Supporting Information

$Pb_2Al_2B_3O_8F_3$: Structure and Properties of a New Fluoroaluminoborate with Non-traditional Chain-like B_3O_8 Group

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Table S1 The final Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Pb_2Al_2B_3O_8F_3$, U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor ($\times 10^3$), and the Bond Valence Sum for each atom in the asymmetric unit.

Atom	x	y	z	U_{eq}	BVS
Pb(1)	2084(1)	5119(1)	6456(1)	10(1)	2.05
Al(1)	5252(2)	6491(2)	5659(2)	6(1)	2.84
B(1)	8083(7)	7286(8)	5961(6)	8(1)	3.00
B(2)	5000	3556(10)	7500	3(2)	2.89
F(1)	5612(4)	8470(4)	5168(3)	12(1)	0.84
F(2)	5000	7182(5)	7500	8(1)	0.92
O(1)	3411(4)	6993(5)	5297(4)	9(1)	2.22
O(2)	4661(4)	4482(5)	6212(4)	6(1)	1.90
O(3)	7095(4)	6173(5)	6027(4)	9(1)	1.96
O(4)	3791(4)	2541(5)	7787(4)	10(1)	2.04

Table S2 Bond lengths [Å] and angles [deg] for $Pb_2Al_2B_3O_8F_3$.

Pb(1)-F(1)#1	2.423(3)	O(3)#2-Pb(1)-O(3)#3	144.36(17)
Pb(1)-O(1)	2.343(4)	O(4)#4-Pb(1)-O(2)	122.57(13)
Pb(1)-O(1)	2.945(4)	O(4)#4-Pb(1)-O(3)#3	148.15(12)
Pb(1)-O(2)	2.610(4)	O(4)#4-Pb(1)-O(3)#2	52.90(12)
Pb(1)-O(3)#2	2.642(4)	F(1)-Al(1)-F(2)	87.48(19)
Pb(1)-O(3)#3	2.692(4)	F(1)-Al(1)-O(1)	85.84(18)
Pb(1)-O(4)#4	2.577(4)	F(1)-Al(1)-O(2)	173.3(2)
Pb(1)-O(4)	3.052(4)	F(1)-Al(1)-O(2)#3	99.97(18)
Al(1)-F(1)	1.802(4)	F(1)-Al(1)-O(3)	89.64(19)
Al(1)-F(2)	1.832(2)	F(2)-Al(1)-Al(1)#3	131.55(17)
Al(1)-O(1)	1.896(4)	F(2)-Al(1)-O(1)	87.83(14)
Al(1)-O(2)#3	1.936(4)	F(2)-Al(1)-O(2)#3	171.6(2)
Al(1)-O(2)	1.899(4)	F(2)-Al(1)-O(2)	90.11(18)
Al(1)-O(3)	1.869(4)	F(2)-Al(1)-O(3)	90.47(13)
B(1)-O(1)#1	1.366(7)	O(1)-Al(1)-O(2)#3	88.92(18)
B(1)-O(3)	1.369(8)	O(1)-Al(1)-O(2)	87.9(2)
B(1)-O(4)#5	1.377(7)	O(2)-Al(1)-O(2)#3	82.07(17)
B(2)-O(2)×2	1.479(6)	O(3)-Al(1)-O(1)	175.2(2)
B(2)-O(4)×2	1.503(6)	O(3)-Al(1)-O(2)#3	93.35(18)
F(1)#1-Pb(1)-O(2)	129.36(12)	O(3)-Al(1)-O(2)	96.6(2)
F(1)#1-Pb(1)-O(3)#2	124.39(12)	O(2)-B(2)-O(2)#2	114.7(6)
F(1)#1-Pb(1)-O(3)#3	81.48(12)	O(2)#2-B(2)-O(4)#2	106.2(2)
F(1)#1-Pb(1)-O(4)#4	72.13(11)	O(2)#2-B(2)-O(4)	110.4(2)
O(1)-Pb(1)-F(1)#1	72.59(13)	O(2)-B(2)-O(4)#2	110.5(2)
O(1)-Pb(1)-O(2)	63.97(13)	O(2)-B(2)-O(4)	106.2(2)
O(1)-Pb(1)-O(3)#2	90.01(13)	O(4)-B(2)-O(4)#2	108.8(6)
O(1)-Pb(1)-O(3)#3	73.85(13)	O(1)#6-B(1)-O(3)	121.7(5)
O(1)-Pb(1)-O(4)#4	81.35(13)	O(1)#6-B(1)-O(4)#8	122.3(6)
O(2)-Pb(1)-O(3)#2	81.45(12)	O(3)-B(1)-O(4)#8	115.8(5)
O(2)-Pb(1)-O(3)#3	62.93(11)		

