Supporting Information

$NaGaI_3O_9F$: A new alkali metal gallium iodate combined with IO_3^- and IO_3F^{2-} units

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Contents.

1. Supplementary Tables.

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of $NaGaI_3O_9F$.

Atom	x	y	z	$U_{(eq)}$[a]
I1	939.7(4)	5743.3(11)	7078.1(4)	11.91(13)
I2	1575.5(4)	-21.2(11)	4921.7(4)	10.95(12)
I3	4898.2(16)	785(5)	6240.8(8)	11.4(3)
I4	5138(16)	80(50)	6331(11)	11.4(3)
Na1	6981(3)	4953(7)	6124(3)	24.1(8)
Ga1	3092.6(7)	5046.2(19)	6619.8(7)	10.7(2)
F1	3590(4)	2702(10)	7825(4)	21.8(12)
O1	2220(4)	7007(11)	7224(5)	16.3(14)
O2	192(5)	7571(13)	5877(5)	26.4(16)
O3	793(5)	7987(12)	8058(5)	20.9(15)
O4	1924(5)	1651(12)	3951(5)	18.5(14)
O5	2717(4)	-2246(11)	5446(5)	13.7(13)
O6	1889(4)	2646(12)	5938(5)	15.3(13)
O7	3864(4)	3339(12)	5863(5)	16.0(13)
O8	5714(4)	2294(11)	7539(4)	12.9(13)
O9	5607(5)	2137(13)	5506(5)	19.9(14)

[a] $U_{(eq)}$ is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond lengths (Å) of $NaGaI_3O_9F$.

Bond	Length/Å
I1-O1	1.847(5)
I1-O2	1.804(6)
I1-O3	1.806(6)
I2-O4	1.783(6)
I2-O5	1.845(5)
I2-O6	1.832(6)
I3-O7	1.840(6)
I3-O8	1.849(6)
I3-O9	1.797(6)
I4-O7	2.31(3)
I4-O8	1.875(14)
I4-O9	1.820(14)
I4-F1	2.07(3)
Ga1-O1	1.979(6)
Ga1-O5	1.987(6)
Ga1-O6	1.977(6)
Ga1-O7	1.958(6)
Ga1-O8	1.966(6)
Ga1-F1	1.902(5)

Table S3. Selected bond angles (°) of $NaGaI_3O_9F$.

Angle	(°)
O1-I1-O3	96.0(3)
O2-I1-O1	97.6(3)
O2-I1-O3	99.9(3)
O4-I2-O6	100.2(3)
O4-I2-O5	96.2(3)
O6-I2-O5	102.4(3)
O8-I3-O9	96.3(3)
O7-I3-O8	97.1(3)
O9-I3-O7	98.4(3)
F1-I4-O7	163.4(7)
F1-I4-O9	102.1(10)
O8-I4-F1	81.6(8)
O7-I4-O8	82.1(9)
O9-I4-O8	94.6(7)
O7-I4-O9	82.8(10)

2. Supplementary Figures.

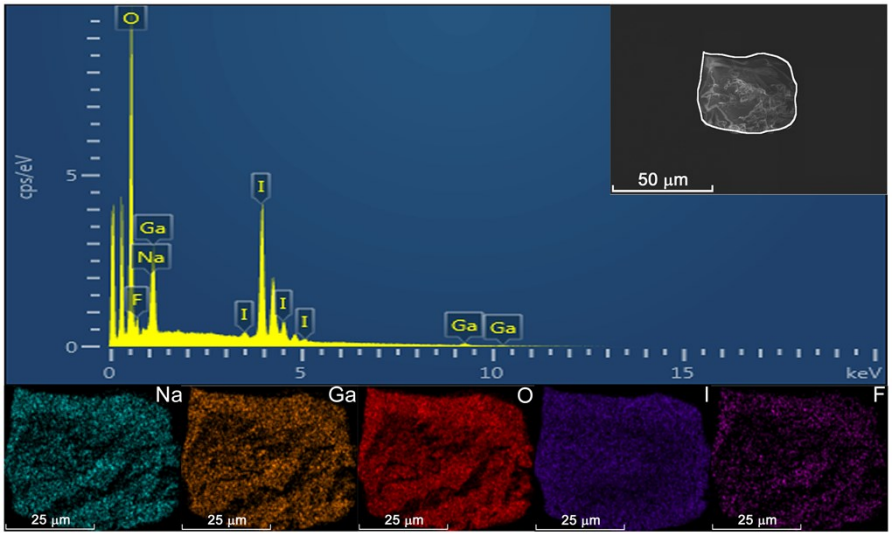

Figure S1. The EDS spectrum of $NaGaI_3O_9F$.

