$KB(PO_4)F$: A novel acentric deep-ultraviolet material

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Table S1. Atomic displacement parameters ($Å^2$) of $KB(PO_4)F$

atoms	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K1	0.0199 (12)	0.0210 (14)	0.0097 (11)	0.0024 (10)	0.0004 (8)	0.0000 (9)
P1	0.0105 (12)	0.0086 (12)	0.0095 (15)	−0.0008 (9)	0.0012 (9)	0.0006 (9)
B1	0.008 (6)	0.013 (5)	0.012 (6)	−0.003 (5)	0.001 (5)	0.008 (4)
F1	0.020 (4)	0.027 (4)	0.009 (4)	0.003 (3)	0.000 (3)	0.000 (3)
O1	0.018 (4)	0.014 (4)	0.011 (4)	0.005 (3)	−0.004 (3)	−0.001 (3)
O2	0.014 (4)	0.012 (3)	0.010 (4)	0.000 (3)	0.006 (3)	−0.004 (3)
O3	0.012 (4)	0.011 (3)	0.023 (5)	−0.003 (3)	0.002 (3)	0.004 (3)
O4	0.019 (4)	0.021 (4)	0.015 (4)	−0.005 (3)	0.004 (3)	0.000 (3)

Table S2. Selected bond lengths and angles (Å, °) for $KB(PO_4)F$.

K1—F1^{i}	2.666 (8)	P1—O4	1.474 (9)
K1—O2^{ii}	2.772 (9)	P1—O2	1.546 (8)
K1—F1	2.785 (7)	P1—O3	1.552 (8)
K1—O4^{iii}	2.792 (9)	P1—O1	1.566 (9)
K1—O4^{iv}	2.802 (9)	B1—F1	1.414 (14)
K1—F1^{v}	2.884 (8)	B1—O2^{vi}	1.447 (15)
K1—O4^{ii}	2.968 (9)	B1—O1	1.449 (15)
K1—O3^{vi}	3.027 (9)	B1—O3^{ix}	1.458 (14)
K1—O1	3.060 (9)	B1^{i}—O3—P1	129.6 (8)
O4—P1—O2	108.8 (5)	F1—B1—O2^{vi}	110.3 (9)
O4—P1—O3	115.6 (5)	F1—B1—O1	104.1 (9)

O2—P1—O3	104.3 (4)	O2^{vi}—B1—O1	114.4 (9)
O4—P1—O1	115.5 (5)	F1—B1—O3^{ix}	109.5 (8)
O2—P1—O1	108.6 (5)	O2^{vi}—B1—O3^{ix}	109.6 (10)
O3—P1—O1	103.3 (5)	O1—B1—O3^{ix}	108.6 (10)
B1—O1—P1	127.2 (8)	B1^{xi}—O2—P1	134.6 (8)

Symmetry codes: (i) x+1/2, y−1/2, z; (ii) x−1, −y+1, z−1/2; (iii) x, −y+1, z−1/2; (iv) x−1/2, −y+1/2, z−1/2; (v) x−1/2, y−1/2, z; (vi) x−1, y, z; (vii) x+1, −y+1, z+1/2; (viii) x+1/2, −y+1/2, z+1/2; (ix) x−1/2, y+1/2, z; (x) x+1/2, y+1/2, z; (xi) x+1, y, z; (xii) x, −y+1, z+1/2.

Table S3. Bond valence sums (BVS) for $KB(PO_4)F$.

	K1	P1	B1	BVS
O1	0.081	1.109	0.810	2.00
O2	0.176	1.171	0.815	2.162
O3	0.088	1.152	0.790	2.030
O4	0.167+0.163+0.104	1.422		1.856
F1	0.161+0.117+0.089		0.754	1.121
BVS	1.146	4.854	3.169	

Table S4. Comparisons of the interlayer bonding in $KBe_2BO_3F_2$ and $KB(PO_4)F$

species	bonds	lengths(Å)	q_1[a]	q_1[a]	|F|[b]
KBBF[c]	K-F1	2.755	0.756	0.901	1
$KBPO_4F$	K-F1^{i}	2.666	1.146	1.121	2.01
	K-F1	2.785	1.146	1.121	1.84
	K-F1^{v}	2.884	1.146	1.121	1.72
	K-O1	3.060	1.146	2.000	2.72
	K-O2	2.772	1.146	2.162	3.58
	K-O3	3.027	1.146	2.030	2.82
	K-O4^{iii}	2.792	1.146	1.856	3.03
	K-O4^{iv}	2.802	1.146	1.856	3.011
	K-O4^{ii}	2.968	1.146	1.856	2.682

[a] In multiples of 1.602×10^{-19}C. [b] In multiples of $|F_{KBBF}|$. [c] Data from ref "L. F. Mei, Y. B. Wang, C. T. Chen and B. C. Wu, *J Appl Phys*, 1993, **74**, 7014-7015".

