$Ba_2Ga_2F_6(IO_3)(PO_4)$: First fluoride-containing iodate-phosphate with 1D $[Ga_2F_6(IO_3)(PO_4)]^{4-}$ helix chain

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Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $Ba_2Ga_2F_6(IO_3)(PO_4)$.

Atom	x	y	z	U(eq)
Ba1	2176.6(9)	1149.5(2)	5374.5(5)	14.47(16)
Ba2	7703.2(9)	2763.4(2)	3435.6(5)	12.31(16)
Ga1	2483.3(16)	5336.0(4)	6970.6(10)	9.7(2)
Ga2	2417.7(16)	2856.3(4)	6258.3(9)	9.8(2)
I1	7531.6(10)	4381.3(2)	7727.7(6)	12.93(17)
P1	2783(4)	4191.2(9)	4728(2)	8.7(5)
O1	6977(11)	3900(3)	9160(6)	19.0(14)
O2	10528(10)	4772(2)	8332(6)	13.9(13)
O3	5423(10)	5094(2)	8168(6)	12.1(13)
O4	5378(10)	4074(2)	4061(6)	12.2(13)
O5	1439(10)	3525(2)	4993(6)	13.0(13)
O6	965(10)	4615(2)	3863(6)	12.4(13)
O7	3324(10)	4552(2)	6023(6)	12.8(13)
F1	776(9)	3291(2)	7680(5)	18.5(11)
F2	5554(9)	3211(2)	6793(5)	18.3(12)
F3	2994(9)	2071(2)	7335(5)	16.9(11)
F4	-601(9)	2358.8(19)	5783(5)	14.3(11)
F5	4010(9)	2344(2)	4929(5)	16.9(11)
F6	1837(9)	6085(2)	8003(5)	17.5(11)

Table S2. Selected bond distances (Å) and calculated bond valences for $Ba_2Ga_2F_6(IO_3)(PO_4)$.

Bond	Bond Distance	BV	BVS
Ba1-O1[2]	2.933(6)	0.174	1.940
Ba1-O1[3]	2.790(6)	0.255	
Ba1-O2[2]	2.892(5)	0.194	
Ba1-O3[4]	2.841(5)	0.223	
Ba1-F1[3]	3.046(5)	0.098	
Ba1-F3	2.741(5)	0.224	
Ba1-F4	2.831(4)	0.176	
Ba1-F5	2.597(4)	0.331	
Ba1-F6[5]	2.679(5)	0.265	
Ba2-O4	2.941(5)	0.170	2.217
Ba2-O5[7]	2.900(5)	0.190	
Ba2-F1[6]	2.746(5)	0.221	
Ba2-F2[3]	2.779(4)	0.263	
Ba2-F3[3]	2.676(4)	0.267	
Ba2-F3[6]	2.988(5)	0.115	
Ba2-F4[7]	2.663(5)	0.277	
Ba2-F4[6]	2.877(5)	0.155	
Ba2-F5	2.600(5)	0.328	
Ba2-F6[8]	2.731(5)	0.230	
Ga1-O2[1]	2.065(6)	0.404	3.188
Ga1-O3	1.988(5)	0.498	
Ga1-O4[8]	1.935(6)	0.575	
Ga1-O6[9]	1.959(5)	0.539	

Ga1-O7	1.890(5)	0.649	
Ga1-F6	1.859(5)	0.524	
Ga2-O5	1.915(5)	0.607	3.006
Ga2-F1	1.904(5)	0.464	
Ga2-F2	1.836(4)	0.558	
Ga2-F3	1.930(4)	0.433	
Ga2-F4	1.898(4)	0.472	
Ga2-F5	1.897(5)	0.473	
I1-O1	1.777(6)	1.842	4.993
I1-O2	1.825(5)	1.618	
I1-O3	1.845(5)	1.533	
P1-O4	1.531(6)	1.262	5.109
P1-O5	1.520(6)	1.300	
P1-O6	1.528(5)	1.272	
P1-O7	1.527(6)	1.275	

Symmetry transformations used to generate equivalent atoms:
[1] 1/2+X, 3/2-Y, 1/2-Z; [2] 1/2+X, +Y, 1/2-Z; [3] +X, 3/2-Y, +Z; [4] 1/2-X, 1/2+Y, -1/2+Z; [5] 1/2-X, 1-Y, -1/2+Z; [6] -1/2+X, +Y, 1/2-Z; [7] -1/2+X, 3/2-Y, 1/2-Z; [8] 1-X, 1-Y, 1-Z; [9] +X, 1/2-Y, +Z.