Symmetry transformations used to generate equivalent atoms:

$^{\#1}$x-1/2,-y+3/2,-z+1, $^{\#2}$-x+1,y,-z+3/2, $^{\#3}$-x+1,-y+1,-z+1, $^{\#4}$-x+1/2,y+1/2,z,

$^{\#5}$x-1/2,y-1/2,-z+3/2, $^{\#8}$ x+1/2,y+1/2,-z+3/2

Table S3 Anisotropic displacement parameters ($\times 10^3$) of $Pb_2Al_2B_3O_8F_3$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pb(1)	11(1)	10(1)	9(1)	0(1)	1(1)	-1(1)
Al(1)	6(1)	7(1)	6(1)	-1(1)	-1(1)	0(1)
B(1)	5(3)	8(3)	10(3)	-1(2)	-2(2)	3(3)
B(2)	3(2)	3(2)	3(2)	0	0(1)	0
F(1)	13(1)	12(1)	12(1)	1(1)	1(1)	0(1)
F(2)	10(2)	9(2)	7(2)	0	2(2)	0
O(1)	7(2)	13(2)	7(2)	1(2)	1(2)	0(2)
O(2)	5(2)	9(2)	5(2)	-2(1)	2(1)	0(2)
O(3)	11(2)	5(2)	11(2)	1(1)	-3(2)	-2(2)
O(4)	13(2)	12(2)	4(2)	1(1)	1(2)	-3(2)

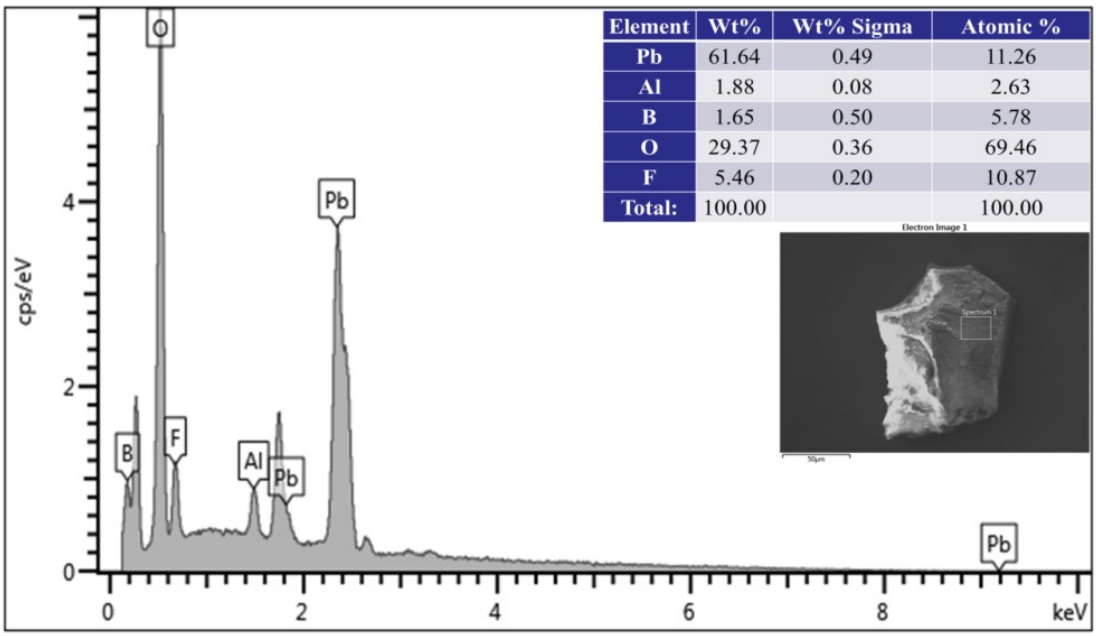
Table S4 Aluminum borates in the reported structures.

