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Crystal growth, structure and characterization of $Er_6B_4O_{15}$ as self-activated infrared eye-safe laser material

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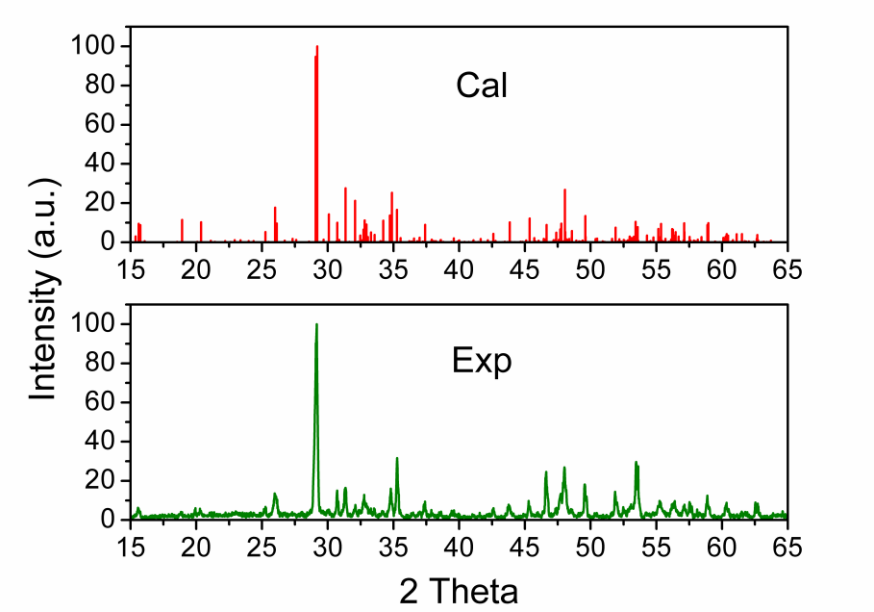

Figure S1. Experimental and calculated powder XRD patterns for $Er_6B_4O_{15}$

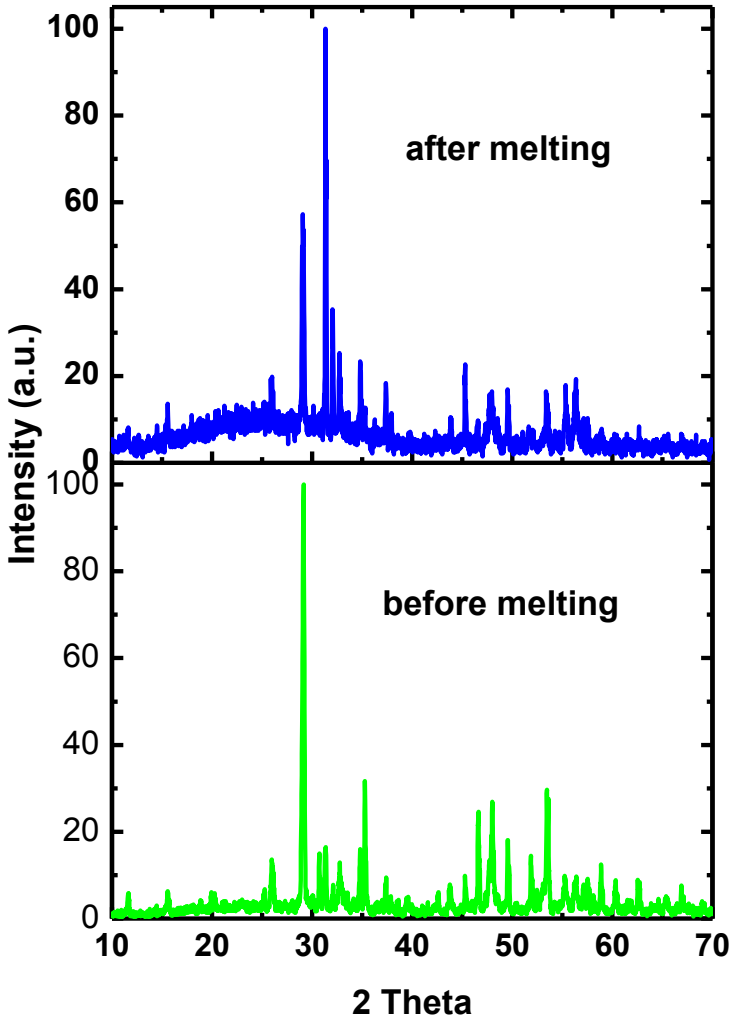

Figure S2. XRD patterns of $Er_6B_4O_{15}$ powders before and after melting during the thermal analysis

