Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

$K_2(BeS)O_4F_2$: A novel fluorosulfate with unprecedented 1D $[(BeO_3F)\text{-}(SO_3F)]_\infty$ chains exhibiting large birefringence

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Table S1. Crystal Data and Structure Refinement for $K_2(BeS)O_4F_2$.

Formula	$K_2(BeS)O_4F_2$
Formula weight (amu)	221.27
Temperature (K)	293(2)
Wavelength (Å)	1.34139
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a (Å)	4.5337(4)
b (Å)	5.4828(6)
c (Å)	12.0877(13)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	300.47(5)
Z	2
Calculated density (g/cm^3)	2.446
Absorption coefficient (mm^{-1})	11.362
F(000)	216
Theta range (θ)	9.091-60.729
Limiting indices	-4<=h<=5 -6<=k<=7 -15<=l<=15
Reflections collected / unique	1008 / 595
R_{int}	0.0230
Completeness to θ = 53.594°(%)	96
GOF on F^2	1.119
R/*wR*(I>2σ(I))	R_1 = 0.0669 wR_2 = 0.1800
R/*wR*(all data)	R_1 = 0.0700 wR_2 = 0.1847
Absolute structure parameter	0.45(11)

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$

[b] ${}_wR_2(F_o^2) = [\sum w (F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$

Table S2. Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $K_2(BeS)O_4F_2$.

Atom	x	y	z	U(eq)
K(001)	2735(4)	7981(3)	6453(2)	29(1)
O(002)	7639(13)	978(11)	6555(4)	23(1)
O(003)	11653(11)	2743(13)	5404(4)	28(2)
S(004)	8288(9)	2851(9)	5692(4)	41(1)
F(005)	7630(17)	5384(11)	6062(7)	55(2)
Be(0)	8288(9)	2851(9)	5692(4)	41(1)

Table S3. Selected Bond lengths [Å] and angles [°] for $K_2(BeS)O_4F_2$.

K(001)-O(002)#1	2.652(6)	O(002)#1-K(001)-O(002)#3	104.90(13)
K(001)-O(002)#2	2.838(6)	O(003)#2-K(001)-O(003)#4	127.18(19)
K(001)-O(002)#3	2.767(6)	F(005)#4-K(001)-O(002)#2	67.86(17)
K(001)-O(003)#4	3.177(7)	K(001)#7-O(002)-K(001)#8	109.32(18)
K(001)-O(003)#2	2.943(7)	O(002)-S(004)-K(001)#11	164.2(3)
K(001)-S(004)#2	3.470(5)	O(002)-S(004)-O(003)	108.7(4)
K(001)-S(004)#1	3.483(5)	O(003)#12-S(004)-K(001)#7	141.8(3)
K(001)-S(004)#5	3.465(5)	F(005)-S(004)-K(001)#9	116.9(4)
K(001)-F(005)#1	3.284(9)	F(005)-S(004)-O(002)	113.1(5)
K(001)-F(005)#5	3.170(9)	K(001)#10-F(005)-K(001)#11	90.3(2)
K(001)-F(005)#4	2.759(7)	K(001)#8-Be(0)-K(001)#9	77.23(10)
K(001)-F(005)	2.679(7)	O(002)-Be(0)-K(001)#7	45.2(3)
O(002)-S(004)	1.493(7)	O(002)-Be(0)-O(003)#12	111.0(4)
O(002)-Be(0)	1.493(7)	O(003)#12-Be(0)-K(001)#11	57.7(3)
O(003)-S(004)#6	1.553(7)	F(005)-Be(0)-K(001)#7	69.9(4)
O(003)-S(004)	1.566(7)	F(005)-Be(0)-O(003)#12	110.9(5)
O(003)-Be(0)	1.566(7)	O(003)#12-Be(0)-O(003)	105.6(3)
S(004)-F(005)	1.489(7)	O(002)-Be(0)-K(001)#8	53.1(3)
F(005)-Be(0)	1.489(7)	K(001)#11-F(005)-K(001)#7	172.5(2)

Table S4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $K_2(BeS)O_4F_2$

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K(001)	23(1)	24(1)	39(1)	7(1)	0(1)	-1(1)
O(002)	21(3)	26(3)	22(2)	9(2)	4(3)	-4(3)
O(003)	12(2)	49(4)	24(2)	1(3)	-2(2)	2(3)
S(004)	31(2)	45(2)	45(2)	3(2)	0(1)	1(2)
F(005)	27(3)	32(3)	106(5)	-17(3)	-6(4)	3(3)
Be(0)	31(2)	45(2)	45(2)	3(2)	0(1)	1(2)

Table S5. The elemental content ICP analysis.

