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Supporting Information

Coordination Units of Mn^{2+} Modulation toward Tunable Emission in Zero-Dimensional Bromides for White Light-Emitting Diodes

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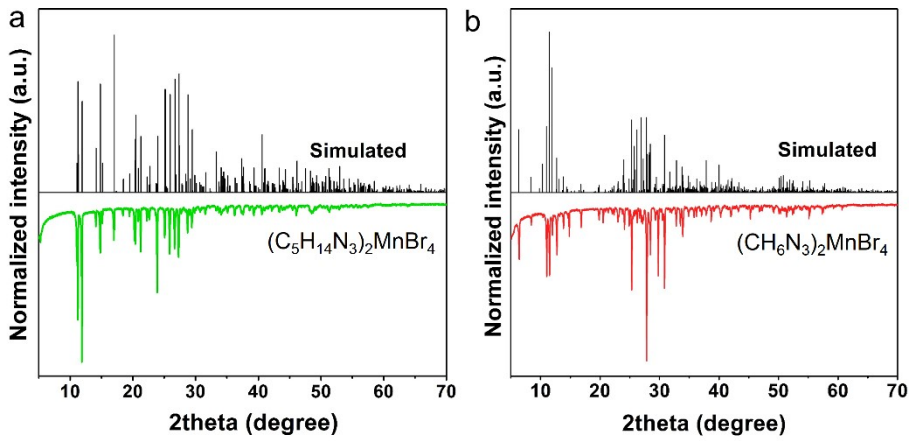

Figure S1. The simulated and experimental X-ray powder patterns of $(C_5H_{14}N_3)_2MnBr_4$ (a) and $(CH_6N_3)_2MnBr_4$ (b).

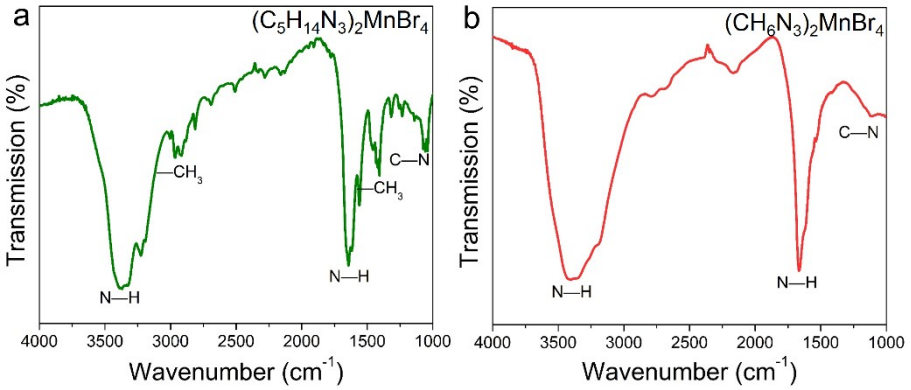

Figure S2. FTIR spectra of $(C_5H_{14}N_3)_2MnBr_4$ (a) and $(CH_6N_3)_2MnBr_4$ (b).

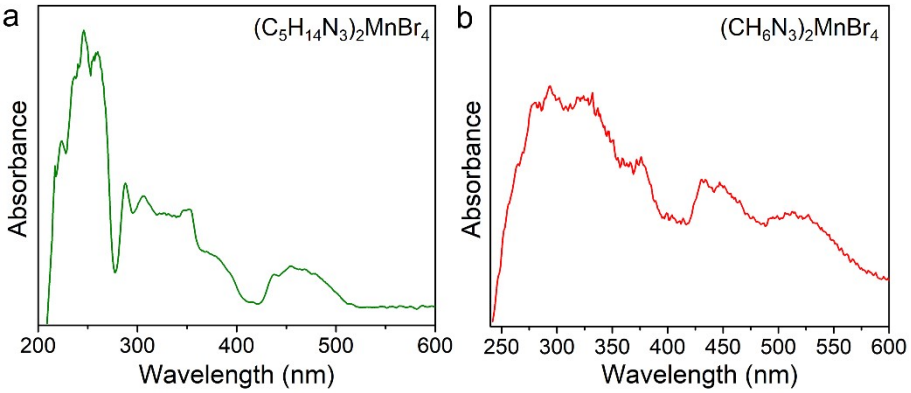

Figure S3. UV-visible absorption spectra of $(C_5H_{14}N_3)_2MnBr_4$ (a) and $(CH_6N_3)_2MnBr_4$ (b).

