Supplementary Information

$YMgB_5O_{10}$ crystal preparation and attractive multi-wavelength emission characteristics of doping Nd^{3+} ions

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Fig. S1. Schematic diagram of crystal growth apparatus.

Fig. S2. (a) The coordination environments of B, Y and Mg atoms. (b) View of the B_5O_{12} cluster.

(c) View of the topological network of B-O layer along [101] direction.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters of YMB crystal.

Table S2. Selected bond distances (Å) of YMB crystal.

Table S3. Indexation results of powder XRD pattern.

Calculations of Judd–Ofelt theory.

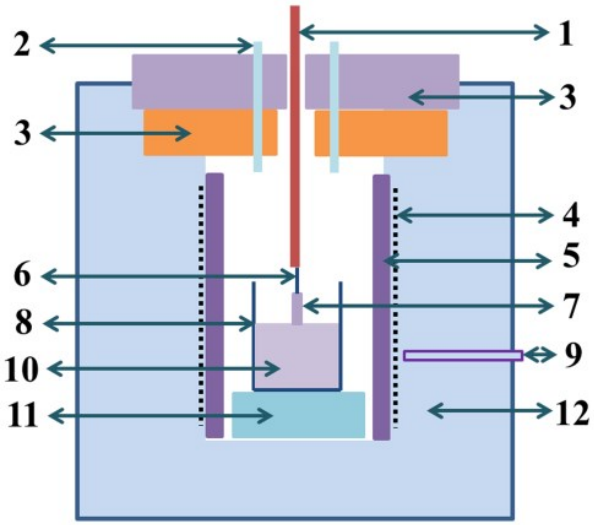

Fig. S1. Schematic diagram of crystal growth apparatus. (1) seed-holder, (2) watch window, (3) furnace cover (thermal insulation materials), (4) nickel-chrome heating wires, (5) Al_2O_3 tube, (6) platinum wires, (7) seed, (8) platinum crucible, (9) thermocouple, (10) solution, (11) thermal insulation materials (the height is based on the thermal field), (12) thermal insulation materials.

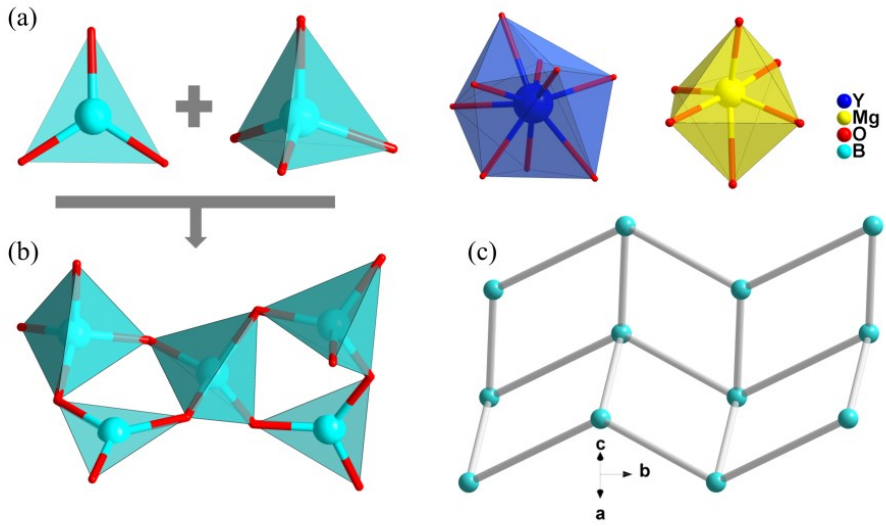

Fig. S2. (a) The coordination environments of B, Y and Mg atoms. (b) View of the B_5O_{12} cluster. (c) View of the topological network of B-O layer along [101] direction.

Table S1. Atomic coordinates and equivalent isotropic displacement parameters of YMB crystal.