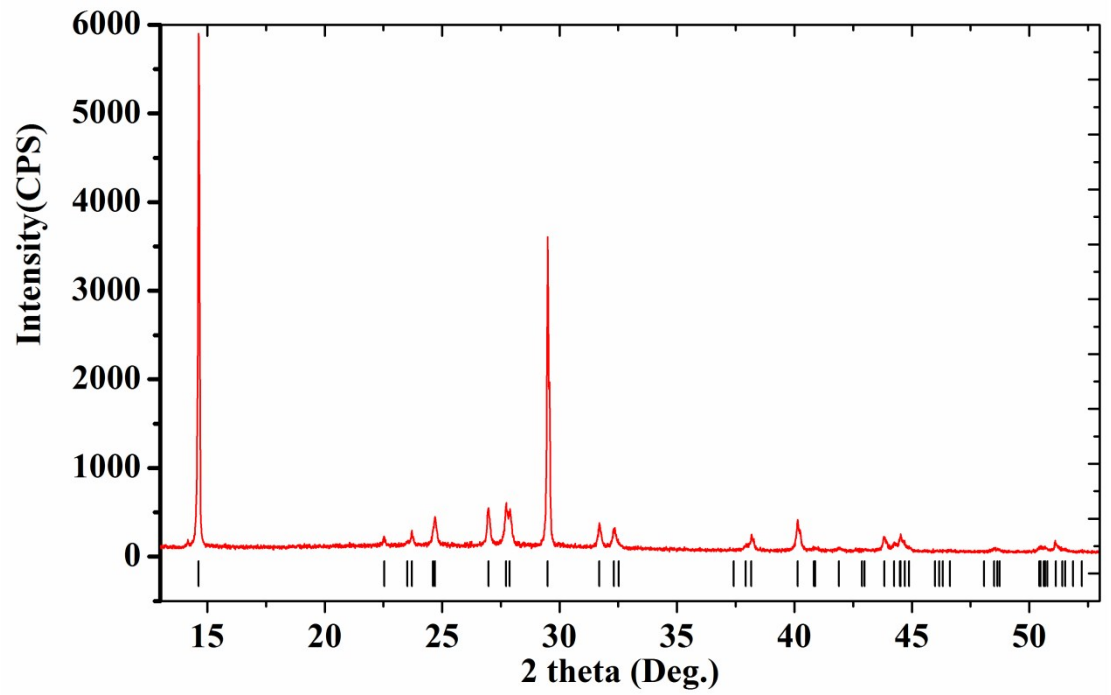

Figure S1 Experimental and calculated PXRD patterns of $KB(PO_4)F$.

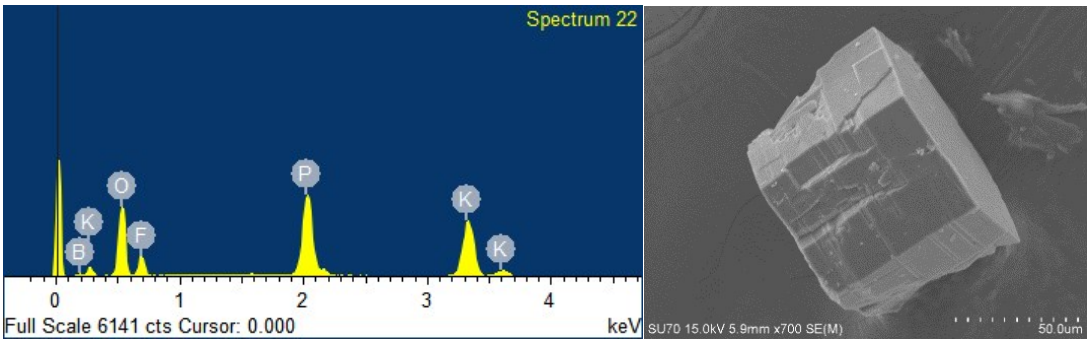

Figure S2 Representative EDX spectrum and SEM image of $KB(PO_4)F$.