No.	Compounds	B-O groups	Space group	A/B
1	$CaZrB(Al_9O_{18})$	Isolated BO_3	$P6_3$	11
2	$Na_2AlBAs_4O_{14}$	Isolated BO_4	$P2_1/c$	7
3	Al_5BO_9	Isolated BO_3	*Pbam*	5
4	$Al_{20}B_4O_{36}$	Isolated BO_3	$Cmc2_1$	5
5	$Al_5O_6(BO_3)$	Isolated BO_3	$Cmc2_1$	5
6	$Pb_6AlF_7B_2O_7$	Isolated BO_3	*Cmca*	3.5
7	$NaFe_3B_3Al_6Si_6O_{30}F$	Isolated BO_3	*R*3*m*	3.3
8	$Li_2(BAlO_4)$	Isolated BO_3	$P2_1/c$	3
9	$Al_4B_2O_9$	Isolated BO_4	*Pbam*	2
10	$Al_4B_2O_9$	Isolated BO_3 and BO_4	*C*2/*m*	2
11	$Li_3(AlB_2O_6)$	Isolated BO_3	*P*-1	2
12	$Li_6Al_2(BO_3)_4$	Isolated BO_3	*P*-1	2
13	$Li(Al_7B_4O_{17})$	Isolated BO_3	*I*4/*m*	2
14	$Na_2Al_2(B_2O_7)$	Isolated BO_3	*P*-31*c*	2
15	$Na_2(Al_2B_2O_7)$	Isolated BO_3	*R*-3c	2
16	$K_2(Al_2B_2O_7)$	Isolated BO_3	*P*321	2
17	$(K_{0.48}Na_{0.52})_2Al_2B_2O_7$	Isolated BO_3	*P*321	2
18	$Rb_2Al_2B_2O_7$	Isolated BO_3	*P*321	2
19	$Rb_2(Al_2B_2O_7)$	Isolated BO_3	$P2_1/c$	2
20	$Cs_2Al_2B_2O_7$	Isolated BO_3	$P2_1/c$	2
21	$CaAlBO_4$	Isolated BO_3	*Ccc*2	2
22	$SrBAlO_4$	Isolated BO_3	*Pccn*	2
23	α-$PbAlBO_4$	Isolated BO_3	*Pnma*	2
24	β-$PbAlBO_4$	Isolated BO_3	*Pbcn*	2
25	$K_3Sr_3Li_2Al_4B_6O_{20}F$	Isolated BO_3	*R*32	2
26	$K_3Ba_3Li_2Al_4B_6O_{20}F$	Isolated BO_3	*P*-62*c*	2
27	$Rb_3Ba_3Li_2Al_4B_6O_{20}F$	Isolated BO_3	*P*-62*c*	2
28	$Rb_3Al_3B_3O_{10}F$	Isolated BO_3	*P*31*c*	2
29	$BaAl(BO_3)F_2$	Isolated BO_3	$P6_3/m$	2
30	$Cu_2(AlBO_5)$	Isolated BO_3	$P2_1/c$	2
31	$Cu_2(Al_6B_4O_{17})$	Isolated BO_3	*I*4/*m*	2
32	$AlMg(BO_4)$	Isolated BO_4	*Pnma*	2
33	$NaCa_{0.5}(Al_2B_2O_7)$	Isolated BO_3	$P6_3/m$	1.75
34	$NaSr_{0.5}(Al_2B_2O_7)$	Isolated BO_3	$P6_3/m$	1.75
35	$K_{0.91}Rb_{1.09}Al_2(B_2O_7)$	Isolated BO_3	*P*321	1.5
36	$Pb_2Bi_2AlB_3O_{11}$	Isolated BO_3	*C*2/*c*	1.6
37	$CaAl_2(BO_3)_2O$	Isolated BO_3	*R*-3*c*	1.5
38	$Ca_{0.05}Na_{1.90}Al_2B_2O_7$	Isolated BO_3	$P6_3/m$	1.5
39	$Ca_{0.69}Na_{0.64}Al_2B_2O_7$	Isolated BO_3	$P6_3/m$	1.5
40	α-$SrAl_2(B_2O_7)$	Isolated BO_3	*R*-3*c*	1.5
41	β-$Sr(Al_2B_2O_7)$	Isolated BO_3	*R*32	1.5
42	$Ba_8(Al_{10}B_{12}O_{41})$	Isolated BO_3	*P*-1	1.5

