

***On the Crystal Structure and Optical Spectroscopy of Rare
Earth Comprising Quaternary Tungstates***



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Supporting tables

Table S1: Interatomic distances (pm) for $\text{Li}_3\text{Ba}_2\text{Pr}_3(\text{WO}_4)_8$. All distances of the first coordination spheres are listed. Standard deviations are given in parentheses.

W1: 1 O1 176(1)	Ba1: 2 O6 273(1)	Pr/Li1: 1 O5 242(1)
1 O3 178.4(9)	2 O8 274(1)	1 O3 245(1)
1 O2 180(1)	2 O1 288(1)	1 O7 248(1)
1 O4 181(1)	2 O5 296(1)	1 O7 248(1)
W2: 1 O8 175.2(9)	Li2: 2 O1 199(3)	1 O4 251(1)
1 O6 175(1)	2 O6 219(3)	1 O2 252(1)
1 O5 178.6(9)	2 O8 237(1)	1 O4 253(1)
1 O7 182(1)		1 O2 255.2(9)

Table S2: Anisotropic displacement parameters (pm^2) of $\text{Li}_3\text{Ba}_2\text{Pr}_3(\text{WO}_4)_8$ and $\text{Li}_3\text{Ba}_2\text{Tb}_3(\text{WO}_4)_8$. Standard deviations are given in parentheses. The Li2 positions (Table 3) were refined isotropically.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
$\text{Li}_3\text{Ba}_2\text{Pr}_3(\text{WO}_4)_8$						
W1	102(2)	133(2)	108(3)	9(2)	22(2)	17(2)
W2	99(2)	117(2)	120(3)	-3(2)	18(2)	6(2)
Ba1	136(5)	116(4)	147(7)	0	13(4)	0
0.75 Pr / 0.25 Li1	99(3)	96(3)	84(5)	7(3)	15(3)	-7(3)
O1	130(40)	190(40)	190(60)	30(30)	60(40)	40(40)
O2	140(40)	110(40)	220(60)	0(30)	40(40)	30(40)
O3	260(50)	110(40)	90(50)	-40(30)	-30(40)	10(30)
O4	220(50)	190(40)	160(60)	20(40)	50(40)	40(40)
O5	180(40)	170(40)	120(60)	30(30)	0(40)	10(40)
O6	210(50)	150(40)	120(60)	20(30)	-20(40)	0(30)
O7	190(40)	250(50)	110(60)	130(40)	90(30)	70(40)
O8	120(40)	190(40)	240(70)	0(30)	20(40)	40(40)
$\text{Li}_3\text{Ba}_2\text{Tb}_3(\text{WO}_4)_8$						
W1	138(1)	125(1)	146(2)	2(1)	-1(1)	11(1)
W2	138(1)	125(1)	150(2)	-3(1)	-2(1)	5(1)
Ba1	182(2)	109(2)	197(3)	0	-10(2)	0
0.75 Tb / 0.25 Li1	133(2)	106(2)	133(2)	2(1)	-5(1)	-3(1)
O1	190(20)	170(20)	250(30)	19(18)	0(20)	21(19)
O2	180(20)	210(20)	190(30)	-42(19)	11(19)	47(19)
O3	200(20)	180(20)	170(30)	-40(18)	20(18)	15(18)
O4	220(20)	190(20)	170(30)	13(19)	-30(19)	-32(18)
O5	200(20)	120(20)	200(30)	15(17)	-5(19)	8(17)
O6	190(20)	160(20)	190(30)	12(18)	-36(19)	-11(18)
O7	160(20)	170(20)	230(30)	13(18)	30(19)	51(19)
O8	170(20)	170(20)	200(30)	12(17)	-32(19)	35(18)