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Supporting information for article:

A new langbeinite-type phosphate K2GdHf(PO4)3: aynthesis, crystal structure, band structure and luminescence properties

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Table S1 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) of $K_2GdHf(PO_4)_3$.

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
K1	0.56920 (17)	0.56920 (17)	0.56920 (17)	0.0320 (7)	
K2	0.7035 (2)	0.2035 (2)	0.2965 (2)	0.0410 (9)	
Hf1	0.91688 (3)	0.58312 (3)	0.41688 (3)	0.01225 (14)	0.404(4)
Gd1	0.91688 (3)	0.58312 (3)	0.41688 (3)	0.01225 (14)	0.596(4)
Hf2	0.35145 (3)	0.35145 (3)	0.35145 (3)	0.01377 (14)	0.596(4)
Gd2	0.35145 (3)	0.35145 (3)	0.35145 (3)	0.01377 (14)	0.404(4)
P1	0.62435 (17)	0.53517 (17)	0.23556 (17)	0.0151 (4)	
O1	0.5204 (6)	0.4510 (6)	0.2971 (6)	0.0499 (17)	
O2	0.7445 (7)	0.5203 (7)	0.3167 (7)	0.057 (2)	
O3	0.6512 (6)	0.4885 (5)	0.1003 (6)	0.0437 (15)	
O4	0.5801 (5)	0.6745 (5)	0.2338 (5)	0.0389 (15)	

Table S2 Atomic displacement parameters (Å^2) of $K_2GdHf(PO_4)_3$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0320 (7)	0.0320 (7)	0.0320 (7)	−0.0012 (8)	−0.0012 (8)	−0.0012 (8)
K2	0.0410 (9)	0.0410 (9)	0.0410 (9)	−0.0009 (9)	0.0009 (9)	0.0009 (9)
Hf1	0.01225 (14)	0.01225 (14)	0.01225 (14)	0.00100 (13)	−0.00100 (13)	0.00100 (13)
Gd1	0.01225 (14)	0.01225 (14)	0.01225 (14)	0.00100 (13)	−0.00100 (13)	0.00100 (13)
Hf2	0.01377 (14)	0.01377 (14)	0.01377 (14)	0.00087 (13)	0.00087 (13)	0.00087 (13)
Gd2	0.01377 (14)	0.01377 (14)	0.01377 (14)	0.00087 (13)	0.00087 (13)	0.00087 (13)
P1	0.0132 (10)	0.0158 (9)	0.0161 (9)	−0.0039 (7)	−0.0030 (7)	0.0009 (7)
O1	0.039 (4)	0.054 (4)	0.057 (5)	−0.032 (3)	0.013 (3)	−0.002 (3)
O2	0.043 (4)	0.060 (5)	0.067 (5)	−0.015 (3)	−0.034 (4)	0.020 (4)
O3	0.053 (4)	0.043 (4)	0.035 (3)	−0.003 (3)	0.018 (3)	−0.014 (3)
O4	0.039 (3)	0.024 (3)	0.054 (4)	0.010 (3)	0.012 (3)	−0.006 (3)

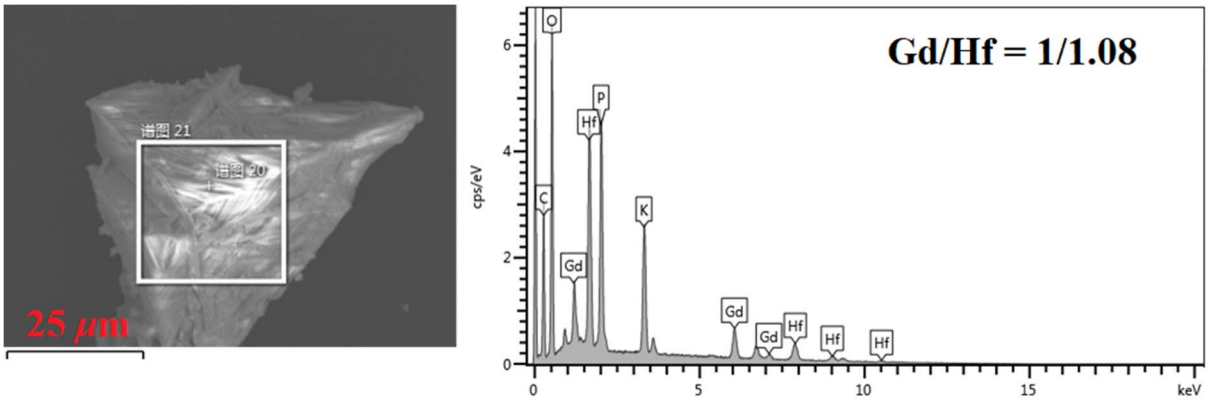

Figure S1 EDS analysis of a $K_2GdHf(PO_4)_2$ crystal.