Supporting Information

KLi_2CO_3F: a Beryllium-free KBBF-type Deep-UV Carbonate with Enhanced Interlayer Interaction and Large Birefringence

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Table of contents

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for KLi_2CO_3F. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	*x*	*y*	*z*	U_{eq} ($Å^2$)	BVS
K1	3333	6667	2500	27.4(3)	0.733
F2	6667	3333	2500	34.1(7)	0.950
O3	2653(3)	2653(3)	5000	24.1(5)	2.071
C4	0	0	5000	13.3(7)	4.027
Li5	6667	3333	4297(4)	16.5(9)	1.163

Table S2. Selected Bond lengths [Å] and angles [°] for KLi_2CO_3F.

K1—F2[1]	2.7841 (5)	K1[11]—F2—K1	120.0
K1—O3	3.0841 (7)	O3[7]—K1—O3	126.337 (14)
F2—K1[10]	2.7841 (5)	O3[5]—K1—O3	60.51 (3)
F2—Li5	1.803 (4)	Li5—F2—K1[10]	90.0
O3—K1[13]	3.0841 (7)	Li5[12]—F2—Li5	180.0
O3—C4	1.2791 (16)	C4—O3—K1	111.53 (3)
O3—Li5[8]	1.9281 (18)	C4—O3—Li5	125.95 (5)
C4—O3[14]	1.2791 (16)	Li5—O3—K1	79.20 (10)
Li5—O3[16]	1.9280 (18)	Li5—O3—Li5[8]	108.09 (10)
F2[1]—K1—F2[2]	120.0	O3—C4—O3[14]	120.0
F2[1]—K1—O3[3]	63.168 (7)	F2—Li5—O3[16]	111.47 (11)
F2—K1—O3[4]	84.71 (3)	O3[6]—K1—O3[5]	114.15 (5)
K1[10]—F2—K1	120.0	Li5[12]—F2—K1[11]	90.0
O3[16]—Li5—O3	107.40 (12)		

Symmetry codes: (1)+X,1+Y,+Z; (2)-1+X,+Y,+Z; (3)1-Y,1+X-Y,+Z; (4)-Y+X,+X,-1/2+Z; (5)+Y-X,1-X,+Z; (6)+Y,1-X+Y,-1/2+Z; (7)1-X,1-Y,-1/2+Z; (8)+Y,+X,1-Z; (9)-Y,1-X,1/2-Z; (10)1+X,+Y,+Z; (11)+X,-1+Y,+Z; (12)1-Y,1-X,1/2-Z; (13)1-X,1-Y,1/2+Z; (14)+Y-X,-X,+Z; (15)-Y,+X-Y,+Z; (16)1+Y-X,1-X,+Z; (17)1-Y,+X-Y,+Z; (18)1+Y,+X,1-Z; (19)+Y,-1+X,1

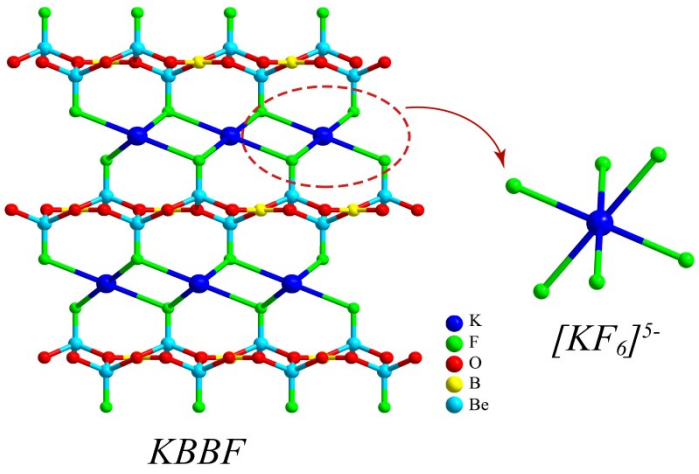

Fig. S1 The coordination mode of K^+ cations in KBBF.

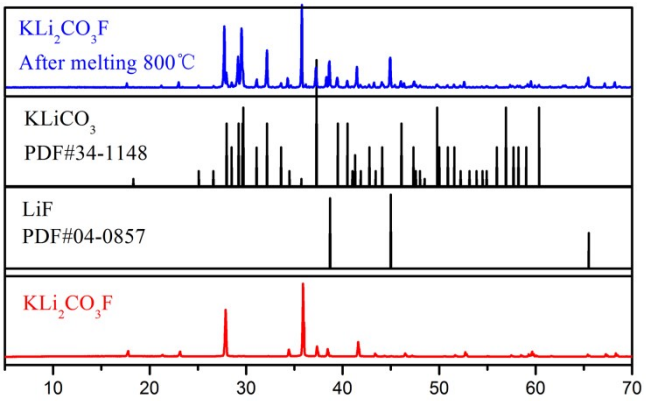

Fig. S2 The XRD analysis of KLi_2CO_3F before and after melting.

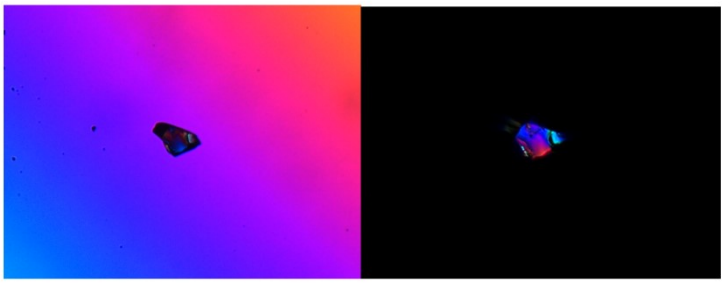

Fig. S3 The birefringence measurements for KLi_2CO_3F.