Crystal structure of NaLuW₂O₈·2H₂O and down/upconversion luminescence of the derived NaLu(WO₄)₂:Yb/Ln phosphors (Ln=Ho, Er, Tm)

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Figure S1. Indexing of the diffraction peaks of NaLuW₂O₈·2H₂O in the 2θ ranges of 5-50° (a) and 50-90° (b).

Table S1. Main bond lengths (Å) and angles (°) of NaLuW₂O₈·2H₂O. Symmetry codes: (i) x, y, z+1; (ii) -x, -y+1, -z; (iii) x, y, z-1.

coordinates condition	bond length (Å)	Coordinates condition	Angle (°)
Lu—O3	2.316 (9)	O3—Lu—O3 ⁱ	103 (4)
Lu—O5	2.012 (16)	O3—Lu—O5	90
W—O2	1.8161 (2)	O2—W—O3	90.6 (5)
W—O3	2.125 (8)	O2—W—O4	89.3 (6)
W—O4	1.623 (16)	O3—W—O3 ⁱⁱ	64.3 (4)
Na—O1	2.350 (5)	O3—W—O4	147.9 (4)
Na—O4	2.370 (14)	O1—Na—O1 ⁱⁱⁱ	101.2 (2)
О5—Н	0.9733	O1—Na—O4	91.4 (4)

Table S2. 2Theta (°), *d*-spacing (Å) and corresponding *h*, *k*, *l* derived from Rietveld refinement of the XRD pattern of NaLuW₂O₈·2H₂O.

2Theta (°)	d-spacing (Å)	h	k	l
8.159	10.8276	2	0	0
16.36	5.4138	4	0	0
17.737	4.9966	1	1	0
21.216	4.1844	3	1	0
24.489	3.632	0	0	1
24.646	3.6092	6	0	0
25.853	3.4434	2	0	1
26.908	3.3107	5	1	0
29.594	3.0161	4	0	1
30.401	2.9379	1	1	1
32.62	2.7429	3	1	1
33.066	2.7069	8	0	0
33.799	2.6499	7	1	0

24.016	2 5 (7 (0	•	0
34.916	2.5676	0	2	0
35.022	2.5601	6	0	l
35.917	2.4983	2	2	0
36.7	2.4468	5	1	1
38.785	2.3199	4	2	0
41.408	2.1788	9	1	0
41.576	2.1704	8	0	1
41.674	2.1655	10	0	0
42.18	2.1407	7	1	1
43.111	2.0966	0	2	1
43.207	2.0922	6	2	0
43.953	2.0584	2	2	1
46.406	1.9551	4	2	1
48.696	1.8684	9	1	1
48.85	1.8629	8	2	0
48.93	1.86	10	0	1
49.549	1.8382	11	1	0
50.197	1.816	0	0	2
50.288	1.8129	6	2	1
50.536	1.8046	12	0	0
50.948	1.791	2	0	2
53.154	1.7217	4	0	2
53.657	1.7068	1	1	2
53.669	1.7064	1	3	0
55.084	1.6659	3	1	2
55.096	1.6655	3	3	0
55.384	1.6576	8	2	1
55 464	1 6554	10	2	0
56 025	1 6401	11	- 1	1
56 698	1 6222	6	0	2
56 932	1 6161	12	ů 0	- 1
57 867	1 5922	5	1	2
57 879	1 5919	5	3	0
58 175	1.5919	13	1	0
59 735	1.5468	13	0	0
59.835	1.5400	1	3	1
61 168	1 5139	3	3	1
61 432	1.5081	8	0	2
61 512	1.5061	10	2	1
61 801	1.0005	7	1	2
61.002	1.498	7	1	2
62 604	1.4977	0	2	2
62.004	1.4820	12	2	2
02.090	1.4/04	12	2	0
03.233	1.4089	2 5	2	2 1
03./84	1.438	5 12	5 1	1
04.004	1.4525	13	1	1
05.18/	1.43	4	2	2
65.541	1.4231	14	0	1

67.035	1.395	9	1	2
67.046	1.3948	1.3948 9		
67.226	1.3915	1.3915 10		
67.318	1.3898	15	1	0
67.603	1.3846	7	3	1
68.343	1.3714	6	2	2
68.554	1.3677	12	2	1
69.38	1.3534	16	0	0
71.095	1.3249	14	2	0
72.54	1.3021	9	3	1
72.651	1.3004	8	2	2
72.803	1.298	15	1	1
73.205	1.2919	11	1	2
73.215	1.2917	11	3	0
73.742	1.2838	0	4	0
73.993	1.2801	12	0	2
74.345	1.2749	2	4	0
74.799	1.2683	16	0	1
76.145	1.2492	4	4	0
76.466	1.2447	14	2	1
76.55	1.2436	1	3	2
77.076	1.2364	17	1	0
77.739	1.2275	3	3	2
78.048	1.2234	10	2	2
78.532	1.217	11	3	1
79.027	1.2107	0	0	3
79.047	1.2104	0	4	1
79.114	1.2096	6	4	0
79.617	1.2032	2	0	3
79.625	1.2031	18	0	0
79.637	1.2029	2	4	1
80.087	1.1973	16	2	0
80.104	1.1971	5	3	2
80.359	1.1939	13	1	2
80.369	1.1938	13	3	0
81.381	1.1815	4	0	3
81.401	1.1812	4	4	1
81.712	1.1775	14	0	2
81.789	1.1766	1	1	3
82.317	1.1704	17	1	1
82.96	1.163	3	1	3
83.223	1.16	8	4	0
83.619	1.1555	7	3	2
84.304	1.1478	6	0	3
84.324	1.1476	6	4	1
84.506	1.1456	12	2	2
84.829	1.142	18	0	1
85.285	1.1371	16	2	1