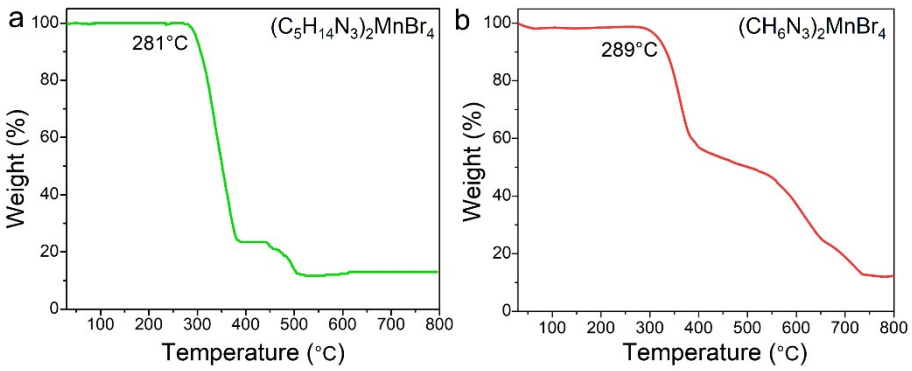

Figure S4. Thermogravimetric (TG) curves for powder sample of $(C_5H_{14}N_3)_2MnBr_4$ (a) and $(CH_6N_3)_2MnBr_4$ (b).

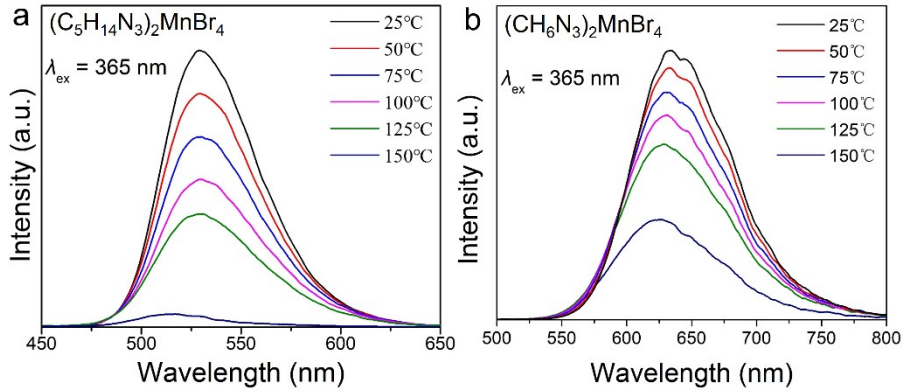

Figure S5. Temperature-dependent PL spectra of $(C_5H_{14}N_3)_2MnBr_4$ (a) and $(CH_6N_3)_2MnBr_4$ (b) under excitation at 365 nm in the temperature range of RT to 150 °C.