Element	Weight(%)	Atomic ratio
K	30.37	0.7767
Be	3.34	0.3711

Table S6. The elemental content EA analysis.

Element	Weight(%)
N	=<0.3
C	=<0.3
H	=<0.3

Table S7. Experimental birefringence of $K_2(BeS)O_4F_2$ at 546.1 nm.

Crystal	ΔR (nm)	T (μm)	Δn
$K_2(BeS)O_4F_2$	516.9	9.22	0.056

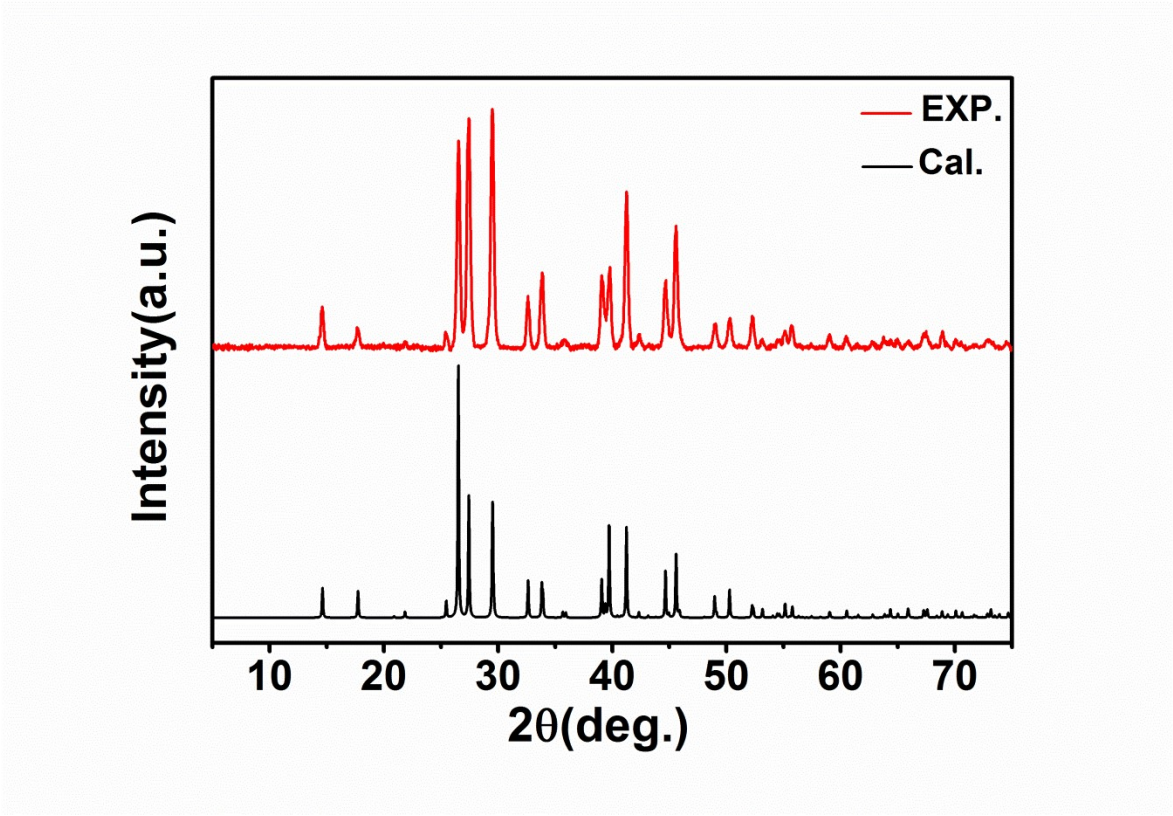

Figure S1. Powder XRD patterns of the simulated and experimental for $K_2(BeS)O_4F_2$