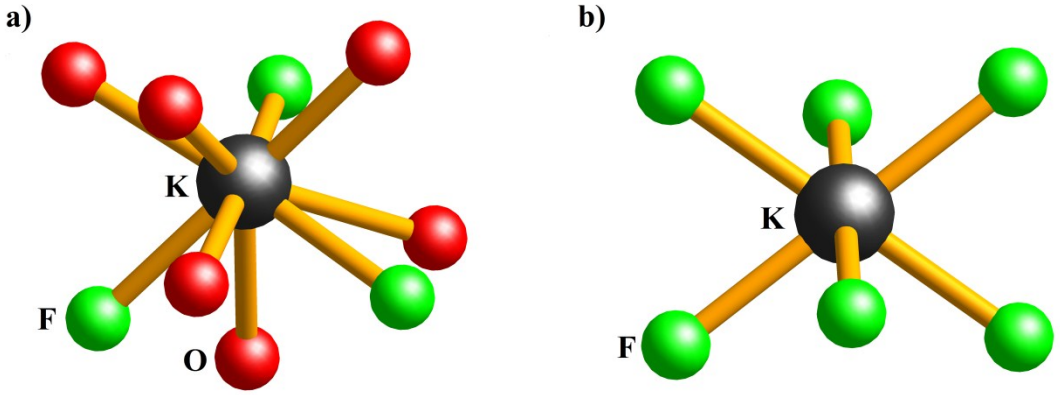

Figure S3 Coordination environments of the K atoms in $KBPO_4F$ (a) and KBBF (b).

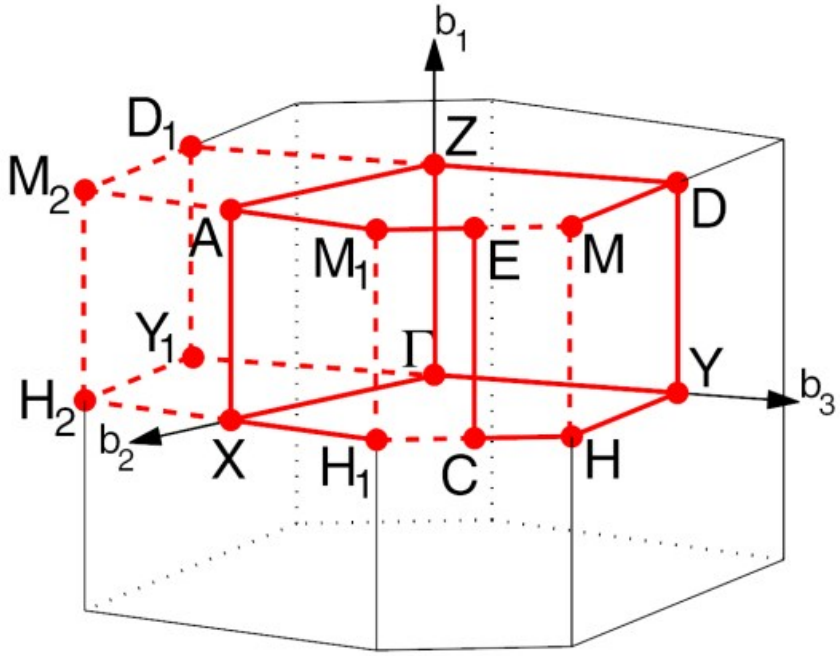

Figure S4 The high symmetry ***k***-path of a monoclinic lattice for the title compound as generated by AFLOW.