Atom	*x*/a	*y*/b	*z*/c	*U*(eq)[Å^2]*
Y(1)	1855(1)	1865(1)	2390(1)	2(1)
Mg(1)	1005(1)	916(2)	6278(1)	4(1)
O(10)	4638(3)	2086(3)	2691(3)	2(1)
O(9)	-843(3)	-275(3)	1484(3)	3(1)
O(8)	1812(3)	3495(3)	6350(3)	4(1)
O(7)	3185(3)	1276(3)	-93(3)	4(1)
O(6)	458(3)	2713(3)	208(3)	4(1)
O(5)	50(3)	1498(3)	4267(3)	4(1)
O(4)	-95(3)	4101(3)	3033(3)	4(1)
O(3)	3142(3)	-332(3)	6267(3)	4(1)
O(2)	2568(3)	-510(3)	3736(3)	4(1)
O(1)	1764(3)	-1073(3)	825(3)	4(1)
B(5)	-178(5)	1741(5)	-1048(5)	3(1)
B(4)	843(5)	4243(5)	7425(5)	4(1)
B(3)	-657(5)	3105(5)	4111(5)	4(1)
B(2)	-2230(5)	315(5)	548(5)	4(1)
B(1)	1599(5)	3997(5)	55(5)	3(1)

* *U*(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond distances (Å) of YMB crystal.

Y(1)-O(2)	2.254(2)	B(5)-O(9)#8	1.482(5)
Y(1)-O(2)#1	2.314(2)	B(1)-O(6)	1.387(5)
Y(1)-O(10)	2.375(3)	B(5)-O(6)	1.461(5)
Y(1)-O(6)	2.385(2)	B(3)-O(5)	1.359(5)
Y(1)-O(5)	2.422(3)	B(3)-O(4)	1.369(5)
Y(1)-O(4)	2.470(2)	B(4)-O(4)#9	1.456(5)
Y(1)-O(1)#1	2.521(3)	B(1)-O(3)#5	1.368(5)
Y(1)-O(1)	2.659(3)	B(4)-O(3)#4	1.488(5)
Y(1)-O(7)	2.686(3)	B(1)-O(2)#5	1.349(5)
Mg(1)-O(3)	2.051(3)	B(5)-O(1)#8	1.469(5)
Mg(1)-O(5)	2.051(3)	B(2)-O(1)#8	1.483(5)
Mg(1)-O(8)	2.066(3)	B(2)-O(9)	1.494(5)
Mg(1)-O(5)#2	2.083(3)	B(2)-O(8)#7	1.455(5)
Mg(1)-O(9)#2	2.162(3)	B(4)-O(8)	1.456(5)
Mg(1)-O(10)#3	2.361(3)	B(3)-O(7)#6	1.356(5)
B(4)-O(10)#6	1.468(5)	B(2)-O(7)#8	1.498(5)
B(5)-O(10)#7	1.477(5)		

Symmetry codes: (#1) -x+3/2,y+1/2,-z+3/2; (#2) -x+1/2,y+1/2,-z+3/2; (#3) x-1/2,-y+1/2,z+1/2; (#4) -x+1/2,y-1/2,-z+3/2; (#5) -x+1,-y,-z+1; (#6) x+1/2,-y+1/2,z-1/2; (#7) -x+1,-y,-z+2; (#8) x-1,y,z; (#9) -x+2,-y,-z+2.

Table S3. Indexation results of powder XRD pattern.

