{*a}

^a College of Chemistry, Sichuan University, Chengdu 610064, P. R. China

^b College of Chemistry and Materials Science, Sichuan Normal University, Chengdu 610066, P. R. China

[+] These authors contributed equally to this work

E-mail: zough@scu.edu.cn

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $\text{Cs}_2\text{Cd}_2\text{BrCl}_5$. $U_{(\text{eq})}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U_{eq} (\AA^2)
Cd1	0.3333	0.6667	0.11709 (6)	0.0170 (3)
Br1	0.16959 (14)	0.3392 (3)	0.2500	0.0279 (5)
Cl1	0.16959 (14)	0.3392 (3)	0.2500	0.0279 (5)
Cl2	0.0000	0.5000	0.0000	0.0283 (6)
Cs1	0.6667	0.3333	0.2500	0.0303 (4)
Cs2	0.0000	0.0000	0.0000	0.0367 (4)

Table S2. Selected bond lengths (\AA) and angles (deg) for $\text{Cs}_2\text{Cd}_2\text{BrCl}_5$.

Cd1—Cl2	2.6046 (4)	Cd1—Br1	2.6912 (15)
Cd1—Cl1 ⁱⁱ	2.6912 (15)	Cl2—Cs1 ^{viii}	3.7993 (1)
Cd1—Cl2 ⁱⁱ	2.6046 (4)	Cs1—Cl1 ^{ix}	3.7287
Cd1—Cl1 ⁱⁱⁱ	2.6912 (15)	Cs1—Br1 ^{ix}	3.7287
Cd1—Br1 ⁱⁱⁱ	2.6912 (15)	Cs1—Br1 ^x	3.7287
Cl2—Cd1—Cl2 ⁱ	91.41 (2)	Br1 ^x —Cs1—Br1 ^{xi}	120.0
Cl2—Cd1—Cl2 ⁱⁱ	91.41 (2)	Cl1 ^{xi} —Cs1—Br1 ^{xi}	0.0
Cl2 ⁱⁱ —Cd1—Cl1 ⁱⁱⁱ	176.06 (4)	Br1 ^x —Cs1—Cl1 ^{xii}	58.84 (6)
Cl2—Cd1—Br1 ⁱⁱⁱ	91.340 (17)	Cl1 ^{xi} —Cs1—Cl1 ^{xii}	178.84 (6)
Br1 ⁱⁱⁱ —Cd1—Br1 ⁱⁱ	85.78 (4)	Cl2—Cd1—Cd1 ⁱⁱⁱ	124.261 (14)
Cl1 ⁱⁱ —Cd1—Br1 ⁱⁱ	0.00 (5)	Cl2 ⁱ —Cd1—Cd1 ⁱⁱⁱ	124.261 (14)
Cl2—Cd1—Br1	91.340 (17)	Cl2 ⁱⁱ —Cd1—Cd1 ⁱⁱⁱ	124.260 (14)
Cl2 ⁱ —Cd1—Br1	176.06 (4)	Cl1 ⁱⁱⁱ —Cd1—Cd1 ⁱⁱⁱ	51.80 (3)
Cs2 ^{iv} —Cd1—Br1—Cs1	-177.611 (18)	Cs2 ^{vi} —Br1—Cs1—Cl1 ⁱⁱ	-124.98 (2)
Cs2—Cd1—Br1—Cs1	89.641 (18)	Cd1 ⁱⁱⁱ —Br1—Cs1—Br1 ⁱⁱ	-38.20 (3)
Cl2—Cd1—Br1—Cs1 ^v	-43.92 (2)	Cd1—Br1—Cs1—Br1 ⁱⁱ	38.20 (3)
Cl1 ⁱⁱ —Cd1—Br1—Cs2 ^{vi}	43.033 (17)	Cd1—Cl2—Cs2—Cl2 ^{xvi}	0.0
Br1 ⁱⁱ —Cd1—Br1—Cs2 ^{vi}	43.033 (17)	Cd1 ^{vii} —Cl2—Cs2—Cl2 ^{xvi}	0.0
Cd1 ⁱⁱⁱ —Cd1—Br1—Cs2 ^{vi}	0.0	Cs2 ^{iv} —Cl2—Cs2—Cl2 ^{xvi}	0.0
Br1 ⁱⁱ —Cd1—Cl2—Cd1 ^{vii}	106 (10)	Cd1—Cl2—Cs2—Cl1 ^{xvii}	-143.54 (2)
Br1—Cd1—Cl2—Cd1 ^{vii}	149 (10)	Cd1 ^{vii} —Cl2—Cs2—Cl1 ^{xvii}	36.46 (2)
Cl2 ⁱ —Cd1—Cl2—Cs1 ^v	-134.276 (11)	Cs1 ^v —Br1—Cs2—Cl2 ⁱⁱ	125.65 (3)

