

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for LnMoBO_6 (Ln=La,Ce)

Atom	Site	x	y	z	U_{eq}^{a}
LaMoBO₆					
La1	4e	0.16948(6)	0.71951(12)	-0.01458(2)	0.0090(2)
La2	4e	0.33106(6)	0.24650(11)	0.26419(2)	0.0091(2)
Mo1	4e	0.03429(9)	0.19089(18)	0.33940(4)	0.0083(3)
Mo2	4e	0.46656(8)	-0.33058(19)	0.41015(3)	0.0078(3)
O1	4e	0.4082(7)	0.7670(13)	0.2073(3)	0.0108(14)
O2	4e	0.3996(8)	-0.2416(13)	0.3278(3)	0.0129(15)
O3	4e	0.0894(7)	1.2675(13)	0.0426(3)	0.0119(14)
O4	4e	0.1022(7)	0.2799(13)	0.4222(3)	0.0116(15)
O5	4e	0.2297(7)	0.8401(13)	0.1001(3)	0.0108(13)
O6	4e	-0.1496(7)	0.2828(14)	0.2912(3)	0.0160(15)
O7	4e	0.3500(8)	0.7469(14)	-0.0558(3)	0.0176(16)
O8	4e	0.6516(7)	-0.2418(14)	0.4590(3)	0.0143(15)
O9	4e	0.4699(9)	-0.7480(14)	0.4030(4)	0.0214(17)
O10	4e	0.1506(8)	0.2753(14)	0.3058(3)	0.0162(15)
O11	4e	0.0320(8)	-0.2256(14)	0.3463(4)	0.0202(17)
O12	4e	0.2681(6)	0.3386(14)	0.1487(3)	0.0118(13)
B1	4e	0.3051(11)	0.666(2)	0.1540(5)	0.011(2)
B2	4e	0.193(1)	1.166(2)	0.0952(4)	0.0080(18)
CeMoBO₆					
Ce1	4e	0.19653(3)	0.28091(7)	0.52922(2)	0.00677(15)
Mo1	4e	0.35455(5)	0.68761(10)	0.81901(4)	0.00573(16)
O1	4e	-0.0044(4)	0.2691(6)	0.5852(3)	0.0074(7)
O2	4e	0.2586(4)	0.7779(7)	0.6528(3)	0.0100(8)
O3	4e	0.4604(5)	0.2674(7)	0.6094(4)	0.0152(8)
O4	4e	0.2654(4)	0.7264(7)	0.4144(3)	0.0133(8)
O5	4e	0.3382(5)	0.2684(8)	0.8036(4)	0.0181(9)
O6	4e	-0.0305(4)	-0.1603(7)	0.7002(3)	0.0091(7)
B1	4e	-0.0041(6)	0.1664(11)	0.6910(5)	0.0087(10)

^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond distances (Å) and angles (°) for LnMoBO₆ (Ln=La,Ce)

