

Supporting Information

Crystal Chemistry and Luminescent Properties of Red-Emitting CsGd_{1-x}Eu_x(MoO₄)₂ Solid-Solution Phosphors

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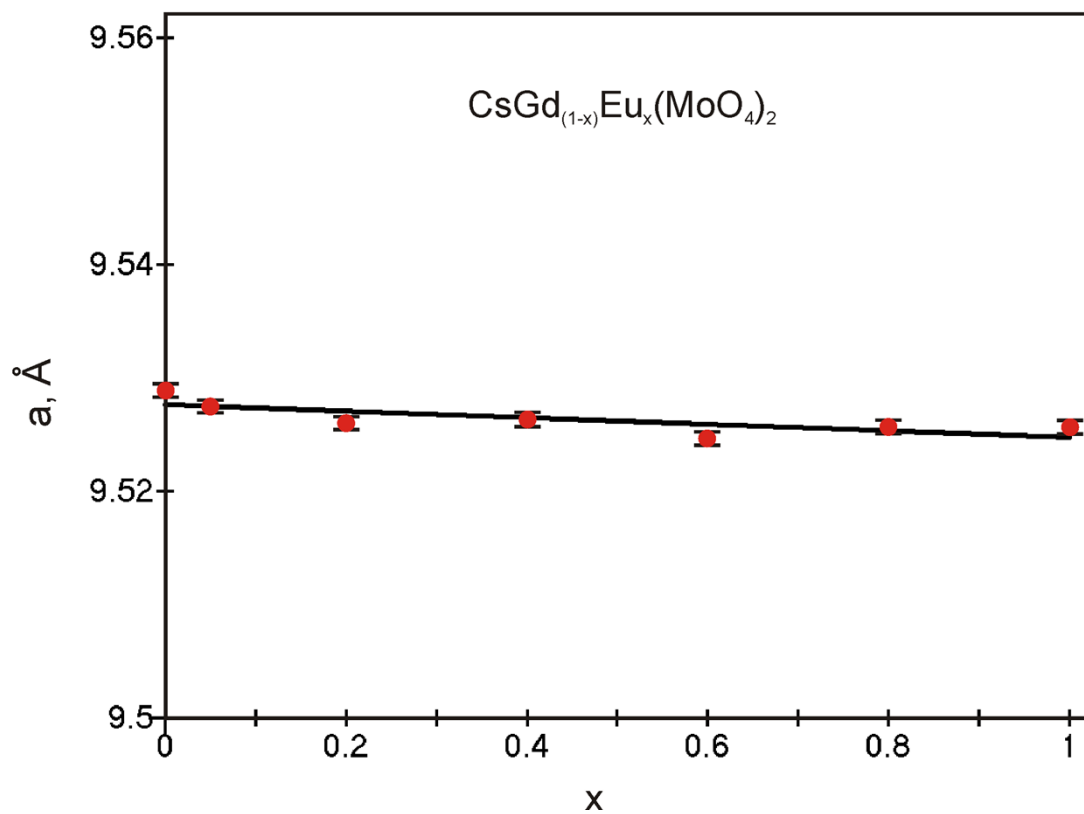


Fig. 1S. Dependence of unit cell parameter a on x in solid solutions $\text{CsGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$.