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $Er_6B_4O_{15}$

Atom	**Wyck.**	**Site**	**x/a**	**y/b**	**z/c**	**U [Å^2]**
Er1	4e	1	0.1991(2)	0.00367(11)	0.93909(17)	
Er2	4e	1	0.1442(2)	0.17793(11)	1.19306(18)	
Er3	4e	1	0.4483(2)	-0.01325(11)	1.28407(18)	
Er4	4e	1	0.0764(2)	-0.16594(11)	1.16681(18)	

Er5	4e	1	0.4573(2)	-0.17469(11)	0.94590(19)	
Er6	4e	1	0.2238(2)	-0.14521(11)	0.57689(18)	
B1	4e	1	0.428(5)	0.174(2)	1.476(4)	0.0010
B2	4e	1	0.069(5)	0.001(2)	1.361(4)	0.0010
B3	4e	1	0.173(5)	-0.306(2)	0.721(4)	0.0010
B4	4e	1	0.436(5)	-0.643(2)	1.212(4)	0.0010
O1	4e	1	0.052(3)	0.2708(14)	0.994(2)	0.0010
O2	4e	1	0.285(3)	0.2052(14)	1.423(2)	0.0010
O3	4e	1	0.460(3)	0.0868(14)	1.490(2)	0.0010
O4	4e	1	0.342(3)	0.0839(15)	1.125(2)	0.0010
O5	4e	1	0.005(3)	0.0916(15)	1.040(2)	0.0010
O6	4e	1	0.649(3)	-0.1065(15)	1.200(2)	0.0010
O7	4e	1	0.303(3)	-0.1005(14)	1.105(2)	0.0010
O8	4e	1	-0.039(3)	-0.0508(15)	1.275(2)	0.0010
O9	4e	1	0.148(3)	-0.2289(15)	1.379(2)	0.0010
O10	4e	1	0.340(3)	-0.0787(14)	0.781(2)	0.0010
O11	4e	1	0.315(3)	-0.2758(14)	0.773(2)	0.0010
O12	4e	1	0.060(3)	-0.2512(14)	0.679(2)	0.0010
O13	4e	1	-0.033(3)	-0.0861(14)	0.618(2)	0.0010
O14	4e	1	0.211(3)	-0.0339(14)	0.407(2)	0.0010
O15	4e	1	-0.175(4)	-0.103(2)	0.436(4)	0.035(8)

Table S2. Selected bond distances (Å) and angles (deg.) for $Er_6B_4O_{15}$

Atom 1	Atom 2	$d_{1,2}$ (Å)	Atom 3	$d_{1,3}$ (Å)	Angle (deg.)
Er1	O10	2.2510	O5	2.2672	95.265
	O5	2.2672	O5	2.3179	163.302
	O5	2.3179	O7	2.3268	78.742
	O7	2.3268	O4	2.3514	117.882

			O8	2.3919	88.519
			O6	2.3991	76.293
			O5	2.3179	79.247
			O7	2.3268	76.321
			O4	2.3514	130.777
			O8	2.3919	81.973
			O6	2.3991	152.342
			O7	2.3268	114.650
			O4	2.3514	76.541
			O8	2.3919	75.154
			O6	2.3991	101.248
			O4	2.3514	75.969
			O8	2.3919	153.562
			O6	2.3991	126.106
	O4	2.3514	O8	2.3919	130.324
			O6	2.3991	74.979
	O8	2.3919	O6	2.3991	71.648
Er2	O5	2.2044	O4	2.2975	79.919
			O2	2.3491	151.266
			O9	2.3609	125.707
			O12	2.3664	102.055
			O1	2.3782	76.305
			O13	2.4013	81.801
	O4	2.2975	O2	2.3491	89.747
			O9	2.3609	77.015
			O12	2.3664	164.761
			O1	2.3782	114.122
			O13	2.4013	95.977
	O2	2.3491	O9	2.3609	76.752