LaMoBO ₆					
La1—O7	2.450(7)	La2—O2	2.457(7)	Mo1—O10	1.739(7)
La1—O3 ⁱ	2.455(7)	La2—O10	2.472(7)	Mo1—O11	1.743(6)
La1—O4 ⁱⁱ	2.486(6)	La2—O1 ^{vii}	2.535(6)	Mo1—O6	1.784(7)
La1—O4 ⁱⁱⁱ	2.491(6)	La2—O2 ^{viii}	2.576(6)	Mo1—O4	1.830(7)
La1—O5	2.582(6)	La2—O12	2.617(6)	Mo1—O11 ^{viii}	2.436(6)
La1—O8 ^{iv}	2.598(6)	La2—O6 ^{ix}	2.717(6)	Mo2—O7 ^{xi}	1.746(8)
La1—O3 ^v	2.655(6)	La2—O1 ^v	2.845(6)	Mo2—O9	1.748(6)
La1—O8 ^{vi}	2.844(6)	La2—O1	2.847(6)	Mo2—O8	1.797(7)
La1—O3	2.952(6)	La2—O6 ^x	2.993(8)	Mo2—O2	1.820(7)
La1—O11 ⁱⁱ	2.999(8)	La2—O9 ^{viii}	2.457(7)	Mo2—O9 ^{viii}	2.433(6)
B1—O1	1.327(12)	B1—O5	1.388(11)	B1—O12	1.408(11)
B2—O3	1.319(11)	B2—O5	1.401(11)	B2—O12 ^{viii}	1.377(11)
O10—Mo1—O11	106.5(3)	O4—Mo1—O11 ^{viii}	74.6(3)	O8—Mo2—O9 ^{viii}	78.3(3)
O10—Mo1—O6	114.1(3)	O7 ^{xi} —Mo2—O9	106.8(3)	O2—Mo2—O9 ^{viii}	74.4(3)
O11—Mo1—O6	102.8(3)	O7 ^{xi} —Mo2—O8	114.0(3)	O1—B1—O5	128.6(8)
O10—Mo1—O4	115.9(3)	O9—Mo2—O8	102.0(3)	O1—B1—O12	117.9(8)
O11—Mo1—O4	96.5(3)	O7 ^{xi} —Mo2—O2	116.3(3)	O5—B1—O12	113.5(8)
O6—Mo1—O4	117.5(3)	O9—Mo2—O2	96.4(3)	O3—B2—O12 ^{viii}	128.2(8)
O10—Mo1—O11 ^{viii}	81.8(3)	O8—Mo2—O2	117.7(3)	O3—B2—O5	117.9(8)
O11—Mo1—O11 ^{viii}	170.1(4)	O7 ^{xi} —Mo2—O9 ^{viii}	82.3(3)	O12 ^{viii} —B2—O5	113.8(7)
O6—Mo1—O11 ^{viii}	78.0(3)	O9—Mo2—O9 ^{viii}	169.5(4)		
CeMoBO ₆					
Ce1—O1	2.427(4)	Ce1—O1 ⁱⁱⁱ	2.619(3)	Mo1—O4 ^v	1.780(4)
Ce1—O3	2.438(4)	Ce1—O4 ⁱ	2.918(3)	Mo1—O2	1.823(4)
Ce1—O2	2.450(3)	Ce1—O1 ⁱⁱ	2.929(3)	Mo1—O5 ^{vi}	2.417(3)
Ce1—O2 ⁱ	2.472(3)	Ce1—O5	2.939(4)	B1—O1	1.330(6)
Ce1—O6 ⁱⁱ	2.556(3)	Mo1—O3 ^{iv}	1.734(4)	B1—O6 ^x	1.386(6)
Ce1—O4	2.577(3)	Mo1—O5	1.750(3)	B1—O6	1.396(5)
O3 ^{iv} —Mo1—O5	105.98(18)	O5—Mo1—O2	96.25(17)	O4 ^v —Mo1—O5 ^{vi}	79.10(14)
O3 ^{iv} —Mo1—O4 ^v	113.81(19)	O4 ^v —Mo1—O2	118.12(17)	O2—Mo1—O5 ^{vi}	74.10(13)
O5—Mo1—O4 ^v	102.37(18)	O3 ^{iv} —Mo1—O5 ^{vi}	82.60(15)	O1—B1—O6 ^x	127.9(4)
O3 ^{iv} —Mo1—O2	116.47(18)	O5—Mo1—O5 ^{vi}	169.4(2)	O1—B1—O6	117.8(4)
O6 ^x —B1—O6	114.1(4)				

Symmetry codes: LaMoBO₆: (i) -x, 2-y, -z; (ii) x, 0.5-y, -0.5+z; (iii) x, 1.5-y, -0.5+z; (iv) 1-x, 0.5+y, 0.5-z;

(v) $x, -1+y, z$; (vi) $1-x, 1.5+y, 0.5-z$; (vii) $1-x, -0.5+y, 0.5-z$; (viii) $x, 1+y, z$; (ix) $-x, -0.5+y, 0.5-z$; (x) $-x, 0.5+y, 0.5-z$; (xi) $x, 0.5-y, 0.5+z$; (xii) $x, 1.5-y, 0.5+z$; (xiii) $1-x, -1.5+y, 0.5-z$.

CeMoBO₆: (i) $x, -1+y, z$; (ii) $-x, -y, 1-z$; (iii) $-x, 1-y, 1-z$; (iv) $1-x, 0.5+y, 1.5-z$; (v) $x, 1.5-y, 0.5+z$; (vi) $x, 1+y, z$; (vii) $1-x, -0.5+y, 1.5-z$; (viii) $x, 1.5-y, -0.5+z$; (ix) $-x, -0.5+y, 1.5-z$; (x) $-x, 0.5+y, 1.5-z$.

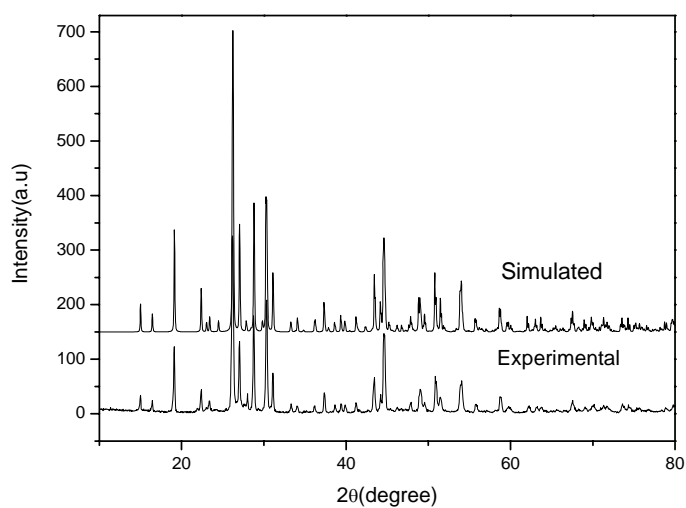


Figure S1. Experimental and simulated X-ray powder diffraction patterns of LaMoBO₆