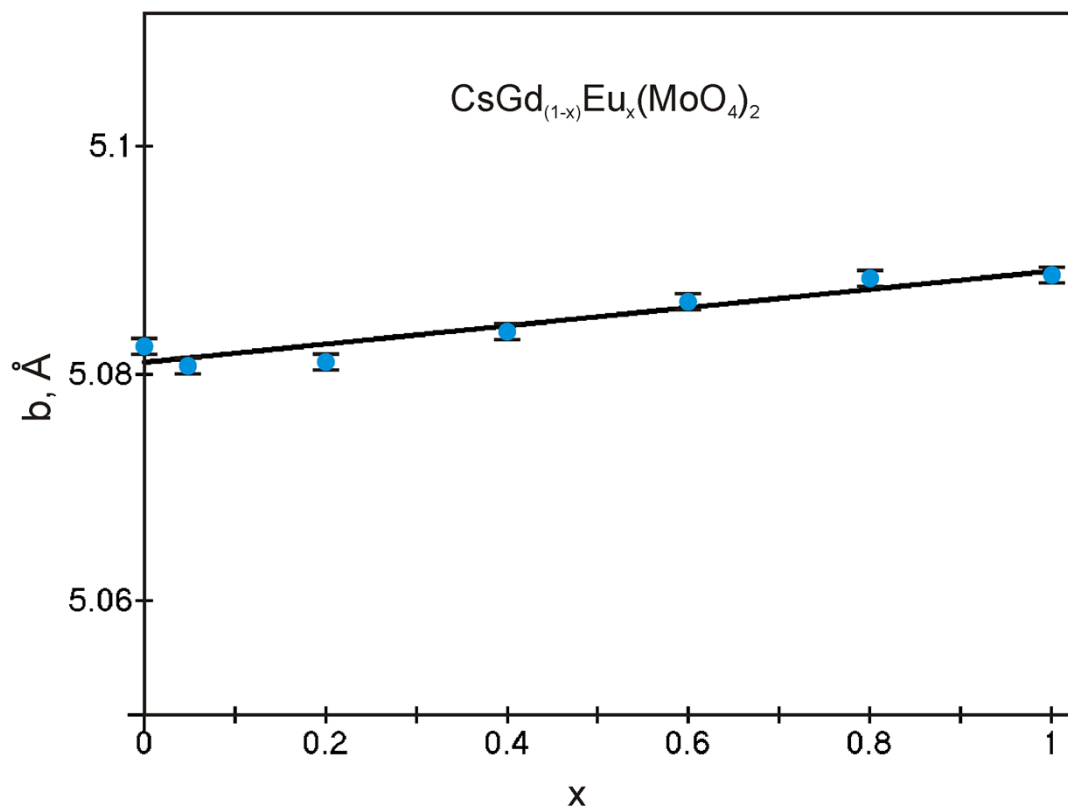


Fig. 2S. Dependence of unit cell parameter b on x in solid solutions $\text{CsGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$.

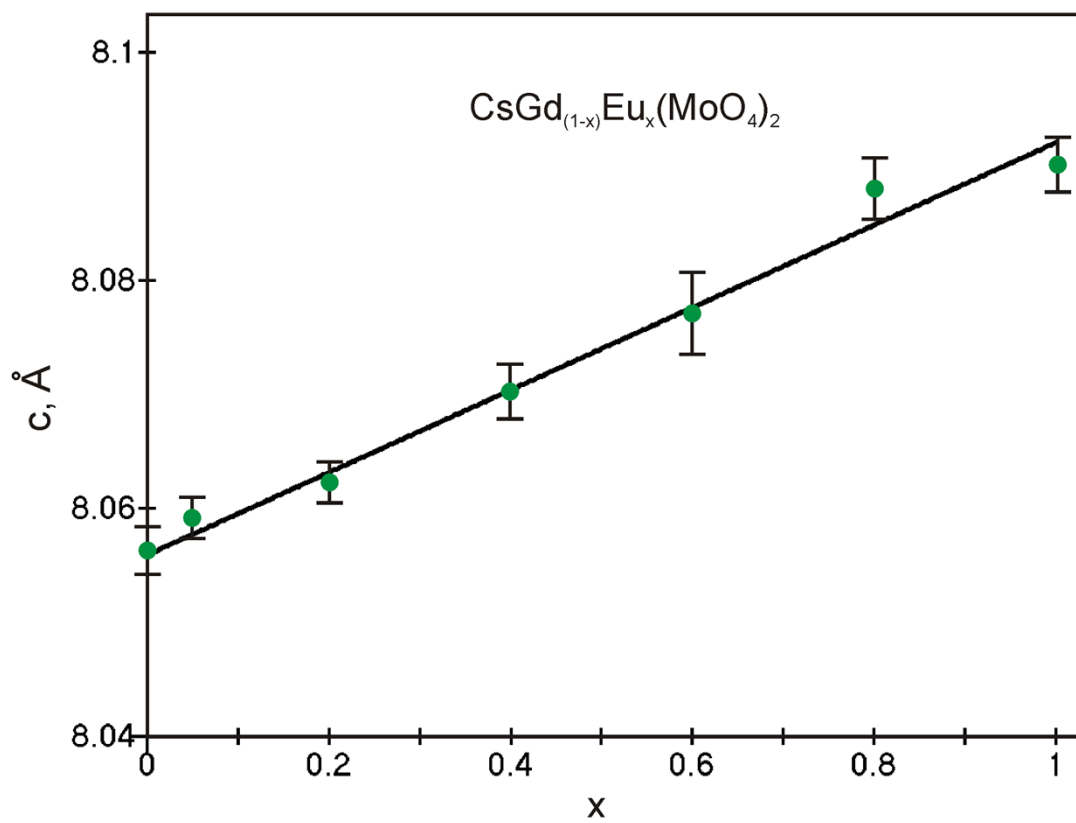


Fig. 3S. Dependence of unit cell parameter c on x in solid solutions $\text{CsGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$.

