Electronic Supplementary Information

High-Temperature, High-Pressure Hydrothermal Synthesis, Crystal Structure and Photoluminescent Properties of $K_3[Gd_{1-x}Tb_xGe_3O_8(OH)_2]$ (x = 0, 0.3, 0.1, 1)

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Contents

Table S1. Bond lengths [Å] and angles [deg] for $K_3[GdGe_3O_8(OH)_2]$.

bond	bond length (Å)	bond angle	value (deg)
Gd(1)-O(6)#1	2.224(3)	O(6)#7-Gd(1)-O(1)	171.33(12)
Gd(1)-O(1)	2.264(3)	O(6)#7-Gd(1)-O(2)#2	88.28(8)
Gd(1)-O(2)#2	2.290(2)	O(1)-Gd(1)-O(2)#2	97.54(8)
Gd(1)-O(2)#3	2.290(2)	O(6)#7-Gd(1)-O(2)#3	88.28(8)
Gd(1)-O(3)	2.340(2)	O(1)-Gd(1)-O(2)#3	97.54(8)
Gd(1)-O(3)#4	2.340(2)	O(2)#8-Gd(1)-O(2)#3	95.27(12)
Ge(2)-O(1)	1.702(3)	O(6)#7-Gd(1)-O(3)	88.16(8)
Ge(2)-O(6)	1.703(3)	O(1)-Gd(1)-O(3)	85.67(8)
Ge(2)-O(4)	1.779(2)	O(2)#8-Gd(1)-O(3)	175.31(8)
Ge(2)-O(4)#4	1.779(2)	O(2)#9-Gd(1)-O(3)	87.68(9)
Ge(1)-O(2)	1.716(2)	O(6)#7-Gd(1)-O(3)#4	88.16(8)
Ge(1)-O(3)	1.729(2)	O(1)-Gd(1)-O(3)#6	85.67(8)
Ge(1)-O(4)	1.766(2)	O(2)#8-Gd(1)-O(3)#4	87.68(9)
Ge(1)-O(5)	1.789(2)	O(2)#9-Gd(1)-O(3)#4	175.31(8)
		O(3)-Gd(1)-O(3)#4	89.16(12)
		O(1)-Ge(2)-O(6)	116.86(15)
		O(1)-Ge(2)-O(4)	113.01(9)
		O(6)-Ge(2)-O(4)	104.83(10)
		O(1)-Ge(2)-O(4)#4	113.01(9)
		O(6)-Ge(2)-O(4)#4	104.83(10)
		O(4)-Ge(2)-O(4)#4	102.95(16)
		O(2)-Ge(1)-O(3)	113.54(11)
		O(2)-Ge(1)-O(4)	112.84(11)
		O(3)-Ge(1)-O(4)	111.47(10)
		O(2)-Ge(1)-O(5)	109.75(11)
		O(3)-Ge(1)-O(5)	110.72(11)
		O(4)-Ge(1)-O(5)	97.38

Symmetry transformations used to generate equivalent atoms

#1 x+1/2,y,-z+3/2 #2 x,-y+1/2,z+1 #3 x,y,z+1 #4 x,-y+1/2,z

Table S2. Bond lengths [Å] and angles [deg] for $K_3[TbGe_3O_8(OH)_2]$.