43	$SnAl_2(BO_3)_2F_2$	Isolated BO_3	$I4_1/amd$	1.5
44	$Ba(Al_2B_2O_7)$	Isolated BO_3	R-3c	1.5
45	$Al_8(BO_3)_4(B_2O_5)F_8$	Isolated BO_3 and B_2O_5	$P42/nmc$	1.33
46	$Pb_2Al_2B_3O_8F_3$	IsolatedB_3O_8	$Pbcn$	1.33
47	$Li_4NaKAl_4Be_3B_{10}O_{27}$	Isolated BO_3	P-43m	1.3
48	$Al_6(BO_3)_5F_3$	Isolated BO_3	$P6_3/m$	1.2
49	$AlBO_3$	Isolated BO_3	R-3c	1
50	$Li(AlB_2O_5)$	Isolated B_2O_5	$C2/c$	1
51	$YAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
52	α-$NdAl_3(BO_3)_4$	Isolated BO_3	$C2/c$	1
53	β-$NdAl_3(BO_3)_4$	Isolated BO_3	$C2/c$	1
54	α-$GdAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
55	β-$GdAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
56	$PrAl_3(BO_3)_4$	Isolated BO_3	$C2/c$	1
57	$HoAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
58	α-$ErAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
59	β-$ErAl_3(BO_3)_4$	Isolated BO_3	$C2$	1
60	$TmAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
61	$YbAl_3(BO_3)_4$	Isolated BO_3	$R32$	1
62	$NaBa_4Al_2B_8O_{18}Cl_3$	Isolated B_4O_9	$P4_2nm$	0.875
63	$NaBa_4(A0.875lB_4O_9)_2Br_3$	Isolated B_4O_9	$P4_2nm$	0.875
64	$Li_7BaAlB_{12}O_{24}$	B_6O_{14} chain	R-3	0.75
65	$Li_7SrAlB_{12}O_{24}$	B_6O_{14} chain	R-3	0.75
66	$Li_5MgSrAlB_{12}O_{24}$	B_2O_6 chain	R-3	0.75
67	$Li_5ZnSrAlB_{12}O_{24}$	B_2O_6 chain	R-3	0.75
68	$Cs(Al_4Be_4B_{12}O_{28})$	BO_4 3D-network	P-43m	0.75
69	$Ba_2AlB_4O_9Cl$	Isolated B_4O_9	$P4_2nm$	0.75
70	$CsAlB_3O_6F$	Isolated B_3O_6	$Pna2_1$	0.75
71	RbAlB3O6F	Isolated B_3O_6	$Pna2_1$	0.75
72	Cs0.5Rb0.5AlB3O6F	Isolated B_3O_6	P-62c	0.75
73	$Cs_{0.55}Al_4B_{12}Be_5O_{28}$	BO_4 3D-network	P-43m	0.7125
74	$Ba_6Al_4B_{14}O_{33}$	Isolated B_6O_{14}	P-1	0.714
75	$Al_4(B_6O_{15})$	Isolated B_2O_5	$R3$	0.66
76	$Cs_3AlB_6O_{12}$	Isolated $B_{12}O_{24}$	$P2_1/c$	0.66
77	$CaAl(B_3O_7)$	BO_4 layer	$Cmma$	0.66
78	$SrAlB_3O_6F_2$	B_3O_6 chain	$P2_1/c$	0.66
79	$Cs_3AlB_6O_{12}$	Isolated $B_{12}O_{24}$	$P2_1/c$	0.66
80	$Li_2(AlB_5O_{10})$	Isolated B_5O_{10}	$P2_1/c$	0.6
81	$Cs_2AlB_5O_{10}$	Isolated B_5O_{10}	$P3_121$	0.6
82	$NaSr_7Al(B_{18}O_{36})$	Isolated $B_{18}O_{36}$	R-3c	0.5
83	$K_3AlB_8O_{15}$	B_8O_{15} chain	$P2_1/c$	0.5