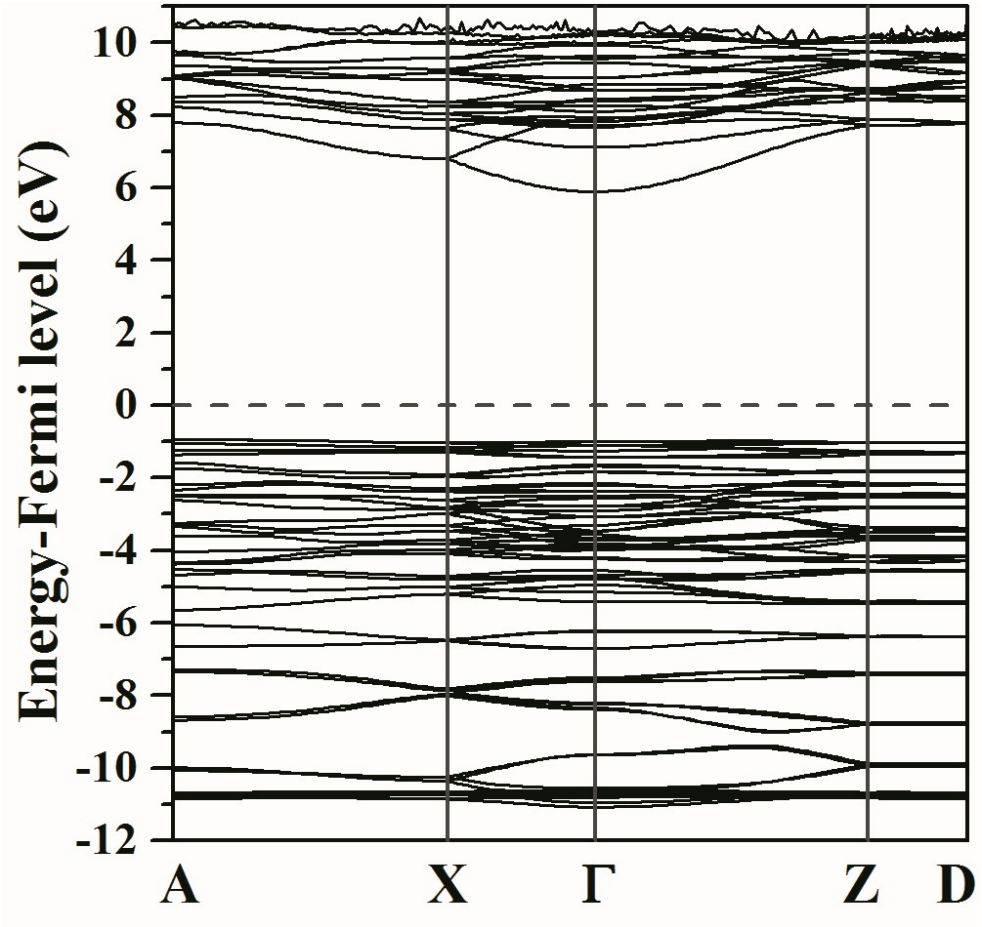

Figure S5. The calculated electronic band structure of $KB(PO_4)F$.

