Supplementary Materials

Growth Peculiarities and Properties of KR_3F_{10} (*R* = Y, Tb) Single Crystals

Denis N. Karimov [1,*], Irina I. Buchinskaya [1], Natalia A. Arkharova [1], Anna G. Ivanova [1], Alexander G. Savelyev [1], Nikolay I. Sorokin [1], Pavel A. Popov [2]

[1] Shubnikov Institute of Crystallography of Federal Scientific Research Center «Crystallography and Photonics», Russian Academy of Sciences, Leninskiy Prospekt 59, Moscow 119333, Russia; buchinskayaii@gmail.com (I.I.B.); natalya.arkharova@yandex.ru (N.A.A.); ani.crys.ras@gmail.com (A.G.I.); a.g.savelyev@gmail.com (A.G.S.); nsorokin1@yandex.ru(N.I.S.)

[2] Department of Physics and Mathematics, Petrovsky Bryansk State University, Bezhitskaya str. 14, Bryansk 241036, Russia; tfbgubry@mail.ru

* Correspondence: dnkarimov@gmail.com; Tel.: +7-903-778-74-89

Single-crystal x-ray diffraction study of KR_3F_{10} (R = Y, Tb)

CCDC–2062503 (KTb_3F_{10}) and CCDC–2062504 (KY_3F_{10}) contain the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters U_{eq} (Å^2 ×10^3) for KR_3F_{10} (*R* = Tb, Y). U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Table S2. Selected bond lengths (Å) for KTb_3F_{10} crystal.

Table S3. Selected bond lengths (Å) for KY_3F_{10} crystal.

CIF file for KTb_3F_{10} single crystal.

CIF file for KY_3F_{10} single crystal.

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters U_{eq} (Å^2 ×10^3) for KR_3F_{10} (*R* = Tb, Y). U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom label for KTb_3F_{10}	**Wyckoff position**	**x**	**y**	**z**	**U_{eq}**
Tb	24e	0.24034 (2)	0.00000	0.00000	0.00703 (6)
K	8c	0.25000	0.25000	0.25000	0.0269 (4)
F1	48i	0.50000	0.16670 (10)	0.16670 (10)	0.0185 (3)
F2	32f	0.11219 (8)	0.11219 (8)	0.11219 (8)	0.0108 (3)
Atom label for KY_3F_{10}	**Wyckoff position**	**x**	**y**	**z**	**U_{eq}**
Y	24e	0.24032 (2)	0.000000	0.000000	0.00605 (8)
K	8c	0.250000	0.250000	0.250000	0.0225 (2)
F1	48i	0.500000	0.16576 (7)	0.16576 (7)	0.0142 (2)
F2	32f	0.11162 (7)	0.11162 (7)	0.11162 (7)	0.0100 (2)

Table S2. Selected bond lengths (Å) for KTb_3F_{10} crystal.

Tb—Tb^{i}	3.9674 (3)	K—F1^{v}	3.2259 (7)
Tb—Tb^{ii}	3.9674 (3)	K—F1^{xii}	3.2259 (7)
Tb—Tb^{iii}	3.9674 (3)	K—F1^{xiii}	3.2259 (7)
Tb—Tb^{iv}	3.9674 (3)	K—F1^{xiv}	3.2259 (7)
Tb—F1^{v}	2.2279 (4)	K—F1^{vii}	3.2259 (7)
Tb—F1^{vi}	2.2279 (4)	K—F1^{xv}	3.2259 (7)

Tb—F1^{vii}	2.2279 (4)	K—F1^{xvi}	3.2259 (7)
Tb—F1^{viii}	2.2279 (4)	K—F1^{xvii}	3.2259 (7)
Tb—F2	2.3806 (5)	K—F2^{xviii}	2.7862 (17)
Tb—F2^{ix}	2.3806 (5)	K—F2	2.7862 (17)
Tb—F2^{x}	2.3806 (5)	K—F2^{xix}	2.7862 (17)
Tb—F2^{xi}	2.3806 (5)	K—F2^{xx}	2.7862 (17)

Symmetry codes: (i) -*y*, -*z*, -*x*; (ii) *y*, *z*, *x*; (iii) *z*, *x*, *y*; (iv) -*z*, -*x*, -*y*; (v) -*y*+1/2, *z*, -*x*+1/2; (vi) -*z*+1/2, -*x*+1/2, -*y*; (vii) -*z*+1/2, *x*-1/2, *y*; (viii) -*y*+1/2, -*z*, -*x*+1/2; (ix) *x*, *y*, -*z*; (x) *x*, -*y*, -*z*; (xi) *x*, -*y*, *z*; (xii) -*x*+1, -*y*+1/2, -*z*+1/2; (xiii) -*y*+1/2, -*z*+1/2, -*x*+1; (xiv) *z*, -*x*+1/2, -*y*+1/2; (xv) *y*, -*z*+1/2, *x*-1/2; (xvi) -*z*+1/2, -*x*+1, -*y*+1/2; (xvii) *x*-1/2, *y*, -*z*+1/2; (xviii) *x*, -*y*+1/2, -*z*+1/2; (xix) -*x*+1/2, *y*, -*z*+1/2; (xx) -*x*+1/2, -*y*+1/2.

Table S3. Selected bond lengths (Å) for KY_3F_{10} crystal.

Y—Y^{i}	3.9215 (3)	K—F1^{xii}	3.1954 (5)
Y—Y^{ii}	3.9215 (3)	K—F1^{v}	3.1954 (5)
Y—Y^{iii}	3.9215 (3)	K—F1^{xiii}	3.1954 (5)
Y—Y^{iv}	3.9215 (3)	K—F1^{xiv}	3.1954 (5)
Y—F1^{v}	2.1983 (3)	K—F1^{xv}	3.1954 (5)
Y—F1^{vi}	2.1983 (3)	K—F1^{vii}	3.1954 (5)
Y—F1^{vii}	2.1983 (3)	K—F1^{xvi}	3.1954 (5)
Y—F1^{viii}	2.1983 (3)	K—F1^{xvii}	3.1954 (5)
Y—F2^{ix}	2.3500 (4)	K—F2	2.7656 (15)
Y—F2^{x}	2.3500 (4)	K—F2^{xviii}	2.7657 (15)
Y—F2	2.3500 (4)	K—F2^{xix}	2.7657 (15)
Y—F2^{xi}	2.3500 (4)	K—F2^{xx}	2.7657 (15)

Symmetry codes: (i) -*y*, -*z*, -*x*; (ii) *y*, *z*, *x*; (iii) *z*, *x*, *y*; (iv) -*z*, -*x*, -*y*; (v) -*y*+1/2, *z*, -*x*+1/2; (vi) -*z*+1/2, -*x*+1/2, -*y*; (vii) -*z*+1/2, *x*-1/2, *y*; (viii) -*y*+1/2, -*z*, -*x*+1/2; (ix) *x*, *y*, -*z*; (x) *x*, -*y*, -*z*; (xi) *x*, -*y*, *z*; (xii) -*x*+1, -*y*+1/2, -*z*+1/2; (xiii) -*y*+1/2, -*z*+1/2, -*x*+1; (xiv) *z*, -*x*+1/2, -*y*+1/2; (xv) *y*, -*z*+1/2, *x*-1/2; (xvi) -*z*+1/2, -*x*+1, -*y*+1/2; (xvii) *x*-1/2, *y*, -*z*+1/2; (xviii) *x*, -*y*+1/2, -*z*+1/2; (xix) -*x*+1/2, *y*, -*z*+1/2; (xx) -*x*+1/2, -*y*+1/2.