Table S5 F-containing aluminum borates in the reported structures.

No.	Compounds	B-O groups	Al-O/F configuration
1	$K_3Sr_3Li_2Al_4B_6O_{20}F$	Isolated BO_3	AlO_4
2	$K_3Ba_3Li_2Al_4B_6O_{20}F$	Isolated BO_3	AlO_4
3	$Rb_3Ba_3Li_2Al_4B_6O_{20}F$	Isolated BO_3	AlO_4
4	$NaFe_3B_3Al_6Si_6O_{30}F$	Isolated BO_3	AlO_6
5	$CsAlB_3O_6F$	Isolated B_3O_6	AlO_3F
6	$RbAlB_3O_6F$	Isolated B_3O_6	AlO_3F
7	$Rb_3Al_3B_3O_{10}F$	Isolated BO_3	AlO_4 andAlO_3F
8	$BaAl(BO_3)F_2$	Isolated BO_3	AlO_3F_2
9	$Al_6(BO_3)_5F_3$	Isolated BO_3	AlO_5F
10	$Al_8(BO_3)_4(B_2O_5)F_8$	Isolated BO_3 and B_2O_5	AlO_4F_2
11	$SnAl_2(BO_3)_2F_2$	Isolated BO_3	AlO_4F_2
12	$Pb_6AlF_7B_2O_7$	Isolated BO_3	AlF_6
13	$Pb_2Al_2B_3O_8F_3$	IsolatedB_3O_8	AlO_4F_2



Element	Wt%	Wt% Sigma	Atomic %
Pb	61.64	0.49	11.26
Al	1.88	0.08	2.63
B	1.65	0.50	5.78
O	29.37	0.36	69.46
F	5.46	0.20	10.87
Total:	100.00		100.00

Figure S1 X-ray energy dispersive spectrum of $Pb_2Al_2B_3O_8F_3$ crystal.