d (Å)	2 θ(deg.)	h	k	l	d (Å)	2 θ(deg.)	h	k	l
6.5086	13.5935	-1	0	1	1.9295	47.0558	2	1	4
6.1102	14.4843	1	0	1	1.9256	47.1574	-1	3	3
5.8754	15.0665	0	1	1	1.9233	47.2178	-4	1	2
5.6584	15.6478	1	1	0	1.9120	47.515	1	2	4
4.9321	17.9701	-1	1	1	1.8957	47.9475	4	0	2
4.7518	18.6577	1	1	1	1.8925	48.0353	1	3	3
4.6695	18.9896	0	0	2	1.8896	48.1115	0	4	0
4.2671	20.7993	2	0	0	1.8861	48.2071	3	3	0
3.9726	22.3606	0	1	2	1.8815	48.3322	-3	2	3
3.7793	23.52	0	2	0	1.864	48.8152	-3	3	1
3.7159	23.9274	2	1	0	1.8579	48.9862	4	2	0
3.6781	24.1767	-1	1	2	1.8521	49.1503	0	4	1
3.5295	25.2111	1	1	2	1.8492	49.232	-1	0	5
3.5199	25.2808	-2	1	1	1.8449	49.3535	1	4	0
3.5033	25.4027	0	2	1	1.8417	49.445	-4	2	1
3.4556	25.7592	1	2	0	1.839	49.5226	-2	2	4
3.389	26.2745	2	1	1	1.8388	49.5306	4	1	2
3.2683	27.2636	-1	2	1	1.8339	49.6709	3	3	1
3.2543	27.3831	-2	0	2	1.8147	50.2327	-1	4	1
3.2142	27.7316	1	2	1	1.8132	50.2759	0	1	5
3.0551	29.2067	2	0	2	1.8093	50.3915	-3	1	4
2.989	29.8673	-2	1	2	1.8074	50.4489	-2	3	3
2.986	29.8979	-1	0	3	1.8053	50.5133	1	4	1
2.9377	30.4017	0	2	2	1.8033	50.5731	4	2	1
2.8784	31.043	0	1	3	1.8009	50.6437	1	0	5
2.8666	31.1739	1	0	3	1.7962	50.7853	-1	1	5
2.8325	31.5597	2	1	2	1.7929	50.8859	3	2	3
2.8292	31.5974	2	2	0	1.7749	51.4402	-3	3	2
2.8124	31.7908	-1	2	2	1.7647	51.7586	2	2	4
2.7772	32.2052	-1	1	3	1.7642	51.7766	-4	1	3
2.7706	32.2831	-3	0	1	1.7599	51.9096	-4	2	2
2.7443	32.6019	1	2	2	1.7536	52.1107	2	3	3
2.7398	32.6569	-2	2	1	1.7519	52.1664	1	1	5
2.6804	33.4018	1	1	3	1.7516	52.1743	0	4	2
2.6767	33.4493	2	2	1	1.7278	52.9499	2	4	0
2.6745	33.4773	3	0	1	1.7239	53.0771	-1	4	2
2.6624	33.6335	3	1	0	1.7239	53.0797	3	3	2
2.6014	34.447	-3	1	1	1.7125	53.46	0	3	4
2.5213	35.5769	3	1	1	1.7079	53.6158	1	4	2
2.466	36.4021	-2	2	2	1.707	53.6455	-2	1	5
2.4538	36.5897	-2	1	3	1.7068	53.6527	-2	4	1
2.4325	36.9208	0	3	1	1.706	53.681	3	1	4
2.4164	37.1764	1	3	0	1.6981	53.9486	-5	0	1
2.4028	37.3947	0	2	3	1.6945	54.0745	4	2	2
2.3759	37.8345	2	2	2	1.6943	54.0815	-1	3	4
2.3742	37.8621	-3	1	2	1.6912	54.1874	2	4	1
2.3496	38.2738	-1	3	1	1.6744	54.7754	0	2	5

2.343	38.3869	-1	2	3	1.6714	54.8843	-3	2	4
2.3347	38.5273	0	0	4	1.6679	55.0073	4	1	3
2.3293	38.6213	1	3	1	1.6649	55.1159	5	1	0
2.324	38.7123	2	1	3	1.6642	55.1417	1	3	4
2.2839	39.4191	1	2	3	1.661	55.2554	-1	2	5
2.2728	39.6202	3	2	0	1.6605	55.274	5	0	1
2.256	39.9271	3	1	2	1.6568	55.4072	-5	1	1
2.2345	40.3291	-3	2	1	1.644	55.8777	-3	3	3
2.2307	40.3997	0	1	4	1.6356	56.1914	-4	2	3
2.2173	40.6547	0	3	2	1.6341	56.2456	-2	4	2
2.1909	41.1672	-1	1	4	1.6331	56.2848	2	1	5
2.1831	41.3207	3	2	1	1.6282	56.4687	4	3	0
2.1696	41.591	2	3	0	1.6271	56.5092	-4	0	4
2.1695	41.5921	-3	0	3	1.6258	56.5601	1	2	5
2.162	41.7439	-1	3	2	1.6218	56.7095	5	1	1
2.1389	42.2161	-2	2	3	1.6173	56.8845	-4	3	1
2.1335	42.3265	4	0	0	1.6154	56.9549	-2	3	4
2.1305	42.3889	1	3	2	1.6153	56.9594	0	4	3
2.1284	42.433	-2	3	1	1.6088	57.2131	-3	0	5
2.127	42.4636	1	1	4	1.6071	57.279	2	4	2
2.1051	42.9265	-2	0	4	1.5998	57.5643	-5	1	2
2.0984	43.0696	2	3	1	1.5968	57.6833	-1	4	3
2.0855	43.3495	-3	2	2	1.591	57.9105	4	3	1
2.0853	43.3545	-3	1	3	1.5907	57.9247	-4	1	4
2.0533	44.0651	4	1	0	1.5897	57.9628	-2	2	5
2.0513	44.1115	2	2	3	1.5889	57.9965	3	2	4
2.0367	44.4431	3	0	3	1.5839	58.1958	3	3	3
2.0315	44.5623	-4	1	1	1.5777	58.4472	1	4	3
2.0279	44.6464	-2	1	4	1.574	58.5972	3	4	0
2.0041	45.2066	3	2	2	1.5735	58.6177	-3	1	5
1.9957	45.4079	2	0	4	1.5644	58.994	2	3	4
1.9922	45.4909	-2	3	2	1.5611	59.1294	-3	4	1
1.9888	45.5743	-4	0	2	1.561	59.1325	-4	3	2
1.9863	45.6345	0	2	4	1.558	59.2587	4	2	3
1.9803	45.7811	4	1	1	1.5565	59.3228	0	0	6
1.9666	46.1179	3	1	3	1.5555	59.3622	5	2	0
1.9584	46.3206	0	3	3	1.549	59.64	-5	2	1
1.958	46.3317	-1	2	4	1.5433	59.8816	3	4	1
1.9438	46.6907	2	3	2					