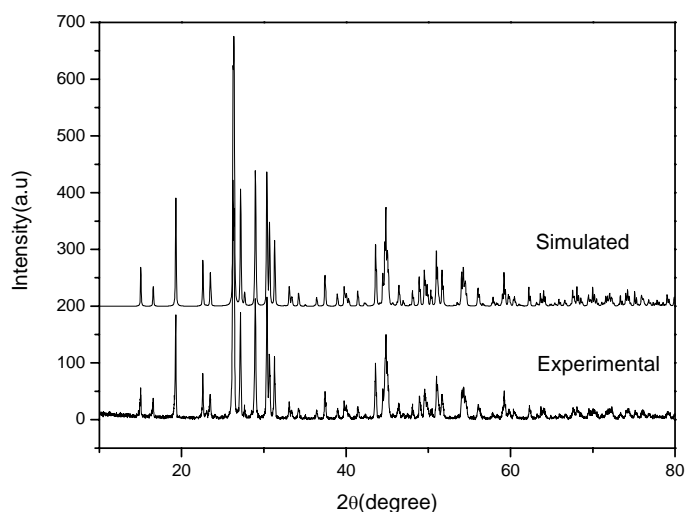


Figure S2. Experimental and simulated X-ray powder diffraction patterns of CeMoBO₆