			O12	2.3664	81.394
			O1	2.3782	132.024
			O13	2.4013	72.630
	O9	2.3609	O12	2.3664	112.554
			O1	2.3782	69.798
			O13	2.4013	148.625
	O12	2.3664	O1	2.3782	80.853
			O13	2.4013	69.598
	O1	2.3782	O13	2.4013	138.360
Er5	O7	2.2521	O9	2.2757	156.427
	O7	2.2521	O10	2.2786	79.740
	O7	2.2521	O4	2.2913	107.230
	O7	2.2521	O11	2.4641	115.818
	O7	2.2521	O12	2.4829	84.785
	O9	2.2757	O10	2.2786	123.547
	O9	2.2757	O4	2.2913	78.864
	O9	2.2757	O11	2.4641	75.530
	O9	2.2757	O12	2.4829	71.680
	O10	2.2786	O4	2.2913	74.249
	O10	2.2786	O11	2.4641	80.274
	O10	2.2786	O12	2.4829	163.701
	O4	2.2913	O11	2.4641	124.304
	O4	2.2913	O12	2.4829	105.889
	O11	2.4641	O12	2.4829	111.419
Er3	O4	2.2224	O14	2.3134	93.368
			O6	2.3517	119.403
			O10	2.3566	74.012
			O7	2.3807	77.355
			O3	2.3872	92.657

			O3	2.3990	162.927
	O14	2.3134	O6	2.3517	133.954
			O10	2.3566	149.269
			O7	2.3807	78.836
			O3	2.3872	75.357
			O3	2.3990	78.467
	O6	2.3517	O10	2.3566	75.257
			O7	2.3807	78.197
			O3	2.3872	128.827
			O3	2.3990	76.047
	O10	2.3566	O7	2.3807	123.490
			O3	2.3872	77.344
			O3	2.3990	105.525
			O3	2.3872	151.695
	O7	2.3807	O3	2.3990	115.051
	O3	2.3872	O3	2.3990	70.866
Er4	O9	2.1766	O7	2.2310	101.676
			O5	2.2436	175.093
			O8	2.2542	95.716
			O1	2.3874	108.145
			O2	2.4521	78.105
	O7	2.2310	O5	2.2436	78.756
			O8	2.2542	97.032
			O1	2.3874	122.148
			O2	2.4521	82.942
	O5	2.2436	O8	2.2542	79.388
			O1	2.3874	75.397
			O2	2.4521	106.780
	O8	2.2542	O1	2.3874	126.841

			O2	2.4521	173.652
	O1	2.3874	O2	2.4521	57.459
Er6	O9	2.2483	O10	2.2648	169.025
	O9	2.2483	O14	2.2844	85.407
	O9	2.2483	O12	2.3368	74.974
	O9	2.2483	O13	2.3717	96.215
	O9	2.2483	O1	2.3812	71.638
	O10	2.2648	O14	2.2844	100.821
	O10	2.2648	O12	2.3368	104.728
	O10	2.2648	O13	2.3717	93.959
	O10	2.2648	O1	2.3812	97.874
	O14	2.2844	O12	2.3368	140.147
	O14	2.2844	O13	2.3717	77.647
	O14	2.2844	O1	2.3812	105.079
	O12	2.3368	O13	2.3717	70.602
	O12	2.3368	O1	2.3812	101.147
	O13	2.3717	O1	2.3812	167.059
O10	Er1	2.2510	Er6	2.2648	122.075
	Er1	2.2510	Er5	2.2786	101.365
	Er1	2.2510	Er3	2.3566	102.742
	Er6	2.2648	Er5	2.2786	112.004
	Er6	2.2648	Er3	2.3566	112.749
	Er5	2.2786	Er3	2.3566	103.847
O4	Er3	2.2224	Er5	2.2913	107.881
	Er3	2.2224	Er2	2.2975	122.690
	Er3	2.2224	Er1	2.3514	105.402
	Er5	2.2913	Er2	2.2975	102.803
	Er5	2.2913	Er1	2.3514	119.555
	Er2	2.2975	Er1	2.3514	99.450