Calculations of Judd–Ofelt theory

The experimental absorption line strength S_{exp} from the ground state to the excited states can be calculated by the following equation (S1).

$$S_{\exp} = \frac{9n}{\left(n^2+2\right)^2} \cdot \frac{3hc\left(2J+1\right)}{8\pi^3 e^2 \bar{\lambda} N_0} \cdot \int \alpha(\lambda) d\lambda \quad \text{(S1)}$$

Where n is the refractive index (n=1.5, RHG-181 refractive index instrument), h is the Planck constant, J is the total angular momentum of the initial level (J=9/2 for Nd^{3+}), e is the electric charge, c is the velocity of light, N_0 is the Nd^{3+} concentrations, $\bar{\lambda}$ is the average wavelength of the absorption band, $\alpha(\lambda)$ is the absorption coefficient at the wavelength λ.

The line strength S_{exp} can also be expressed with the three-parameter formula (S2)

$$S_{cal} = \sum_{2,4,6} \Omega_\lambda \left| \left\langle (S,L)J \left\| U^{(\lambda)} \right\| (S',L')J' \right\rangle \right|^2 \quad \text{(S2)}$$

Where $\|U^{(\lambda)}\|$ are the double reduce matrix elements of unit tensor operators.

The J-O intensity parameters Ω_λ (λ=2, 4, 6) can be calculated using the least-squares-fit method. The effective J-O intensity parameters for the biaxial crystal are determined as $\Omega_{eff}=1/3(\Omega_{E//X}+\Omega_{E//Y}+\Omega_{E//Z})$.

The electric-dipole radiative transition rates A_r corresponding to transitions from the excited state $|(S', L')J'\rangle$ to all possible lower lying states $|(S'', L'')J''\rangle$ can be calculated by equation (S3).

$$A_r\left[(S'L')J',(S''L'')J''\right] = \frac{n\left(n^2+2\right)^2}{9} \times \frac{64\pi^2 e^2}{3h\left(2J'+1\right)\bar{\lambda}^3} \times \sum_{\lambda=2,4,6} \Omega_\lambda \left| \left\langle (S'L')J' \left\| U^{(\lambda)} \right\| (S''L'')J'' \right\rangle \right|^2 \quad \text{(S3)}$$

The fluorescence branching ratio β can be calculated by equations (S4)

$$\beta_r\left[(S',L')J';(S'',L'')J''\right] = \frac{A_r\left[(S',L')J';(S'',L'')J''\right]}{\sum_{S'',L'',J''} A_r\left[(S',L')J';(S'',L'')J''\right]} \quad \text{(S4)}$$

The radiative lifetime τ_r can be calculated by equation (S5)

$$\tau_r = \frac{1}{\sum_{S'',L'',J''} A_r\left[(S',L')J';(S'',L'')J''\right]} \quad \text{(S5)}$$