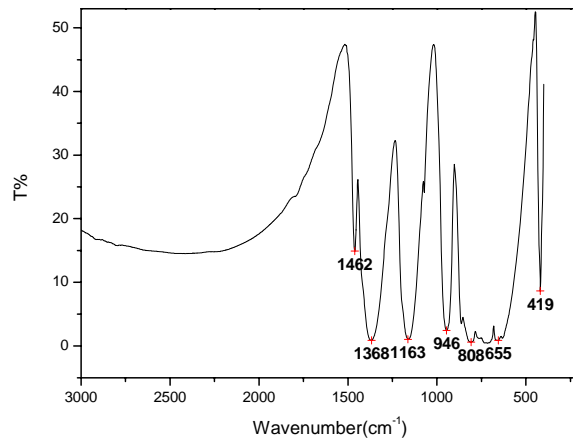


Figure S3. The IR spectrum of LaMoBO₆

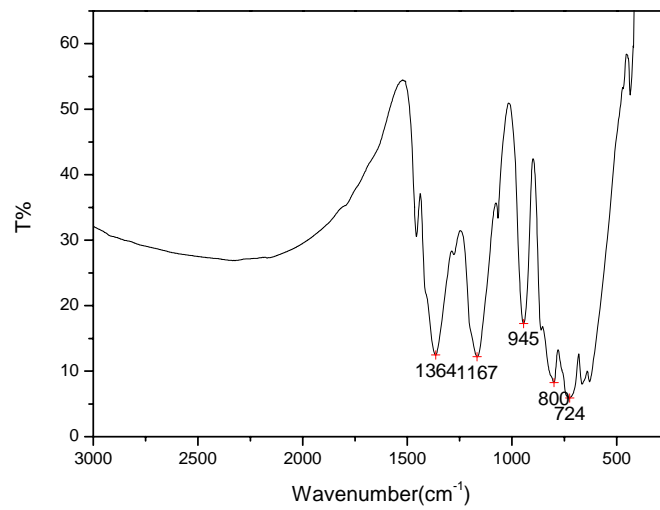


Figure S4. The IR spectrum of CeMoBO₆

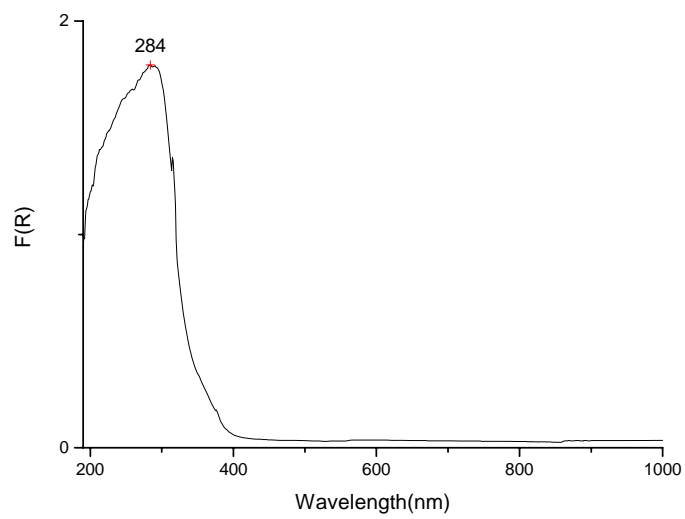
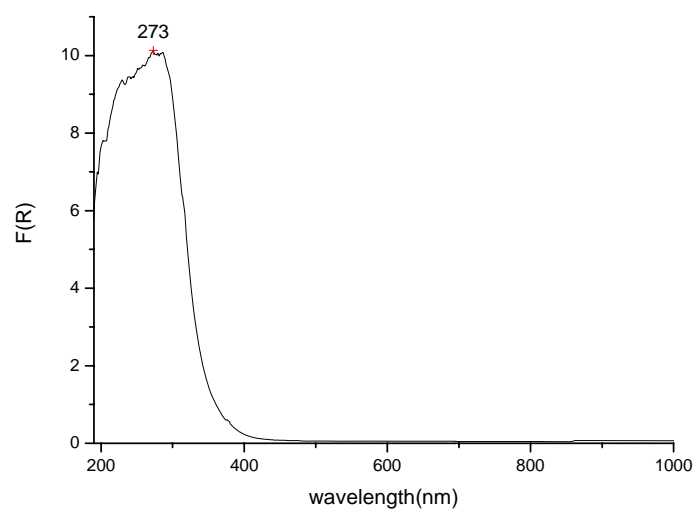


Figure S5. The absorption spectra of compounds LaMoBO_6



(b)

Figure S6. The absorption spectra of compounds CeMoBO_6

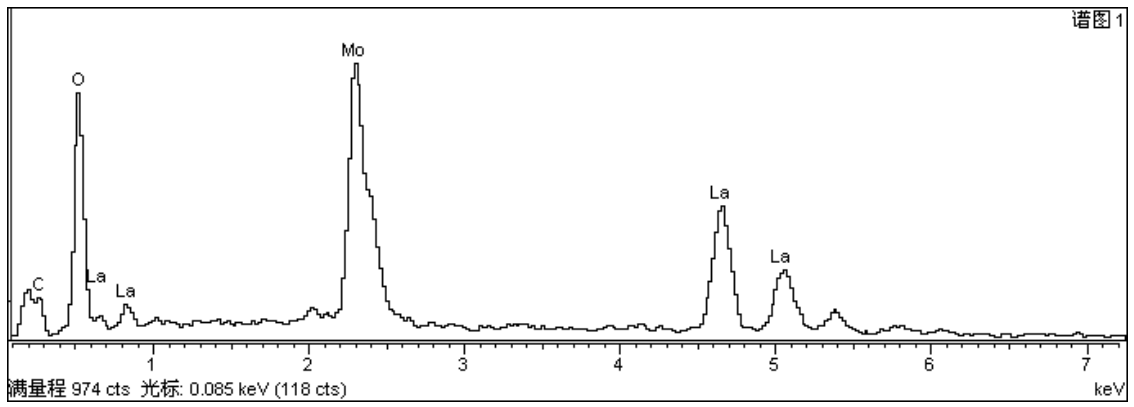


Figure S7. Full results of elemental analysis for LaMoBO₆

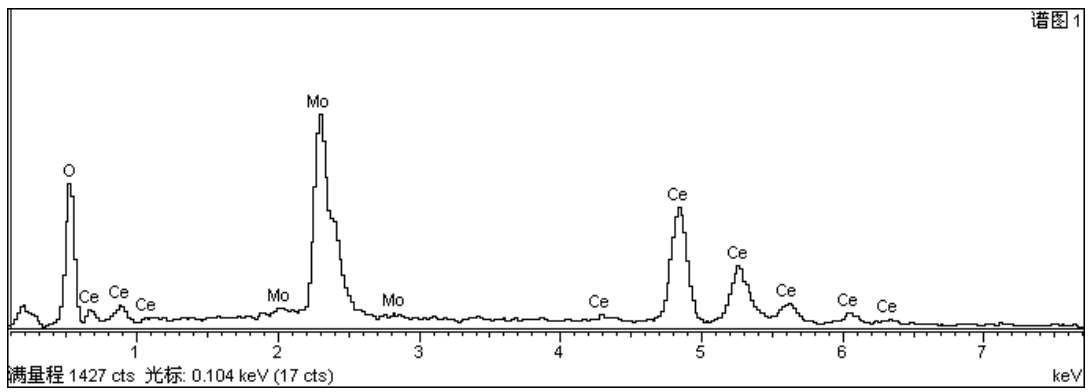


Figure S8. Full results of elemental analysis for CeMoBO₆