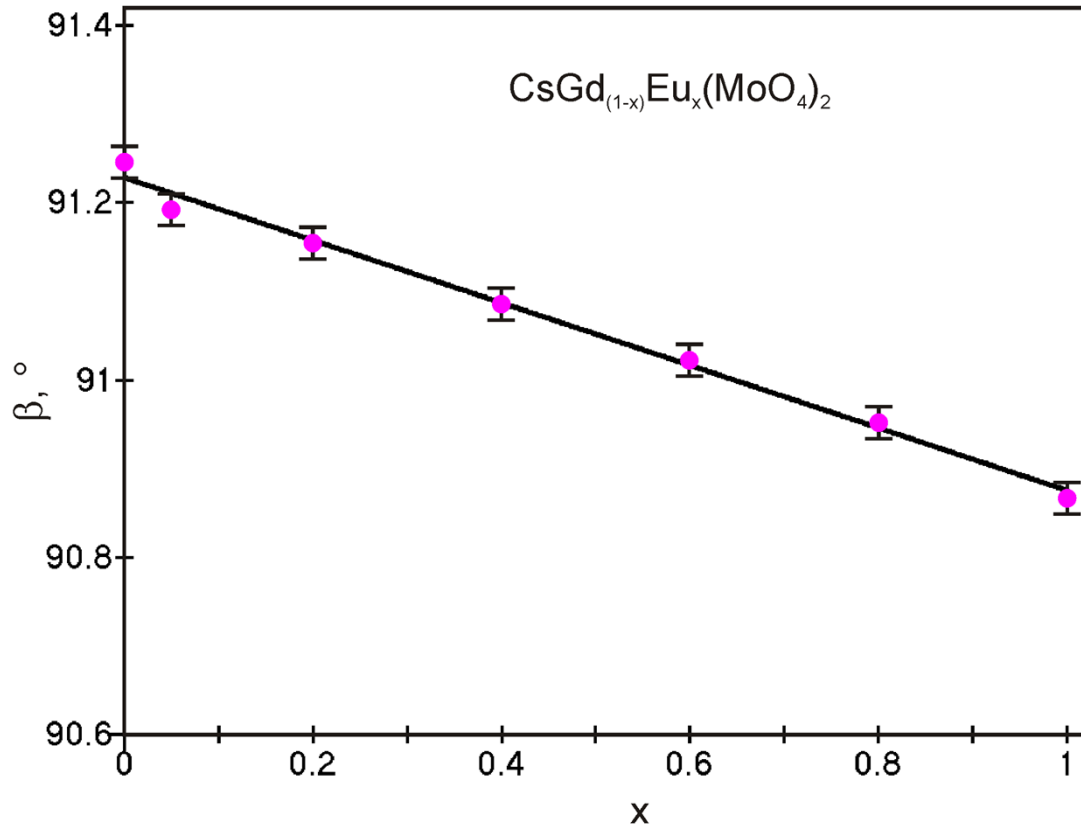


Fig. 4S. Dependence of monoclinic angle β on x in solid solutions $\text{CsGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$.

Table S1 The coordinates of atoms, isotropic thermal parameters (B_{iso}) and atom position occupations in the $\text{CsGd}_{(1-x)}\text{Eu}_x(\text{MoO}_4)_2$ structure at room temperature

CsEu(MoO ₄) ₂ , x=1					
	<i>x</i>	<i>y</i>	<i>z</i>	B_{iso}	Occupation
Eu	0	-0.044 (2)	0.25	0.85 (9)	1
Cs	0.5	0.000 (2)	0.25	1.85 (7)	1
Mo	0.19657 (15)	0.473 (2)	0.0038 (8)	1.04 (8)	1
O1	0.0690 (8)	0.743 (7)	-0.003 (5)	0.8 (2)	1
O2	0.1932 (19)	0.229 (9)	0.890 (7)	0.8 (2)	1
O3	0.3640 (9)	0.684 (6)	0.010 (5)	0.8 (2)	1
O4	0.1868 (19)	0.213 (8)	0.204 (7)	0.8 (2)	1
CsGd _{0.2} Eu _{0.8} (MoO ₄) ₂ , x=0.8					
	<i>x</i>	<i>y</i>	<i>z</i>	B_{iso}	Occupation
Gd	0	-0.036 (3)	0.25	0.98 (8)	0.2
Eu	0	-0.036 (3)	0.25	0.98 (8)	0.8
Cs	0.5	-0.014 (3)	0.25	2.30 (6)	1
Mo	0.19683 (15)	0.475 (2)	0.0054 (8)	1.02 (7)	1
O1	0.0653 (8)	0.736 (7)	0.001 (5)	1.5 (3)	1
O2	0.198 (2)	0.244 (9)	0.884 (8)	1.5 (3)	1
O3	0.3582 (8)	0.671 (6)	0.009 (6)	1.5 (3)	1
O4	0.184 (2)	0.233 (7)	0.206 (8)	1.5 (3)	1