bond	bond length (Å)	bond angle	value (deg)
Tb(1)-O(2)#1	2.211(4)	O(2)#1-Tb(1)-O(1)	171.41(13)
Tb(1)-O(1)	2.253(3)	O(2)#1-Tb(1)-O(4)#2	88.36(9)
Tb(1)-O(4)#2	2.277(3)	O(1)-Tb(1)-O(4)#2	97.42(9)
Tb(1)-O(4)#3	2.277(3)	O(2)#1-Tb(1)-O(4)#3	88.36(9)
Tb(1)-O(6)	2.321(2)	O(1)-Tb(1)-O(4)#3	97.42(9)
Tb(1)-O(6)#4	2.321(2)	O(4)#2-Tb(1)-O(4)#3	95.01(14)
Ge(2)-O(2)	1.701(4)	O(2)#1-Tb(1)-O(6)	88.19(9)
Ge(2)-O(1)	1.702(3)	O(1)-Tb(1)-O(6)	85.70(9)
Ge(2)-O(5)	1.778(2)	O(4)#2-Tb(1)-O(6)	87.71(10)
Ge(2)-O(5)#4	1.778(2)	O(4)#3-Tb(1)-O(6)	175.54(9)
Ge(3)-O(4)	1.712(2)	O(2)#1-Tb(1)-O(6)#4	88.19(9)
Ge(3)-O(6)	1.728(2)	O(1)-Tb(1)-O(6)#4	85.70(9)
Ge(3)-O(5)	1.765(2)	O(4)#2-Tb(1)-O(6)#4	175.54(9)
Ge(3)-O(3)	1.785(3)	O(6)-Tb(1)-O(6)#4	89.35(13)
		O(2)-Ge(2)-O(1)	116.74(17)
		O(2)-Ge(2)-O(5)	104.99(11)
		O(1)-Ge(2)-O(5)	113.09(10)
		O(2)-Ge(2)-O(5)#4	104.99(11)
		O(1)-Ge(2)-O(5)#4	113.09(10)
		O(5)-Ge(2)-O(5)#4	102.56(17)
		O(4)-Ge(3)-O(6)	113.68(12)
		O(4)-Ge(3)-O(5)	113.05(12)
		O(6)-Ge(3)-O(5)	111.28(11)
		O(4)-Ge(3)-O(3)	109.66(12)
		O(6)-Ge(3)-O(3)	110.68(13)
		O(5)-Ge(3)-O(3)	97.32(12)

Symmetry transformations used to generate equivalent atoms

#1 x+1/2,y,-z+3/2 #2 x,y,z+1 #3 x,-y+1/2,z+1 #4 x,-y+1/2,z

Table S3. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $K_3[GdGe_3O_8(OH)_2]$.

	x	y	z	U(eq)
Gd(1)	0.458173	0.250000	0.912183	0.00750
Ge(1)	0.400742	0.099771	0.409040	0.00955
Ge(2)	0.244916	0.250000	0.585821	0.00951
O(1)	0.296124	0.250000	0.843473	0.01473
O(2)	0.468473	0.130076	0.639114	0.01717
O(3)	0.458613	0.126591	0.167052	0.01749
O(4)	0.281993	0.147307	0.423864	0.01876
O(5)	0.367972	-0.027966	0.412826	0.01788
O(6)	0.120639	0.250000	0.574222	0.02209
K(1)	0.135087	0.016618	0.410827	0.02906
K(2)	0.130232	0.250000	0.082573	0.02848

Table S4. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $K_3[TbGe_3O_8(OH)_2]$.

	x	y	z	U(eq)
Tb(1)	0.458263	0.250000	0.911147	0.00605
Ge(1)	0.244483	0.250000	0.586383	0.00772
Ge(2)	0.400869	0.100214	0.408091	0.00787
O(1)	0.296661	0.250000	0.841605	0.01365
O(2)	0.119799	0.250000	0.575470	0.02100
O(3)	0.368485	-0.026446	0.412446	0.01520
O(4)	0.458785	0.126737	0.164955	0.01587
O(5)	0.280948	0.148067	0.422984	0.01539
O(6)	0.468216	0.130497	0.640207	0.01509
K(1)	0.130593	0.250000	0.082887	0.02571
K(2)	0.135261	0.015877	0.410223	0.02757

Table S5. EDS analysis data of K_3 [$GdGe_3O_8$ (OH) $_2$] and K_3 [$TbGe_3O_8$ (OH) $_2$], K_3 [$Gd_{0.7}Tb_{0.3}Ge_3O_8$ (OH) $_2$] and K_3 [$Gd_{0.9}Tb_{0.1}Ge_3O_8$ (OH) $_2$]

	K	Gd	Ge	Tb
$K_3[GdGe_3O_8(OH)_2]$	3.0	1	2.98	0
$K_3[Gd_{0.7}Tb_{0.3}Ge_3O_8(OH)_2]$	3.0	0.7	3.0	0.3
$K_3[Gd_{0.9}Tb_{0.1}Ge_3O_8(OH)_2]$	3.0	0.89	3.0	0.11
$K_3[TbGe_3O_8(OH)_2]$	3.0	0	3.0	1

