Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

$Sc_2F_2(B_2O_5)$: A Deep Ultraviolet Scandium Borate Fluoride Exhibiting Large Birefringence Induced by the Synergistic Effect of B_2O_5 and ScO_nF_2 Groups

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Supplementary Index

Tables and Figures.

Table S1. Selected bond distances (Å) and angles (deg) for $Sc_2F_2(B_2O_5)$.

Sc(1)-F(1)	2.0267(4)	O(1)-B(1)	1.337(6)
Sc(1)-F(1)#1	2.0267(4)	O(2)-B(1)	1.350(6)
Sc(1)-O(2)	2.071(3)	B(1)-O(3)#2	1.418(6)
Sc(1)-O(2)#2	2.157(3)	B(2)-O(5)#3	1.372(6)
Sc(1)-O(4)	2.177(3)	B(2)-O(3)#6	1.412(6)
Sc(1)-O(5)#3	2.188(3)	O(4)-B(2)	1.372(6)
Sc(1)-O(3)	2.410(3)	O(1)-B(1)-O(2)	126.6(4)
Sc(2)-F(2)	2.0201(3)	O(1)-B(1)-O(3)#2	123.2(4)
Sc(2)-F(2)#1	2.0201(3)	O(2)-B(1)-O(3)#2	110.2(4)
Sc(2)-O(5)	2.047(3)	O(4)-B(2)-O(5)#3	114.9(4)
Sc(2)-O(4)	2.056(3)	O(4)-B(2)-O(3)#6	120.8(4)
Sc(2)-O(1)	2.120(3)	O(6)#3-B(2)-O(3)#6	124.2(4)
Sc(2)-O(1)#4	2.124(3)		

Symmetry transformations used to generate equivalent atoms:
#1 x, y, z+1 #2 -x,-y,-z+1 #3 x-1/2,-y+1/2, z #4 -x+1,-y,-z+1 #5 x, y, z-1 #6 x+1/2,-y+1/2, z

Table S2. Atomic coordinates (× 10^4), equivalent isotropic displacement parameters (Å^2 × 10^3) and bond valence sums (BVS) for $Sc_2F_2(B_2O_5)$.

Atom	x/a	y/b	z/c	U(eq)	BVS
Sc(1)	318(1)	1183(1)	5000	10(1)	2.988
Sc(2)	4364(1)	1094(1)	5000	9(1)	3.104
F(1)	195(3)	1266(2)	0	32(1)	0.990
F(2)	4326(3)	1101(2)	0	30(1)	0.973
O(1)	3741(3)	-338(2)	5000	15(1)	2.053
O(2)	1278(3)	-121(2)	5000	17(1)	2.042
O(3)	-2090(3)	1622(2)	5000	20(1)	1.995
O(4)	2435(3)	1704(2)	5000	18(1)	1.981
O(5)	5558(3)	2285(2)	5000	18(1)	1.983
B(1)	2437(5)	-651(4)	5000	14(1)	3.035
B(2)	1970(6)	2617(4)	5000	21(1)	2.890

Table S3. Configuration, anion groups, space group and synthesis condition of known rare earth borate fluorides.

Compound	Metal coordination	Anion groups	Space group	Synthesis condition
LnB_2O_4F (Ln= La, Ce)	LnO_7F_3	BO_3^{3-}	*Pbca*	high temperature and high pressure
$Eu_5(BO_3)_3F$	EuO_8F, EuO_7F, EuO_7	BO_3^{3-}	*Pnma*	boron nitride crucible, argon flow
$RE_2(BO_3)F_3$ (*RE*=La, Tb, Dy, Ho)	REO_4F_5, REO_7F_2, REO_3F_4, REO_4F_3	BO_3^{3-}	$P2_1/c$	traditional high temperature solid-state method
$Gd_4(BO_2)O_5F$	GdO_6F, GdO_5F_2	BO_2^-	*Pmmn*	boron nitride crucible, argon flow
$RE_4B_4O_{11}F_2$ (*RE* = La, Pr, Nd, Sm, Eu, Ga, Tb, Dy, Ho, Er)	REO_6F_3, REO_8F_2, REO_{10}, REO_9F, REO_7F_3, REO_9F_2, REO_7F_2	$B_4O_{11}^{10-}$	*C2/c*	high temperature and high pressure
$Ln_3(BO_3)_2F_3$ (Ln =Sm, Eu, and Gd)	LnO_4F_5, LnO_7F_2.	BO_3^{3-}	*C2/c*	traditional high temperature solid-state method
$Pr_4B_3O_{10}F$	PrO_7F_2, PrO_8F, PrO_9	BO_3^{3-}	$P\bar{1}$	high temperature and high pressure
$RE_5(BO_3)_2F_9$ (*RE*=Dy, Er, Yb, Ho, Tm)	REO_3F_5, REO_3F_4, REO_4F_3	BO_3^{3-}	*C2/c*	high temperature and high pressure

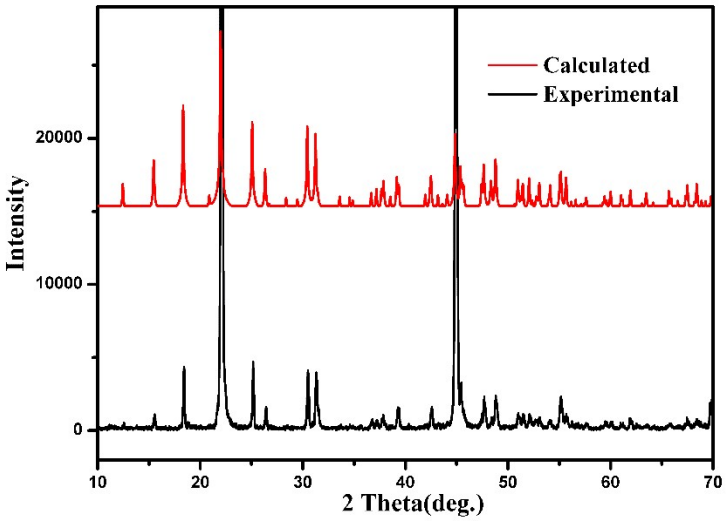

Figure S1. Simulated and experimental powder X−ray diffraction patterns of $Sc_2F_2(B_2O_5)$.