CsGd _{0.4} Eu _{0.6} (MoO ₄) ₂ , x=0.6					
	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso}	Occupation
Gd	0	-0.040 (3)	0.25	0.79 (9)	0.4
Eu	0	-0.040 (3)	0.25	0.79 (9)	0.6
Cs	0.5	-0.004 (3)	0.25	2.14 (7)	1
Mo	0.19691 (17)	0.472 (3)	0.0029 (9)	0.48 (8)	1
O1	0.0664 (9)	0.724 (9)	0.005 (7)	1.5 (3)	1
O2	0.193 (2)	0.224 (11)	0.874 (10)	1.5 (3)	1
O3	0.3536 (10)	0.674 (7)	0.012 (7)	1.5 (3)	1
O4	0.187 (3)	0.225 (9)	0.199 (10)	1.5 (3)	1
CsGd _{0.6} Eu _{0.4} (MoO ₄) ₂ , x=0.4					
	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso}	Occupation
Gd	0	-0.043 (2)	0.25	0.73 (10)	0.6
Eu	0	-0.043 (2)	0.25	0.73 (10)	0.4
Cs	0.5	-0.004 (2)	0.25	2.26 (8)	1
Mo	0.19642 (17)	0.483 (3)	0.0039 (8)	0.66 (8)	1
O1	0.0645 (9)	0.713 (8)	0.004 (6)	1.5 (3)	1
O2	0.190 (2)	0.216 (9)	0.878 (9)	1.5 (3)	1
O3	0.3537 (11)	0.688 (7)	0.011 (7)	1.5 (3)	1
O4	0.188 (2)	0.209 (8)	0.187 (9)	1.5 (3)	1
CsGd _{0.8} Eu _{0.2} (MoO ₄) ₂ , x=0.2					

	x	y	z	B_{iso}	Occupation
Gd	0	-0.041 (2)	0.25	0.77 (8)	0.8
Eu	0	-0.041 (2)	0.25	0.77 (8)	0.2
Cs	0.5	-0.005 (2)	0.25	2.14 (7)	1
Mo	0.19658 (15)	0.479 (2)	0.0046 (7)	0.67 (7)	1
O1	0.0651 (8)	0.710 (7)	0.009 (5)	1.5 (3)	1
O2	0.192 (2)	0.231 (9)	0.880 (8)	1.5 (3)	1
O3	0.3573 (9)	0.698 (6)	0.015 (6)	1.5 (3)	1
O4	0.188 (2)	0.226 (8)	0.205 (8)	1.5 (3)	1
CsGd _{0.95} Eu _{0.05} (MoO ₄) ₂ , x=0.05					
	x	y	z	B_{iso}	Occupation
Gd	0	-0.042 (2)	0.25	0.95 (9)	0.95
Eu	0	-0.042 (2)	0.25	0.95 (9)	0.05
Cs	0.5	0.001 (2)	0.25	2.39 (9)	1
Mo	0.19689 (17)	0.480 (2)	0.0048 (7)	0.89 (8)	1
O1	0.0653 (9)	0.731 (7)	0.003 (5)	1.5 (3)	1
O2	0.198 (2)	0.234 (8)	0.889 (7)	1.5 (3)	1
O3	0.356 (1)	0.676 (6)	0.013 (5)	1.5 (3)	1
O4	0.180 (2)	0.241 (7)	0.203 (6)	1.5 (3)	1
CsGd(MoO ₄) ₂ , x=0					
	x	y	z	B_{iso}	Occupation

Gd	0	-0.038 (3)	0.25	0.82 (10)	1
Cs	0.5	-0.005 (3)	0.25	2.19 (9)	1
Mo	0.19657 (19)	0.480 (3)	0.0043 (9)	0.66 (9)	1
O1	0.0653 (9)	0.715 (9)	0.007 (6)	1.5 (3)	1
O2	0.192 (3)	0.231 (10)	0.897 (9)	1.5 (3)	1
O3	0.3571 (11)	0.690 (7)	0.012 (7)	1.5 (3)	1
O4	0.187 (3)	0.227 (9)	0.205 (9)	1.5 (3)	1