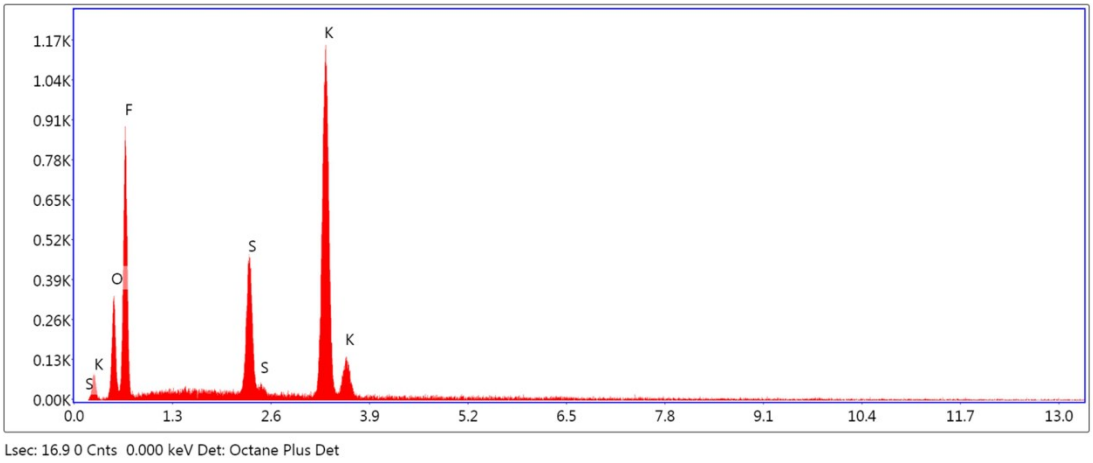

Figure S2. EDS analysis of single crystal for $K_2(BeS)O_4F_2$

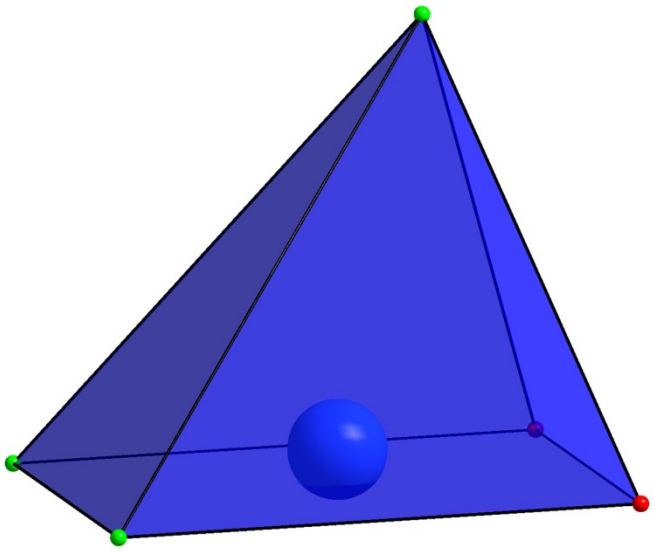