Table S3. The assignments of the infrared absorption peaks for $Ba_2Ga_2F_6(IO_3)(PO_4)$.

	Wavelength (cm^{-1})
I-O	818, 641, 538, 455, 429
P-O	1030, 999, 612, 570, 511,492
Ga-F	1114, 1074
Ga-O	774, 702

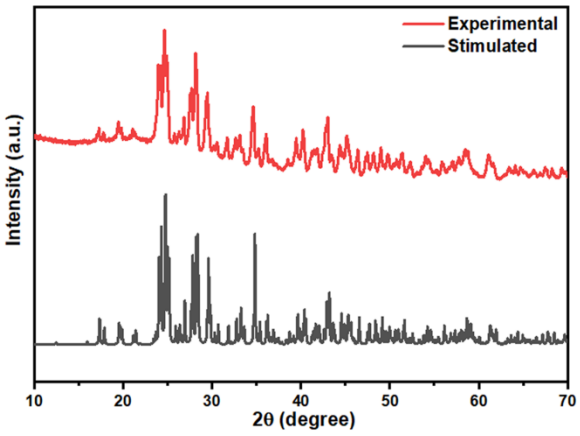

Figure S1. Simulated and measured powder X-ray diffraction patterns for $Ba_2Ga_2F_6(IO_3)(PO_4)$

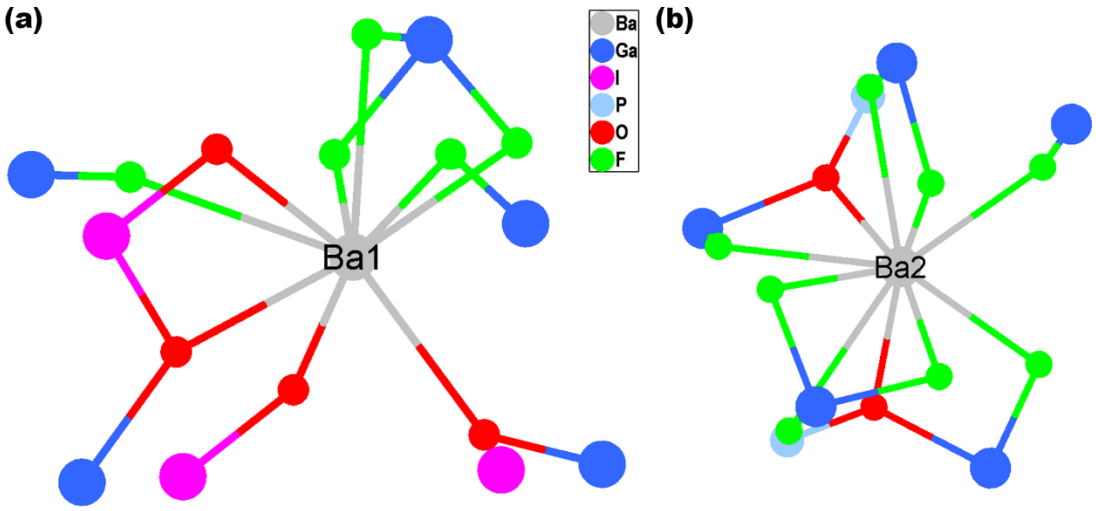

Figure S2. Views of the coordination geometries of Ba(1) and Ba(2)