Table S1. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
		$(C_5H_{14}N_3)_2MnBr_4$		
Mn	0.5000	0.30574 (18)	0.2500	0.0366 (5)
Br1	0.43480 (8)	0.15992 (11)	0.08398 (7)	0.0640 (4)
Br2	0.61714 (7)	0.45894 (14)	0.27426 (8)	0.0654 (5)
N1	0.7497 (6)	0.5136 (11)	0.5496 (8)	0.079 (3)
H11	0.7041	0.4831	0.4911	0.094*
H12	0.7988	0.4807	0.5701	0.094*
N2	0.6696 (5)	0.6630 (8)	0.5784 (6)	0.0491 (18)
N3	0.8158 (5)	0.6566 (9)	0.7007 (6)	0.056 (2)
C2	0.7440 (6)	0.6109 (10)	0.6080 (7)	0.0470 (19)
C3	0.5894 (6)	0.5865 (14)	0.5009 (8)	0.066 (3)
H31	0.5420	0.6405	0.4893	0.080*
H32	0.5831	0.5764	0.4345	0.080*
H33	0.5906	0.4926	0.5282	0.080*
C4	0.6517 (7)	0.8140 (11)	0.5919 (10)	0.069 (3)
H41	0.5923	0.8235	0.5635	0.083*
H42	0.6861	0.8385	0.6664	0.083*
H43	0.6650	0.8779	0.5543	0.083*
C5	0.8285 (8)	0.6862 (13)	0.8013 (8)	0.080 (4)
H51	0.8863	0.7171	0.8528	0.097*
H52	0.7899	0.7610	0.7915	0.097*
H53	0.8177	0.6003	0.8266	0.097*
C6	0.9002 (7)	0.6405 (14)	0.7193 (11)	0.077 (4)
H61	0.9439	0.6782	0.7886	0.093*
H62	0.9110	0.5402	0.7160	0.093*
H63	0.9003	0.6927	0.6654	0.093*
		$(CH_6N_3)_2MnBr_4$		
Mn1	0.73990 (12)	0.45012 (4)	0.27726 (7)	0.0345 (3)
Mn2	0.72539 (13)	0.56746 (5)	0.20649 (7)	0.0390 (3)
Mn3	0.74383 (13)	0.33480 (5)	0.35697 (7)	0.0408 (3)
Br1	0.75425 (8)	0.42247 (3)	0.43455 (4)	0.0357 (2)
Br2	0.72681 (8)	0.48030 (3)	0.11877 (4)	0.0367 (2)
Br3	0.94408 (8)	0.51830 (3)	0.30396 (5)	0.0369 (2)
Br4	0.53277 (8)	0.51612 (3)	0.30429 (5)	0.0359 (2)
Br5	0.53122 (8)	0.38113 (3)	0.24909 (5)	0.0383 (2)
Br6	0.94102 (8)	0.38063 (3)	0.24732 (5)	0.0378 (2)
Br7	0.73537 (10)	0.25907 (3)	0.26142 (5)	0.0470 (2)
Br8	0.73018 (9)	0.63436 (3)	0.31958 (5)	0.0469 (2)
Br9	0.96698 (10)	0.30553 (4)	0.45428 (5)	0.0528 (3)
Br10	0.92066 (10)	0.60706 (4)	0.11286 (5)	0.0556 (3)
Br11	0.53972 (11)	0.30543 (4)	0.45445 (5)	0.0571 (3)

Br12	0.50016 (10)	0.59736 (4)	0.11062 (5)	0.0596 (3)
C1A	0.2229 (8)	0.4689 (3)	0.1057 (5)	0.040 (2)
N1A	0.0950 (7)	0.4600 (3)	0.0664 (4)	0.066 (3)
H11A	0.0924	0.4477	0.0174	0.079*
H12A	0.0136	0.4666	0.0895	0.079*
N2A	0.3454 (8)	0.4589 (3)	0.0705 (4)	0.060 (2)
H21A	0.4294	0.4632	0.0972	0.072*
H22A	0.3424	0.4481	0.0204	0.072*
N3A	0.2303 (8)	0.4851 (3)	0.1808 (5)	0.069 (3)
H31A	0.3153	0.4891	0.2067	0.083*
H32A	0.1502	0.4919	0.2051	0.083*
C1B	0.7461 (8)	0.5648 (3)	0.5451 (4)	0.0364 (18)
N1B	0.6149 (7)	0.5568 (3)	0.5074 (4)	0.059 (2)
H11B	0.6090	0.5466	0.4570	0.071*
H12B	0.5354	0.5618	0.5333	0.071*
N2B	0.8675 (8)	0.5573 (3)	0.5062 (4)	0.066 (3)
H21B	0.8622	0.5471	0.4558	0.079*
H22B	0.9527	0.5625	0.5311	0.079*
N3B	0.7544 (8)	0.5780 (3)	0.6241 (4)	0.054 (2)
H31B	0.6746	0.5813	0.6505	0.065*
H32B	0.8395	0.5832	0.6490	0.065*
C1C	0.2419 (9)	0.2557 (4)	0.2969 (7)	0.067 (3)
N1C	0.2404 (9)	0.3000 (3)	0.3139 (6)	0.074 (3)
H11C	0.3222	0.3147	0.3266	0.089*
H12C	0.1576	0.3153	0.3126	0.089*
N2C	0.3625 (10)	0.2314 (4)	0.2979 (6)	0.087 (3)
H21C	0.4461	0.2451	0.3104	0.104*
H22C	0.3598	0.2014	0.2861	0.104*
N3C	0.1150 (11)	0.2325 (4)	0.2774 (6)	0.093 (3)
H31C	0.0318	0.2476	0.2765	0.112*
H32C	0.1165	0.2025	0.2660	0.112*
C1D	0.7669 (8)	0.3730 (3)	0.6727 (5)	0.0408 (19)
N1D	0.6396 (8)	0.3647 (3)	0.6340 (5)	0.062 (2)
H11D	0.5587	0.3709	0.6578	0.074*
H12D	0.6363	0.3531	0.5845	0.074*
N2D	0.7718 (8)	0.3908 (3)	0.7485 (4)	0.059 (2)
H21D	0.6907	0.3970	0.7722	0.070*
H22D	0.8560	0.3963	0.7742	0.070*
N3D	0.8890 (8)	0.3631 (3)	0.6369 (5)	0.062 (2)
H31D	0.9735	0.3682	0.6626	0.074*
H32D	0.8852	0.3515	0.5873	0.074*
C1E	0.7842 (10)	0.1787 (4)	0.5202 (5)	0.051 (2)
N1E	0.7558 (9)	0.1886 (3)	0.4427 (4)	0.064 (2)
H11E	0.7119	0.1678	0.4106	0.076*