Figure S3. Polyhedron of K, F and O atoms for $K_2(BeS)O_4F_2$

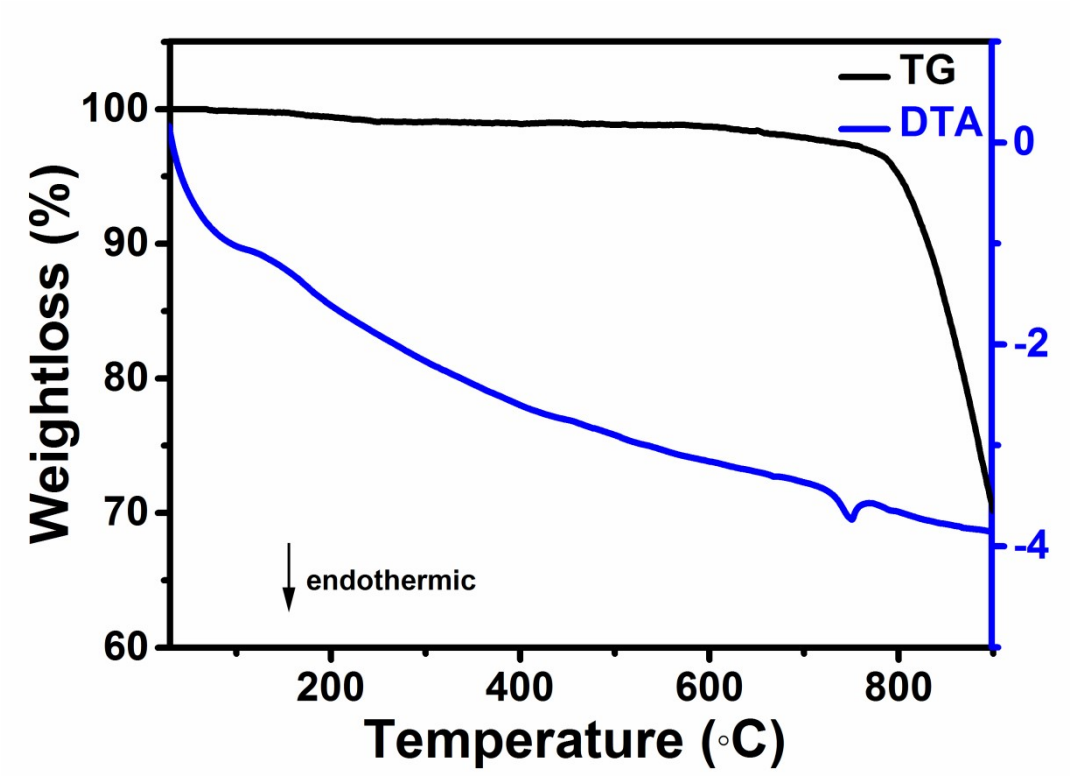

Figure S4. TG and DTA curves of $K_2(BeS)O_4F_2$.