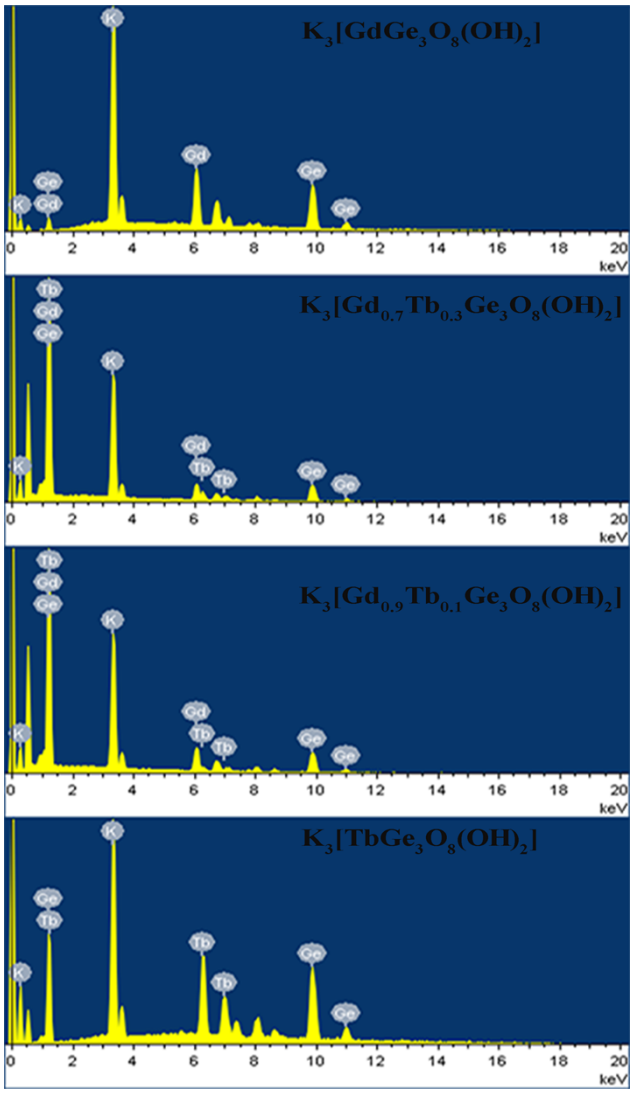

Figure S1. EDS analysis of K_3 [$GdGe_3O_8$ $(OH)_2$] and K_3 [$TbGe_3O_8$ $(OH)_2$], K_3 [$Gd_{0.7}Tb_{0.3}Ge_3O_8$ $(OH)_2$] and K_3 [$Gd_{0.9}Tb_{0.1}Ge_3O_8$ $(OH)_2$]

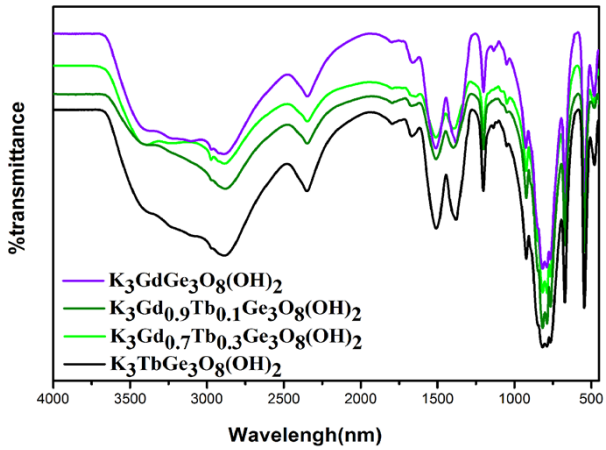

Figure S2. The IR spectra of K_3 [$GdGe_3O_8$ $(OH)_2$] and K_3 [$TbGe_3O_8$ $(OH)_2$], K_3 [$Gd_{0.7}Tb_{0.3}Ge_3O_8$ $(OH)_2$] and K_3 [$Gd_{0.9}Tb_{0.1}Ge_3O_8$ $(OH)_2$]