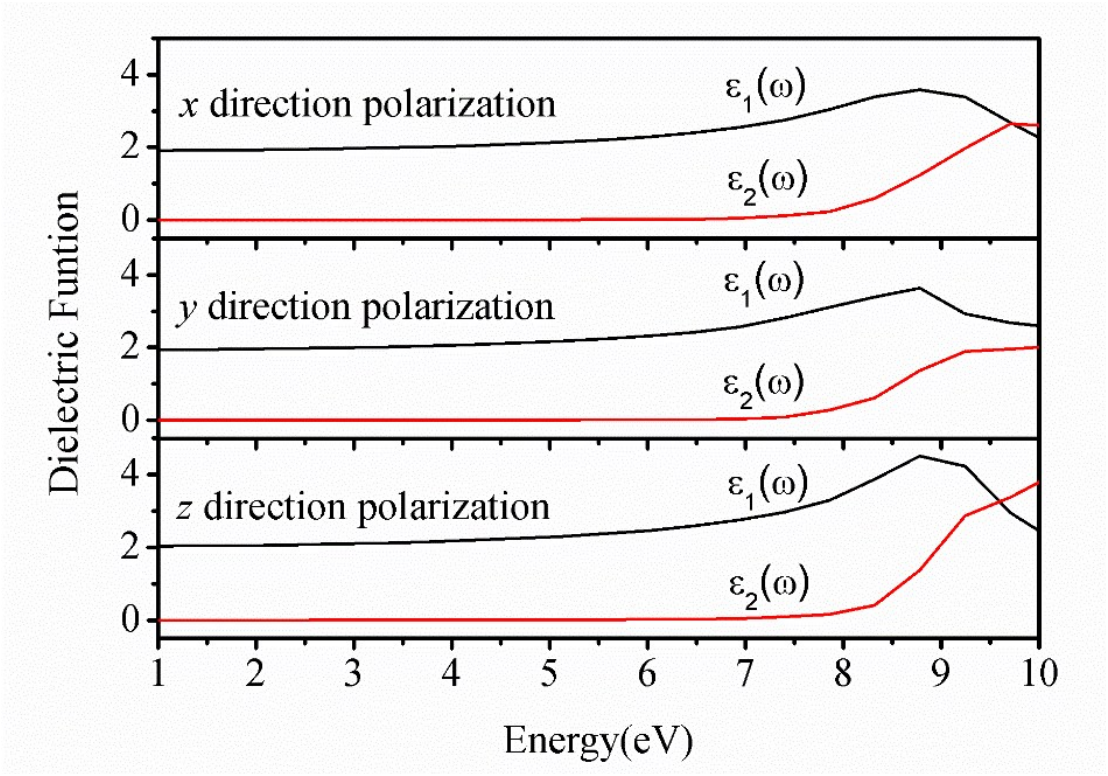

Figure S6 Dielectric function of $KB(PO_4)F$.

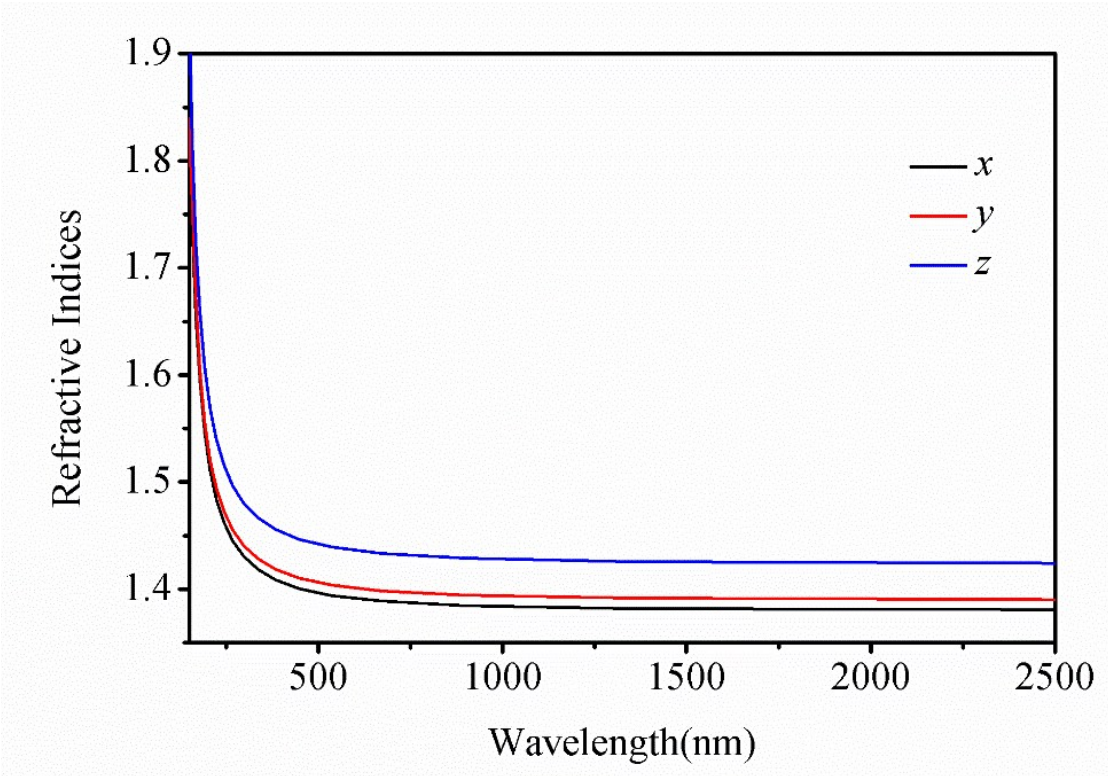

Figure S7 Refractive index curves of $KB(PO_4)F$