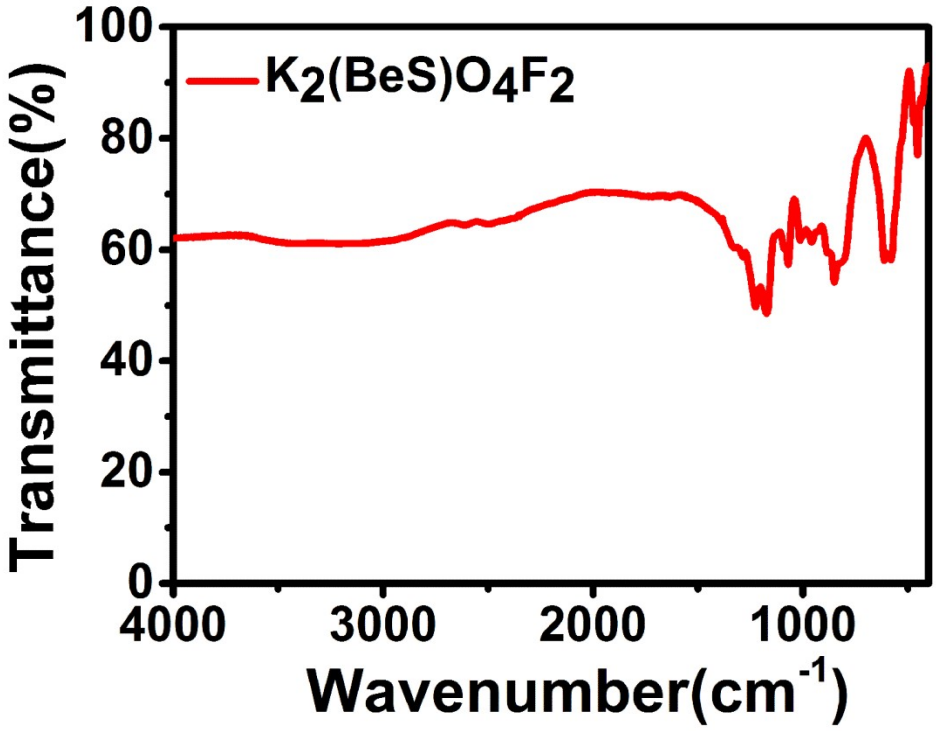

Figure S5. IR transmittance spectra of $K_2(BeS)O_4F_2$

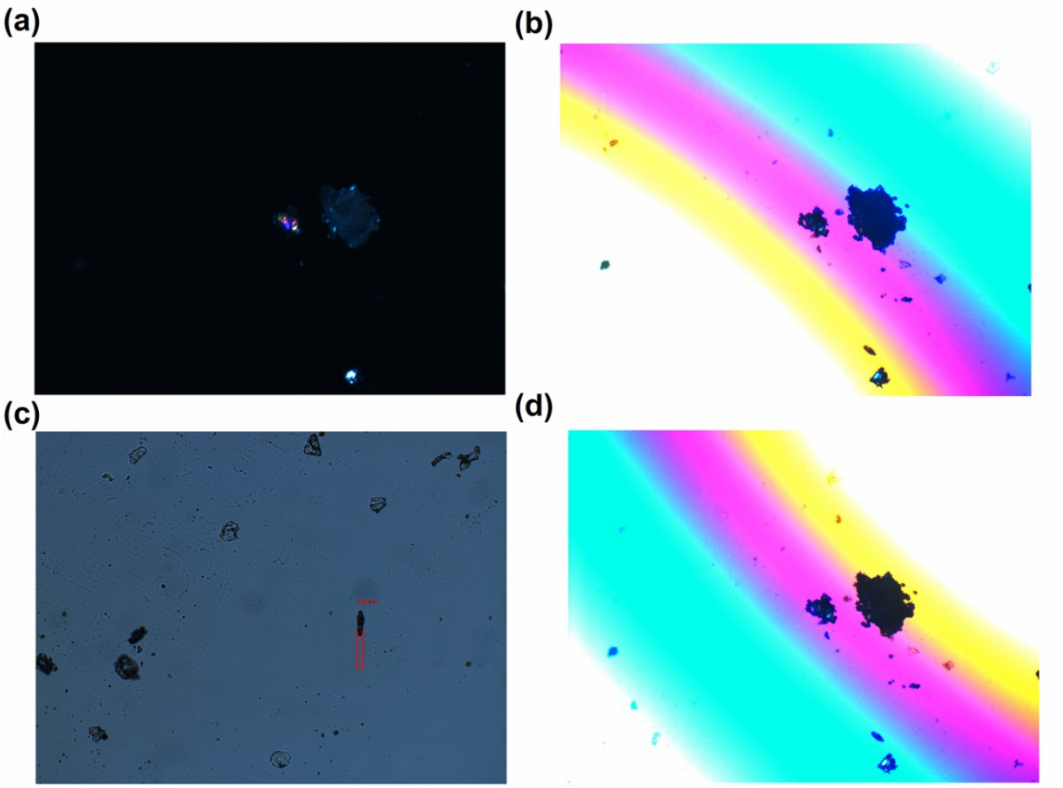

Figure S6. Measurement of birefringence for $K_2(BeS)O_4F_2$.