Table S2 Selected bond lengths (Å) for CsGd_xEu_(1-x)(MoO₄)₂

CsEu(MoO ₄) ₂ , x=1			
Eu—O1 ⁱ	2.42 (4)	Cs—O3 ^v	2.97 (4)
Eu—O1 ⁱⁱ	2.59 (4)	Cs—O4	3.19 (2)
Eu—O2 ⁱⁱⁱ	2.34 (4)	Mo—O1	1.83 (3)
Eu—O4	2.24 (3)	Mo—O2 ^{vi}	1.55 (5)
Cs—O2 ^{iv}	3.36 (3)	Mo—O3	1.921 (19)
Cs—O3 ⁱ	2.82 (4)	Mo—O4	2.10 (5)
CsGd _{0.2} Eu _{0.8} (MoO ₄) ₂ , x=0.8			
Gd(Eu)—O1 ⁱ	2.42 (4)	Cs—O3 ^v	3.06 (4)
Gd(Eu)—O1 ⁱⁱ	2.60 (4)	Cs—O4	3.27 (2)
Gd(Eu)—O2 ⁱⁱⁱ	2.40 (4)	Mo—O1	1.83 (3)
Gd(Eu)—O4	2.26 (3)	Mo—O2 ^{vi}	1.54 (5)
Cs—O2 ^{iv}	3.31 (3)	Mo—O3	1.833 (19)
Cs—O3 ⁱ	2.84 (4)	Mo—O4	2.04 (6)
CsGd _{0.4} Eu _{0.6} (MoO ₄) ₂ , x=0.6			
Gd(Eu)—O1 ⁱ	2.40 (5)	Cs—O3 ^v	3.05 (5)
Gd(Eu)—O1 ⁱⁱ	2.68 (5)	Cs—O4	3.22 (3)
Gd(Eu)—O2 ⁱⁱⁱ	2.28 (5)	Mo—O1	1.79 (3)
Gd(Eu)—O4	2.28 (4)	Mo—O2 ^{vi}	1.64 (7)
Cs—O2 ^{iv}	3.30 (4)	Mo—O3	1.81 (2)

Cs—O3 ⁱ	2.87 (5)	Mo—O4	2.03 (7)
CsGd _{0.6} Eu _{0.4} (MoO ₄) ₂ , x=0.4			
Gd(Eu)—O1 ⁱ	2.43 (4)	Cs—O3 ^v	3.01 (4)
Gd(Eu)—O1 ⁱⁱ	2.71 (4)	Cs—O4	3.19 (3)
Gd(Eu)—O2 ⁱⁱⁱ	2.24 (4)	Mo—O1	1.72 (3)
Gd(Eu)—O4	2.27 (3)	Mo—O2 ^{vi}	1.70 (6)
Cs—O2 ^{iv}	3.33 (3)	Mo—O3	1.83 (2)
Cs—O3 ⁱ	2.83 (4)	Mo—O4	2.03 (6)
CsGd _{0.8} Eu _{0.2} (MoO ₄) ₂ , x=0.2			
Gd(Eu)—O1 ⁱ	2.41 (4)	Cs—O3 ^v	2.99 (4)
Gd(Eu)—O1 ⁱⁱ	2.74 (4)	Cs—O4	3.21 (2)
Gd(Eu)—O2 ⁱⁱⁱ	2.30 (4)	Mo—O1	1.72 (3)
Gd(Eu)—O4	2.28 (3)	Mo—O2 ^{vi}	1.61 (5)
Cs—O2 ^{iv}	3.34 (3)	Mo—O3	1.895 (19)
Cs—O3 ⁱ	2.76 (4)	Mo—O4	2.07 (6)
CsGd(MoO ₄) ₂ , x=0			
Gd—O1 ⁱ	2.41 (5)	Cs—O3 ^v	3.00 (4)
Gd—O1 ⁱⁱ	2.71 (5)	Cs—O4	3.22 (3)
Gd—O2 ⁱⁱⁱ	2.37 (5)	Mo—O1	1.73 (3)
Gd—O4	2.27 (4)	Mo—O2 ^{vi}	1.53 (6)
Cs—O2 ^{iv}	3.39 (4)	Mo—O3	1.87 (2)

Cs—O3 ⁱ	2.80 (4)	Mo—O4	2.07 (6)
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Symmetry codes: (i) $x, y-1, z$; (ii) $-x, -y+1, -z$; (iii) $-x, -y, -z+1$; (iv) $-x+1, -y, -z+1$; (v) $-x+1, -y+1, -z$; (vi) $x, y, z-1$