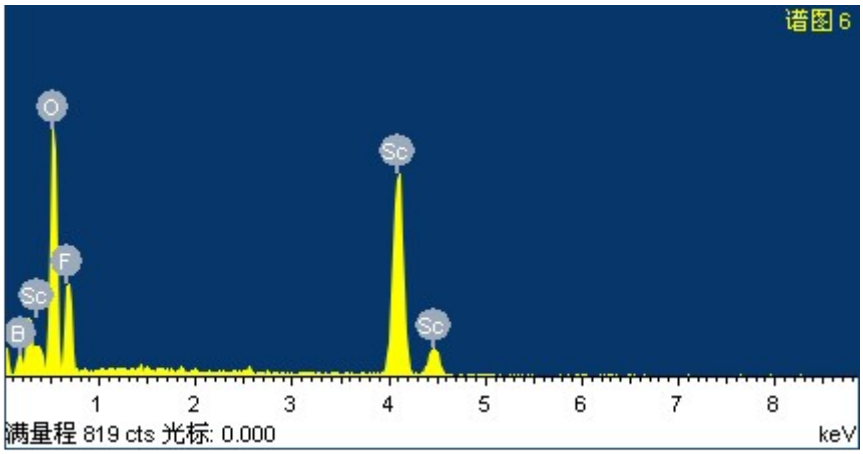

Figure S2. Energy dispersive X-ray spectroscopy (EDX) of $Sc_2F_2(B_2O_5)$.

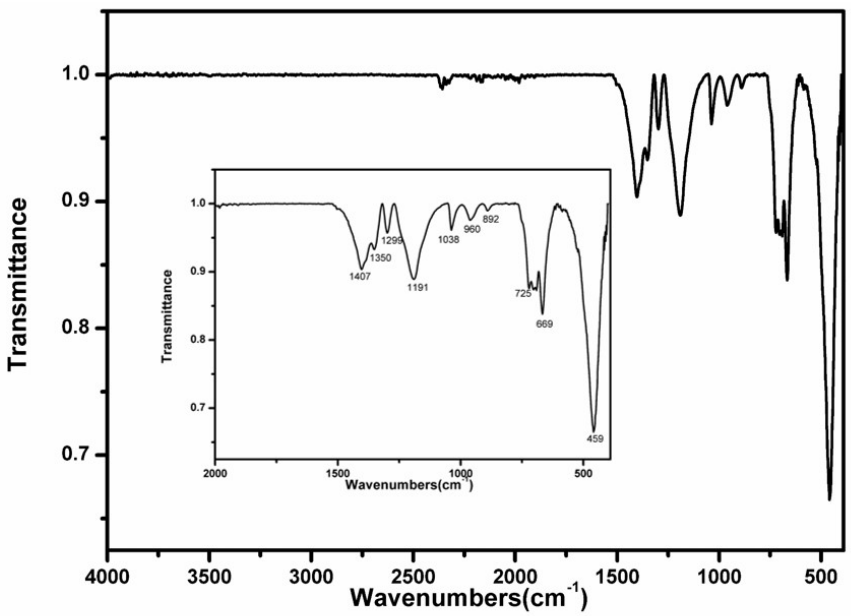

Figure S3. The IR spectrum of $Sc_2F_2(B_2O_5)$.

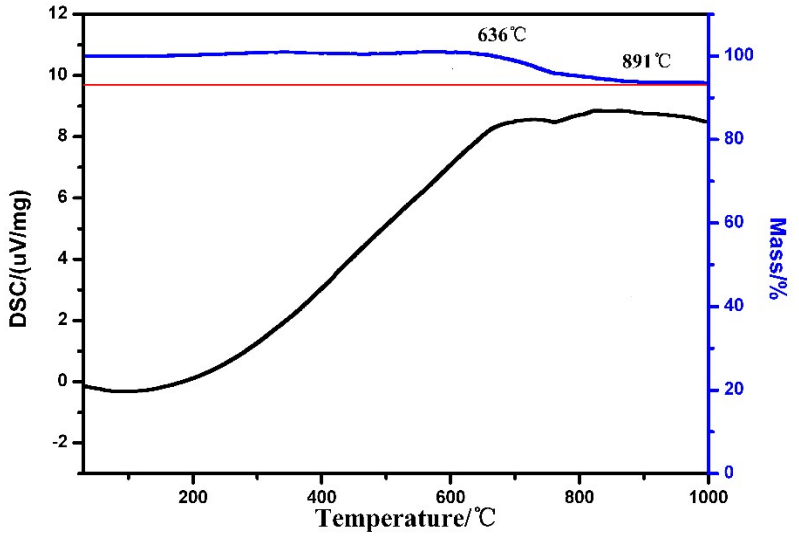

Figure S4. The TG-DSC curves of $Sc_2F_2(B_2O_5)$.