O9	Er4	2.1766	Er6	2.2483	118.141
	Er4	2.1766	Er5	2.2757	110.004
	Er4	2.1766	Er2	2.3609	103.058
	Er6	2.2483	Er5	2.2757	111.014
	Er6	2.2483	Er2	2.3609	111.756
	Er5	2.2757	Er2	2.3609	101.316
O13	B2	1.3659	O15	1.9817	96.240
			Er6	2.3717	126.700
			O14	2.3860	28.538
			O8	2.3897	31.125
			Er2	2.4013	112.669
	O15	1.9817	Er6	2.3717	110.214
			O14	2.3860	70.938
			O8	2.3897	124.978
			Er2	2.4013	104.417
	Er6	2.3717	O14	2.3860	148.303
	Er6	2.3717	O8	2.3897	100.702
	Er6	2.3717	Er2	2.4013	104.494
	O14	2.3860	O8	2.3897	59.559
	O14	2.3860	Er2	2.4013	105.735
	O8	2.3897	Er2	2.4013	110.459
O7	Er4	2.2310	Er5	2.2521	115.369
	Er4	2.2310	Er1	2.3268	99.599
	Er4	2.2310	Er3	2.3807	120.927
	Er5	2.2521	Er1	2.3268	99.858
	Er5	2.2521	Er3	2.3807	114.406
	Er1	2.3268	Er3	2.3807	101.252
O5	Er2	2.2044	Er4	2.2436	109.043
	Er2	2.2044	Er1	2.2672	136.715

	Er2	2.2044	Er1	2.3179	103.292
	Er4	2.2436	Er1	2.2672	101.045
	Er4	2.2436	Er1	2.3179	100.742
	Er1	2.2672	Er1	2.3179	100.753
O1	B1	1.3486	O2	2.3269	30.805
			O3	2.3355	31.609
			Er2	2.3782	134.360
			Er6	2.3812	103.341
			Er4	2.3874	91.889
	O2	2.3269	O3	2.3355	62.157
			Er2	2.3782	125.418
			Er6	2.3812	126.698
			Er4	2.3874	62.667
			Er2	2.3782	132.899
			Er6	2.3812	75.021
	O3	2.3355	Er4	2.3874	119.488
	Er2	2.3782	Er6	2.3812	106.613
			Er4	2.3874	98.941
	Er6	2.3812	Er4	2.3874	123.886
O2	B1	1.3574	O15	2.2300	85.961
			O1	2.3269	30.583
			Er2	2.3491	130.036
			O3	2.4068	28.784
			Er4	2.4521	88.928
	O15	2.2300	O1	2.3269	111.867
			Er2	2.3491	98.631
			O3	2.4068	65.196
			Er4	2.4521	164.952
	O1	2.3269	Er2	2.3491	135.182

			O3	2.4068	59.097
			Er4	2.4521	59.875
	Er2	2.3491	O3	2.4068	110.966
			Er4	2.4521	95.495
	O3	2.4068	Er4	2.4521	114.199
O12	B3	1.3137	O11	2.2924	30.679
	B3	1.3137	O6	2.3314	30.963
	B3	1.3137	Er6	2.3368	97.928
	B3	1.3137	Er2	2.3664	134.276
	B3	1.3137	Er5	2.4829	99.223
	O11	2.2924	O6	2.3314	61.574
	O11	2.2924	Er6	2.3368	72.962
	O11	2.2924	Er2	2.3664	125.687
	O11	2.2924	Er5	2.4829	120.948
	O6	2.3314	Er6	2.3368	120.356
	O6	2.3314	Er2	2.3664	130.432
	O6	2.3314	Er5	2.4829	74.296
	Er6	2.3368	Er2	2.3664	106.717
	Er6	2.3368	Er5	2.4829	101.322
	Er2	2.3664	Er5	2.4829	112.444
O11	B3	1.3419	O12	2.2924	29.967
	B3	1.3419	O15	2.3643	86.798
	B3	1.3419	O6	2.3669	30.126
	B3	1.3419	Er5	2.4641	146.729
	O12	2.2924	O15	2.3643	111.445
	O12	2.2924	O6	2.3669	60.025
	O12	2.2924	Er5	2.4641	122.810
	O15	2.3643	O6	2.3669	64.057
	O15	2.3643	Er5	2.4641	96.984