85.292	1.137	5	1	3
85.564	1.1341	13	3	1
87.624	1.1127	19	1	0
88.272	1.1062	9	3	2
88.373	1.1052	8	0	3
88.393	1.105	8	4	1
88.458	1.1043	10	4	0
88.524	1.1037	15	1	2
88.534	1.1036	15	3	0
88.777	1.1012	7	1	3
89.408	1.095	0	2	3
89.988	1.0895	2	2	3
89.996	1.0894	18	2	0



Figure S2. XRD patterns of NaLuW₂O₈·2H₂O (a) and the NaLu(WO₄)₂ calcined at 600 °C for 2 hours in air (b). The standard diffractions of NaLu(WO₄)₂ are included as bars for comparison (c). The main diffractions of NaLuW₂O₈·2H₂O are indicated in (a) according to the indexing of the diffraction peaks in Figure S1.



Figure S3. SEM morphologies for $Na(Lu_{0.87}Ho_{0.03}Yb_{0.1})W_2O_8 \cdot 2H_2O$ (a) and the $Na(Lu_{0.87}Ho_{0.03}Yb_{0.1})(WO_4)_2$ obtained by calcining $Na(Lu_{0.87}Ho_{0.03}Yb_{0.1})W_2O_8 \cdot 2H_2O$ at 600 °C for 2 h (b).

Table S3. Cell parameters for the synthesized $Na(Lu_{0.87}Ln_{0.03}Yb_{0.1})(WO_4)_2$ (Ln=Ho, Er and Tm) and $NaLu(WO_4)_2$. The data from JCPDS File No. 00-027-0729 for $NaLu(WO_4)_2$ are listed at the bottom for comparison.

Sample	<i>a,b</i> (Å)	c (Å)	$V(\text{\AA}^3)$
$Na(Lu_{0.87}Ho_{0.03}Yb_{0.1})(WO_4)_2$	5.17162 (8)	11.1878 (2)	299.22 (1)
$Na(Lu_{0.87}Er_{0.03}Yb_{0.1})(WO_4)_2$	5.17119 (7)	11.1871 (2)	299.16(1)
$Na(Lu_{0.87}Tm_{0.03}Yb_{0.1})(WO_4)_2$	5.17056 (9)	11.1859 (2)	299.05 (1)
NaLu(WO ₄) ₂	5.16899 (9)	11.1840 (2)	298.82 (1)
PDF No. 00-027-0729	5.166	11.174	298.21



Figure S4. Cell volume V per average ion radii (Lu/Yb/Ho/Er/Tm) of Na(Lu/Yb/Ho/Er/Tm)(WO₄)₂ compounds

Excitation power	Но	Er	Tm
0.6 W	(0.50, 0.49)	(0.33, 0.62)	(0.25, 0.31)
0.8 W	(0.49, 0.50)	(0.28, 0.70)	(0.32, 0.35)
1 W	(0.49, 0.50)	(0.27, 0.71)	(0.29, 0.31)
1.2 W	(0.48, 0.51)	(0.26, 0.72)	(0.26, 0.29)
1.4 W	(0.47, 0.52)	(0.26, 0.72)	(0.24, 0.24)
1.6 W	(0.47, 0.52)	(0.26, 0.72)	(0.22, 0.22)
1.8 W	(0.47, 0.52)	(0.25, 0.72)	(0.20, 0.20)
2 W	(0.47, 0.53)	(0.25, 0.73)	(0.18, 0.18)

Table S4. CIE chromaticity coordinates (x, y) for the upconversion luminescence of $Na(Lu_{0.87}Ln_{0.03}Yb_{0.1})(WO_4)_2$ under varying excitation power.

Table S5. I_{650}/I_{544} , I_{531}/I_{657} and I_{553}/I_{657} , and I_{476}/I_{650} intensity ratios for the Na(Lu_{0.87}Ho_{0.03}Yb_{0.1})(WO₄)₂, Na(Lu_{0.87}Er_{0.03}Yb_{0.1})(WO₄)₂, and Na(Lu_{0.87}Tm_{0.03}Yb_{0.1})(WO₄)₂ phosphors under varying excitation power.

Excitation	Ho	E	lr	Tm	
power	I_{650}/I_{544}	I ₅₃₁ /I ₆₅₇	I553/I657	I_{476}/I_{650}	
0.6 W	3.93	3.88	7.19	1.02	
0.8 W	3.56	7.61	13.79	1.19	
1 W	3.42	9.88	16.46	1.81	
1.2 W	2.97	12.19	18.35	2.56	
1.4 W	2.77	13.55	19.26	3.26	
1.6 W	2.61	15.16	19.91	3.78	
1.8 W	2.53	16.56	20.32	4.92	
2 W	2.52	18.05	20.85	5.57	



Figure S5. CIE chromaticity diagram showing the emission colors of $Na(Lu_{0.87}Ln_{0.03}Yb_{0.1})(WO_4)_2$ (Ln=Ho, Er and Tm) under varying excitation power.



Figure S6. Excitation and emission spectra of NaLu(WO₄)₂.