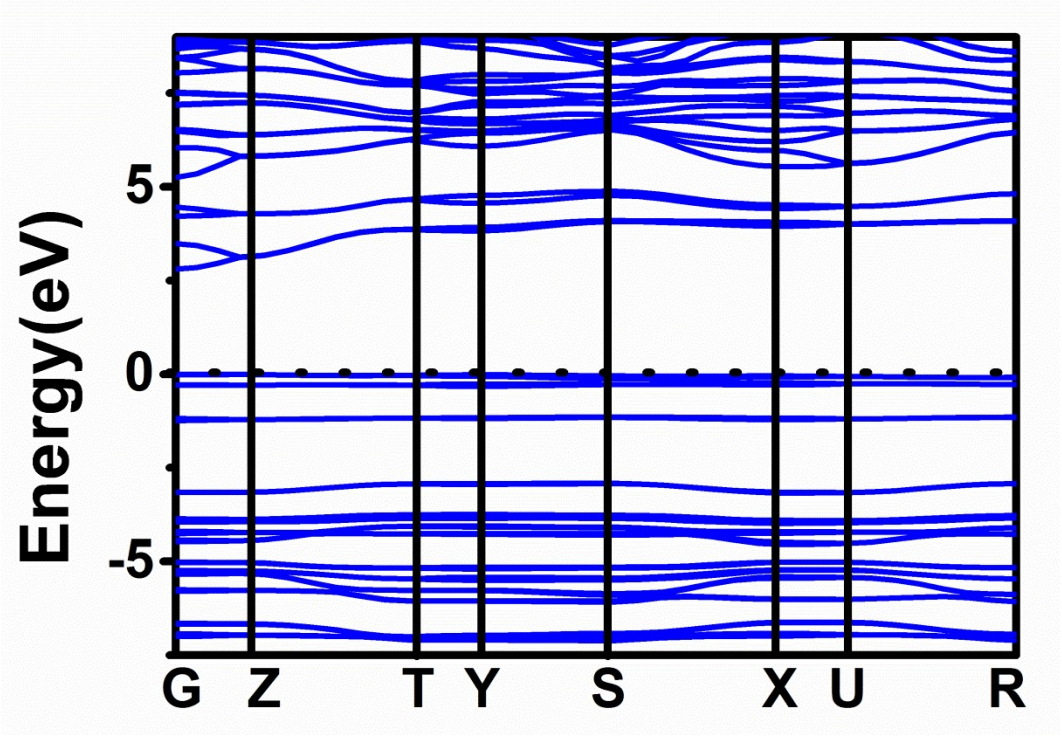

Figure S7. Calculated electronic band structure of $K_2(BeS)O_4F_2$.

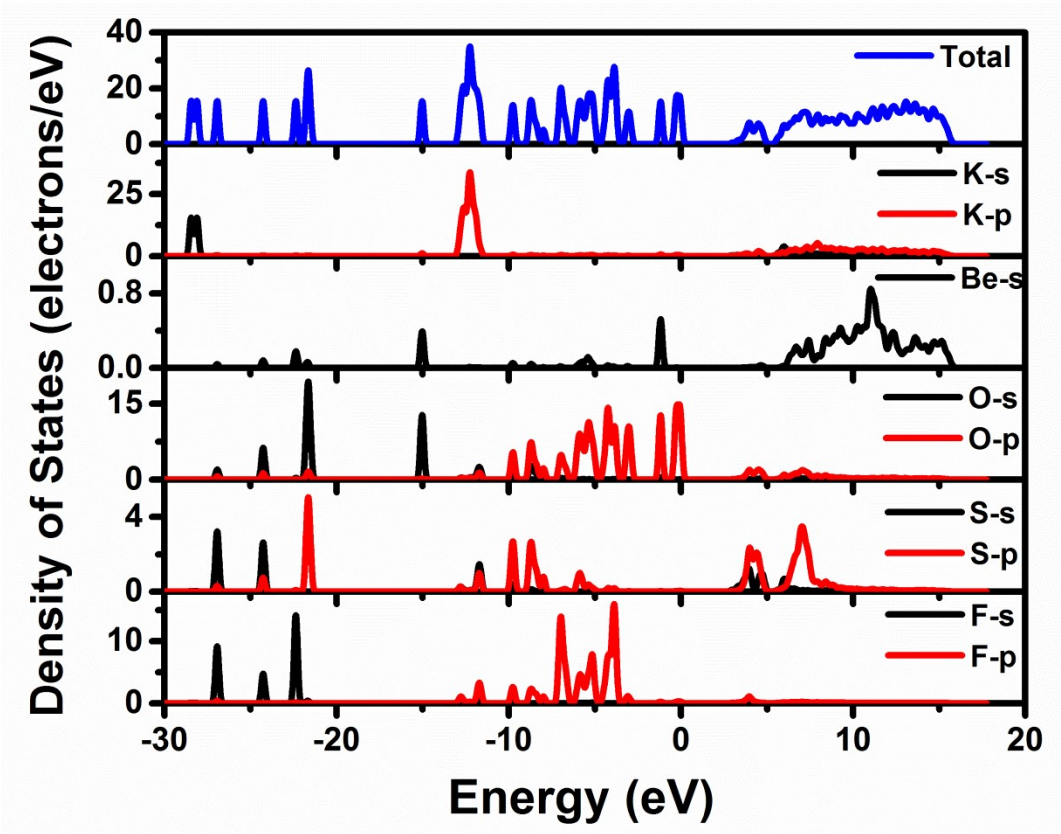

Figure S8. TDOS and PDOS of $K_2(BeS)O_4F_2$.