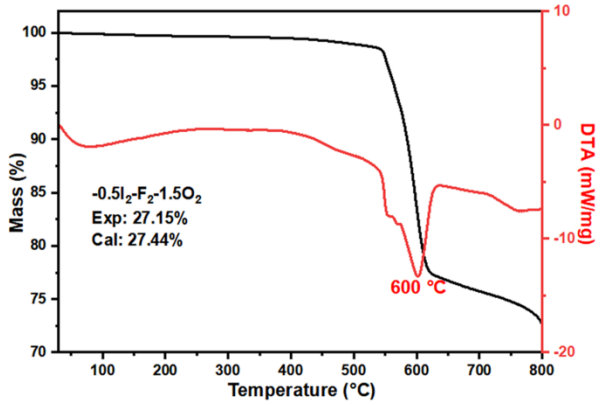

Figure S3. TG-DTA curves for $Ba_2Ga_2F_6(IO_3)(PO_4)$.

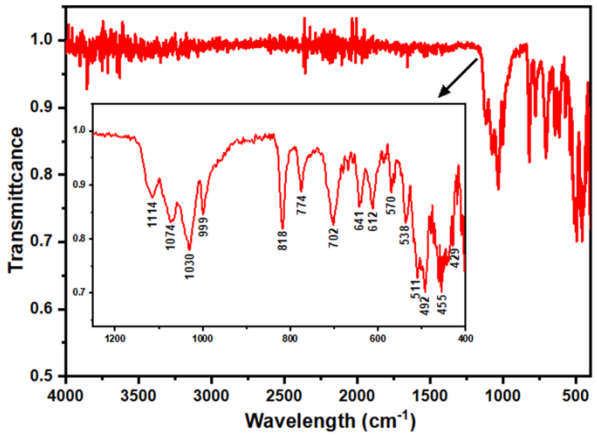

Figure S4. IR spectra for $Ba_2Ga_2F_6(IO_3)(PO_4)$.

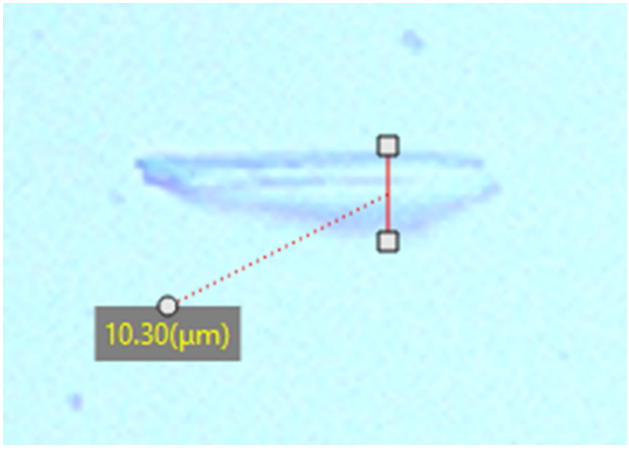

Figure S5. The thickness of $Ba_2Ga_2F_6(IO_3)(PO_4)$ crystal used for birefringence measurements

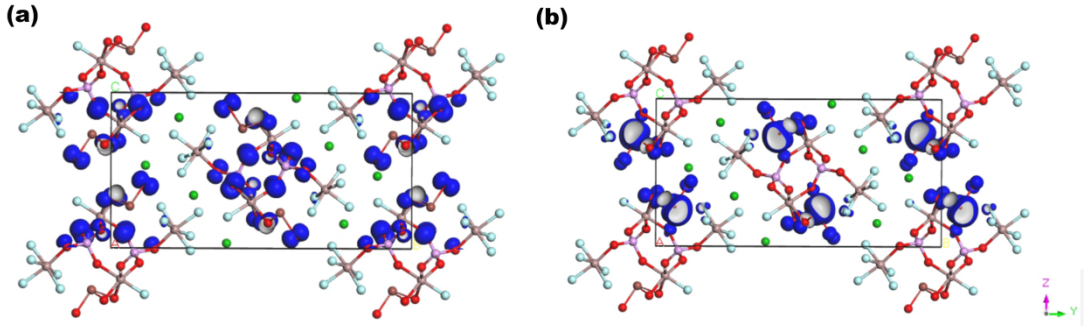

Figure S6. HOMO (a) and LUMO (b) of $Ba_2Ga_2F_6(IO_3)(PO_4)$