H12E	0.7808	0.2159	0.4232	0.076*
N2E	0.7474 (10)	0.1375 (3)	0.5512 (5)	0.074 (3)
H21E	0.7034	0.1164	0.5198	0.089*
H22E	0.7671	0.1315	0.6030	0.089*
N3E	0.8583 (10)	0.2094 (4)	0.5661 (6)	0.094 (3)
H31E	0.8832	0.2026	0.6171	0.113*
H32E	0.8825	0.2365	0.5457	0.113*
C1F	0.3259 (15)	0.2024 (6)	0.5636 (8)	0.107 (4)
N1F	0.4402 (15)	0.2170 (5)	0.6017 (9)	0.144 (5)
H11F	0.4862	0.2416	0.5837	0.173*
H12F	0.4735	0.2026	0.6460	0.173*
N2F	0.2558 (15)	0.2178 (6)	0.4969 (9)	0.151 (5)
H21F	0.2883	0.2424	0.4713	0.181*
H22F	0.1766	0.2035	0.4780	0.181*
N3F	0.2815 (18)	0.1597 (7)	0.5858 (11)	0.193 (7)
H31F	0.3310	0.1442	0.6241	0.231*
H32F	0.2030	0.1473	0.5620	0.231*

Table S2. The main bond lengths (Å) of compound $(C_5H_{14}N_3)_2MnBr_4$ and $(CH_6N_3)_2MnBr_4$.

$(C_5H_{14}N_3)_2MnBr_4$			
Mn—Br1	2.4876 (13)	N1—C2	1.319 (12)
Mn—Br1^{i}	2.4876 (13)	N2—C2	1.315 (12)
Mn—Br2	2.4986 (14)	N2—C3	1.471 (12)
Mn—Br2^{i}	2.4987 (14)	N2—C4	1.483 (13)
		N3—C2	1.352 (11)
		N3—C5	1.445 (13)
		N3—C6	1.481 (15)
$(CH_6N_3)_2MnBr_4$			
Mn1—Br1	2.6446 (13)	C1A—N2A	1.298 (9)
Mn1—Br3	2.6694 (14)	C1A—N3A	1.290 (10)
Mn1—Br4	2.6776 (14)	C1A—N1A	1.310 (9)
Mn1—Br2	2.6845 (13)	C1B—N1B	1.320 (9)
Mn1—Br5	2.7162 (14)	C1B—N2B	1.306 (9)
Mn1—Br6	2.7181 (14)	C1B—N3B	1.322 (9)
Mn2—Br8	2.6093 (15)	C1C—N1C	1.269 (12)
Mn2—Br10	2.6226 (14)	C1C—N2C	1.281 (12)
Mn2—Br12	2.6224 (15)	C1C—N3C	1.339 (12)
Mn2—Br4	2.8011 (14)	C1D—N2D	1.316 (10)
Mn2—Br3	2.8136 (14)	C1D—N1D	1.298 (10)
Mn2—Br2	2.8174 (15)	C1D—N3D	1.299 (10)
Mn3—Br11	2.6133 (14)	C1E—N2E	1.306 (11)
Mn3—Br9	2.6158 (15)	C1E—N1E	1.290 (10)
Mn3—Br7	2.6161 (15)	C1E—N3E	1.295 (12)
Mn3—Br1	2.7510 (15)	C1F—N1F	1.241 (16)
Mn3—Br5	2.8322 (15)	C1F—N2F	1.290 (16)
Mn3—Br6	2.8726 (14)	C1F—N3F	1.314 (19)

Table S3. Hydrogen-bond geometry in the structures (Å, □).