Symmetry codes: (i) $-x+y, -x+1, z$; (ii) $-y+1, x-y+1, z$; (iii) $-x+y, -x+1, -z+1/2$; (iv) $x, y+1, z$; (v) $x-1, y, z$; (vi) $x-y, x, z+1/2$; (vii) $-x, -y+1, -z$; (viii) $-x+1, -y+1, -z$; (ix) $-y+1, x-y, z$; (x) $x+1, y, z$; (xi) $-x+y, -x, -z+1/2$; (xii) $-x+y+1, -x+1, -z+1/2$; (xiii) $-y, x-y, z$; (xiv) $-x+y, -x, z$; (xv) $-x+y-1, -x, z$; (xvi) $x, y-1, z$; (xvii) $-x, -y, -z$; (xviii) $x-y, x, z-1$

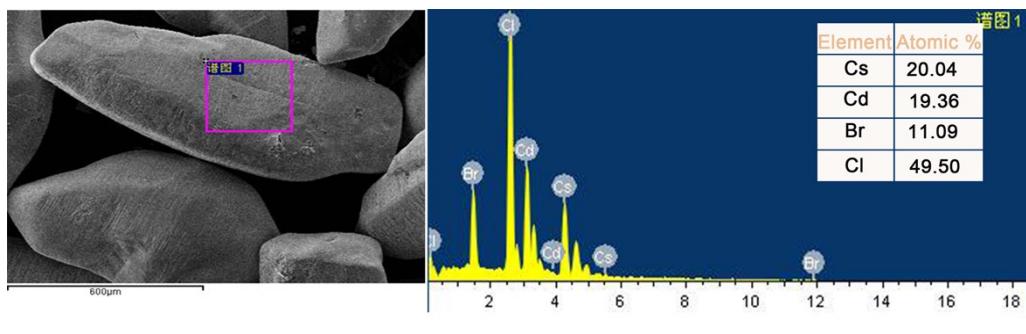


Fig. S1. The energy-dispersive (EDS) analysis for $\text{Cs}_2\text{Cd}_2\text{BrCl}_5$.

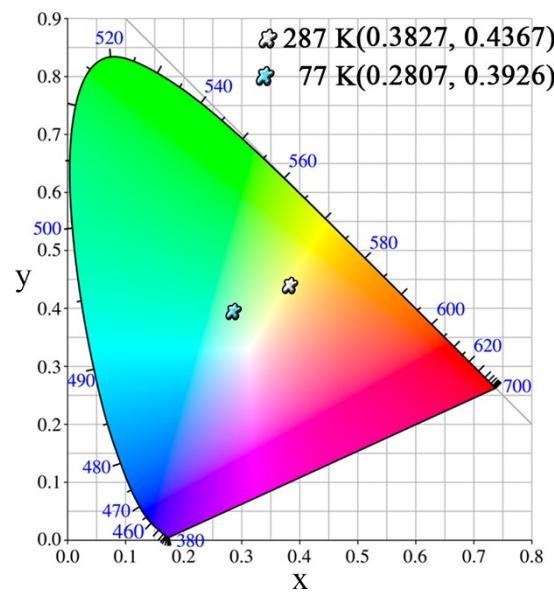


Fig. S2. The CIE chromaticity coordinates of $\text{Cs}_2\text{Cd}_2\text{BrCl}_5$ at 287 K and 77 K.

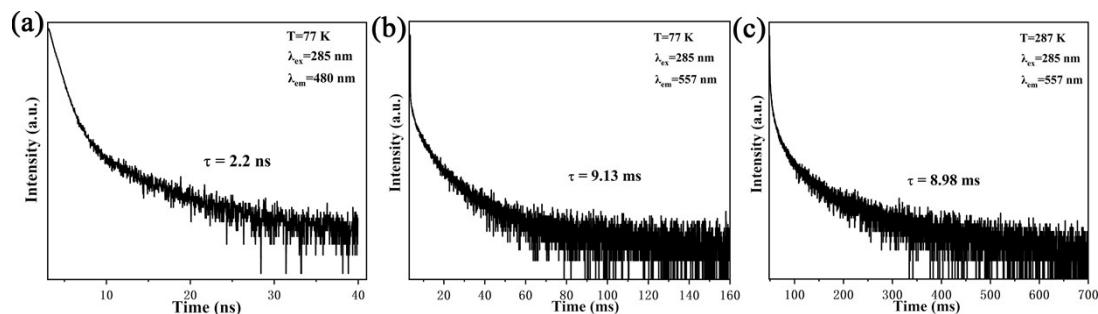


Fig. S3. The time-resolved decay curves of $\text{Cs}_2\text{Cd}_2\text{BrCl}_5$ at 77 K and 287 K.