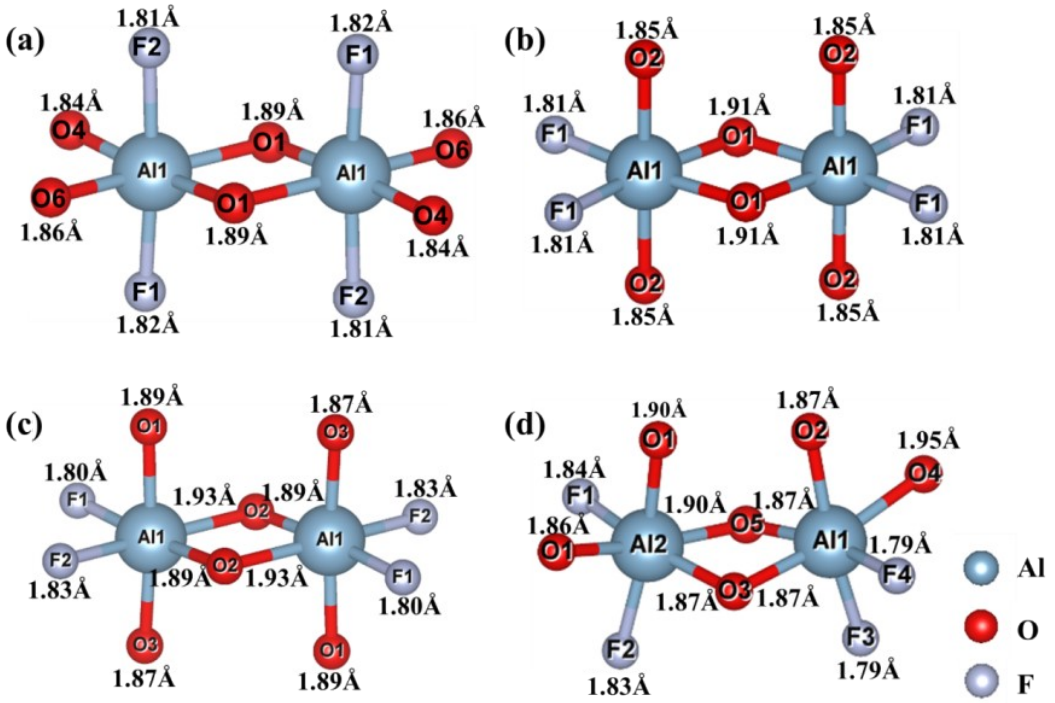


Figure S2 $[AlO_4F_2]^{5-}$ groups in $SrAlB_3O_6F_2$ (a); $Al_8(BO_3)_4(B_2O_5)F_8$ (b); $Pb_2Al_2B_3O_8F_3$ (c); and $SnAl_2(BO_3)_2F_2$ (d).

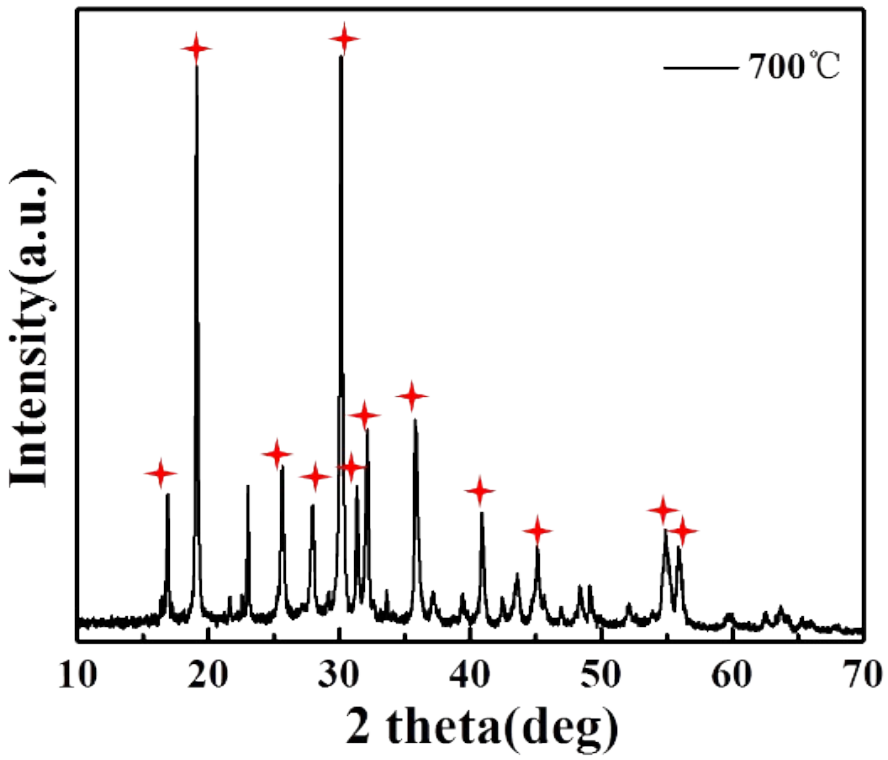


Figure S3 The XRD pattern of calcined sample at 700 °C. The marked asterisks are $Pb_4Al_2B_2O_{10}$ (the PDF card number in the Jade is 43-0022).