D—H	d(D—H)	d(H···A)	□ D—H···A	D···A	A	Transformation for A atom
			$(C_5H_{14}N_3)_2MnBr_4$			
N(1)—H(11)	0.86	2.78	146	3.482(10)	Br(2)	x, y, z
N(1)—H(12)	0.86	2.81	165	3.651(13)	Br(1)	1/2+x, 1/2–y, 1/2+z
			$(CH_6N_3)_2MnBr_4$			
N(1A)—H(11A)	0.86	2.59	167	3.439(7)	Br(10)	x, y, z
N(1B)—H(11B)	0.86	2.66	169	3.505(7)	Br(4)	x, y, z
N(1C)—H(11C)	0.86	2.78	134	3.433(9)	Br(11)	x, y, z
N(1D)—H(11D)	0.86	2.65	156	3.455(7)	Br(8)	x, y, z
N(1E)—H(11E)	0.86	2.75	148	3.516(8)	Br(12)	x, y, z
N(1F)—H(11F)	0.86	2.80	150	3.573(14)	Br(11)	x, y, z
N(1A)—H(12A)	0.86	2.68	164	3.514(6)	Br(2)	x, y, z
N(1B)—H(12B)	0.86	2.72	162	3.552(6)	Br(1)	x, y, z
N(1C)—H(12C)	0.86	2.84	155	3.635(8)	Br(6)	x, y, z
N(1D)—H(12D)	0.86	2.59	159	3.412(8)	Br(11)	x, y, z
N(1E)—H(12E)	0.86	2.88	132	3.519(7)	Br(7)	x, y, z
N(1F)—H(12F)	0.86	2.90	154	3.692(14)	Br(5)	x, y, z
N(2A)—H(21A)	0.86	2.73	157	3.537(7)	Br(2)	x, y, z
N(2B)—H(21B)	0.86	2.71	161	3.537(7)	Br(3)	x, y, z
N(2C)—H(21C)	0.86	2.79	145	3.529(9)	Br(7)	x, y, z
N(2D)—H(21D)	0.86	2.62	159	3.443(7)	Br(12)	x, y, z
N(2E)—H(21E)	0.86	2.77	148	3.524(8)	Br(12)	x, y, z
N(2F)—H(21F)	0.86	2.90	145	3.635(15)	Br(11)	x, y, z
N(2A)—H(22A)	0.86	2.90	148	3.653(7)	Br(12)	x, y, z
N(2B)—H(22B)	0.86	2.70	164	3.539(7)	Br(1)	x, y, z
N(2C)—H(22C)	0.86	2.63	147	3.387(11)	Br(8)	x, y, z
N(2D)—H(22D)	0.86	2.64	161	3.468(7)	Br(10)	x, y, z
N(2E)—H(22E)	0.86	2.76	157	3.563(8)	Br(6)	x, y, z
N(3A)—H(31A)	0.86	2.56	166	3.402(8)	Br(4)	x, y, z
N(3B)—H(31B)	0.86	2.73	161	3.558(7)	Br(5)	x, y, z
N(3C)—H(31C)	0.86	2.69	157	3.499(10)	Br(7)	x, y, z
N(3D)—H(31D)	0.86	2.67	155	3.469(7)	Br(8)	x, y, z
N(3F)—H(31F)	0.86	2.73	164	3.559(17)	Br(5)	x, y, z
N(3A)—H(32A)	0.86	2.62	168	3.463(8)	Br(3)	x, y, z
N(3B)—H(32B)	0.86	2.72	162	3.545(7)	Br(6)	x, y, z
N(3C)—H(32C)	0.86	2.76	143	3.485(11)	Br(8)	x, y, z
N(3D)—H(32D)	0.86	2.64	160	3.457(8)	Br(9)	x, y, z
N(3E)—H(32E)	0.86	2.57	166	3.408(11)	Br(9)	x, y, z