	O6	2.3669	Er5	2.4641	157.552
O14	B2	1.3537	Er6	2.2844	121.297
	B2	1.3537	Er3	2.3134	124.095
	B2	1.3537	O8	2.3720	31.583
	B2	1.3537	O13	2.3860	28.819
	Er6	2.2844	Er3	2.3134	112.929
	Er6	2.2844	O8	2.3720	105.073
	Er6	2.2844	O13	2.3860	131.603
	Er3	2.3134	O8	2.3720	122.661
	Er3	2.3134	O13	2.3860	112.971
	O8	2.3720	O13	2.3860	60.298
O8	B2	1.4100	O15	2.0171	102.398
	B2	1.4100	Er4	2.2542	113.754
	B2	1.4100	O14	2.3720	30.188
	B2	1.4100	O13	2.3897	30.050
	B2	1.4100	Er1	2.3919	125.615
	O15	2.0171	Er4	2.2542	103.876
	O15	2.0171	O14	2.3720	101.894
	O15	2.0171	O13	2.3897	102.584
	O15	2.0171	Er1	2.3919	111.397
	Er4	2.2542	O14	2.3720	85.011
	Er4	2.2542	O13	2.3897	139.774
	Er4	2.2542	Er1	2.3919	98.225
	O14	2.3720	O13	2.3897	60.142
	O14	2.3720	Er1	2.3919	144.513
	O13	2.3897	Er1	2.3919	99.667
O3	B1	1.3815	O1	2.3355	30.772
	B1	1.3815	Er3	2.3872	124.309
	B1	1.3815	Er3	2.3990	126.442

	B1	1.3815	O2	2.4068	28.237
	O1	2.3355	Er3	2.3872	129.025
	O1	2.3355	Er3	2.3990	109.875
	O1	2.3355	O2	2.4068	58.746
	Er3	2.3872	Er3	2.3990	109.134
	Er3	2.3872	O2	2.4068	107.368
	Er3	2.3990	O2	2.4068	137.773
O6	B3	1.3815	O12	2.3314	29.290
	B3	1.3815	Er3	2.3517	131.454
	B3	1.3815	O11	2.3669	29.177
	B3	1.3815	Er1	2.3991	130.006
	O12	2.3314	Er3	2.3517	112.131
	O12	2.3314	O11	2.3669	58.401
	O12	2.3314	Er1	2.3991	139.435
	Er3	2.3517	O11	2.3669	143.588
	Er3	2.3517	Er1	2.3991	98.534
	O11	2.3669	Er1	2.3991	109.588
B3	O12	1.3137	O11	1.3419	119.354
	O12	1.3137	O6	1.3815	119.747
	O11	1.3419	O6	1.3815	120.697
B1	O1	1.3486	O2	1.3574	118.612
	O1	1.3486	O3	1.3815	117.619
	O2	1.3574	O3	1.3815	122.979
B2	O14	1.3537	O13	1.3659	122.643
	O14	1.3537	O8	1.4100	118.228
	O13	1.3659	O8	1.4100	118.826
O15	O13	1.9817	O8	2.0171	100.445
	O13	1.9817	O2	2.2300	83.609
	O13	1.9817	O11	2.3643	127.275

	O8	2.0171	O2	2.2300	158.340
	O8	2.0171	O11	2.3643	84.230
	O2	2.2300	O11	2.3643	76.626

Table S3. Anisotropic displacement parameters for $Er_6B_4O_{15}$

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{12}**	**U_{13}**	**U_{23}**
Er1	0.0073(5)	0.0074(5)	0.0074(5)	0.00001(10)	0.00035(10)	-0.00004(10)
Er2	0.0078(5)	0.0078(5)	0.0079(5)	0.0000(1)	0.00034(10)	-0.00001(10)
Er5	0.0108(5)	0.0109(5)	0.0108(5)	0.00008(10)	0.00041(10)	-0.00002(10)
Er3	0.0092(5)	0.0093(5)	0.0093(5)	0.0000(1)	0.00038(10)	0.00002(10)
Er4	0.0088(5)	0.0088(5)	0.0089(5)	0.00001(10)	0.00035(10)	0.00003(10)
Er6	0.0098(5)	0.0098(5)	0.0099(5)	-0.00001(10)	0.00038(10)	-0.00002(10)