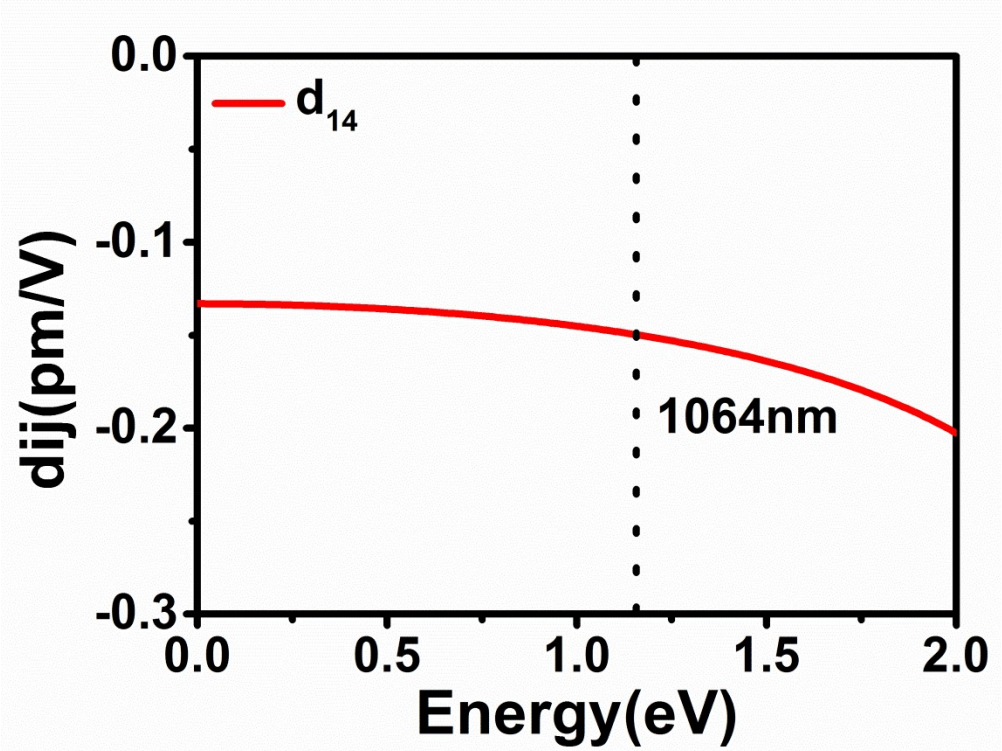

Figure S9. The calculated SHG coefficient of $K_2(BeS)O_4F_2$.

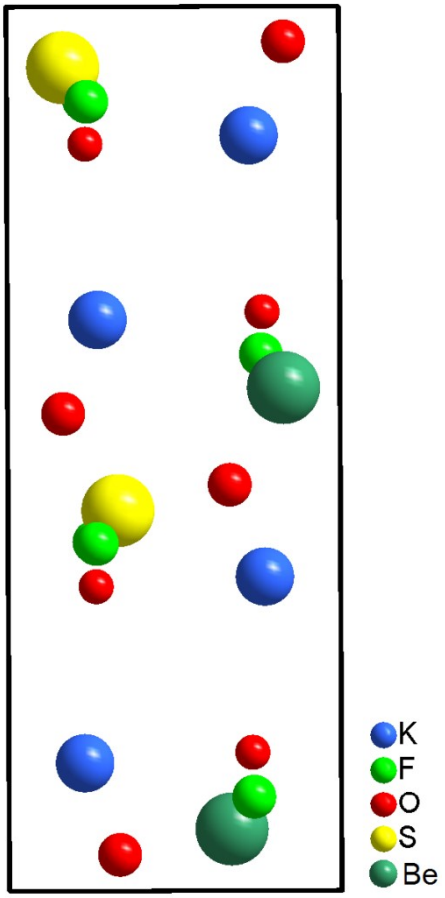

Figure S10. The identified way about Be and S atoms in calculating part.