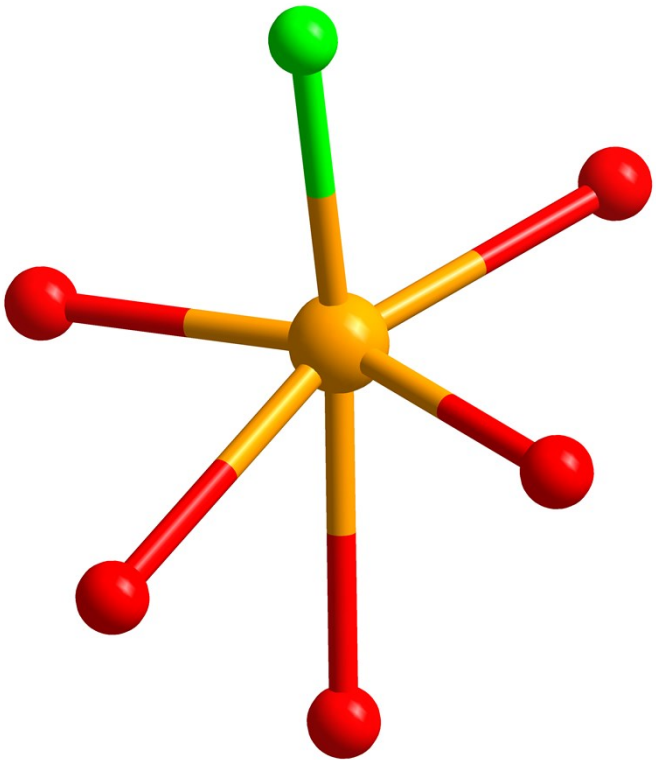

Figure S2. The coordination environment of Na atom.

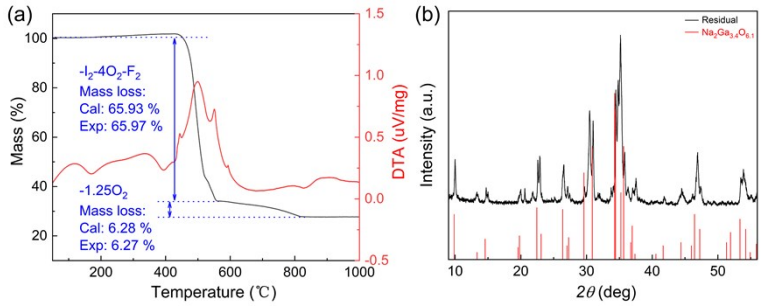

Figure S3. The TG and DTA curves (a) and PXRD patterns for the residual (b) of $NaGaI_3O_9F$.

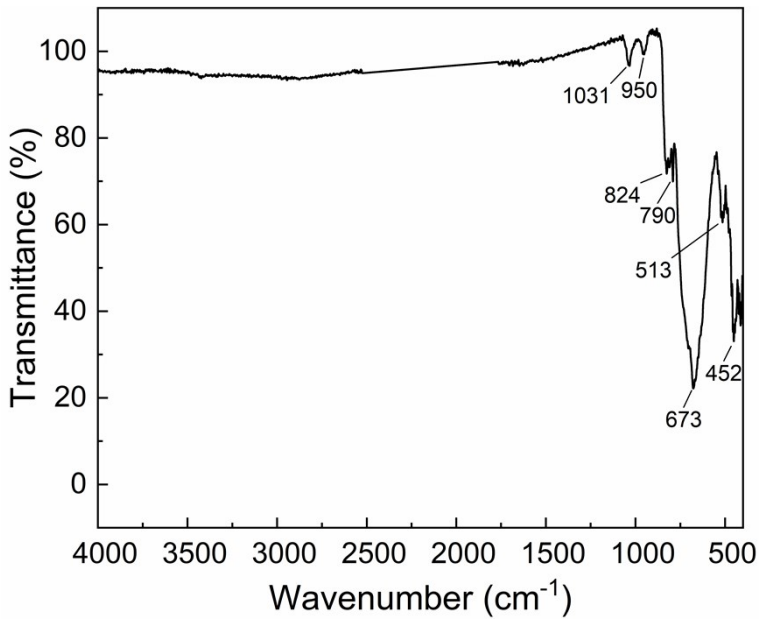

Figure S4. The IR spectrum of $NaGaI_3O_9F$.

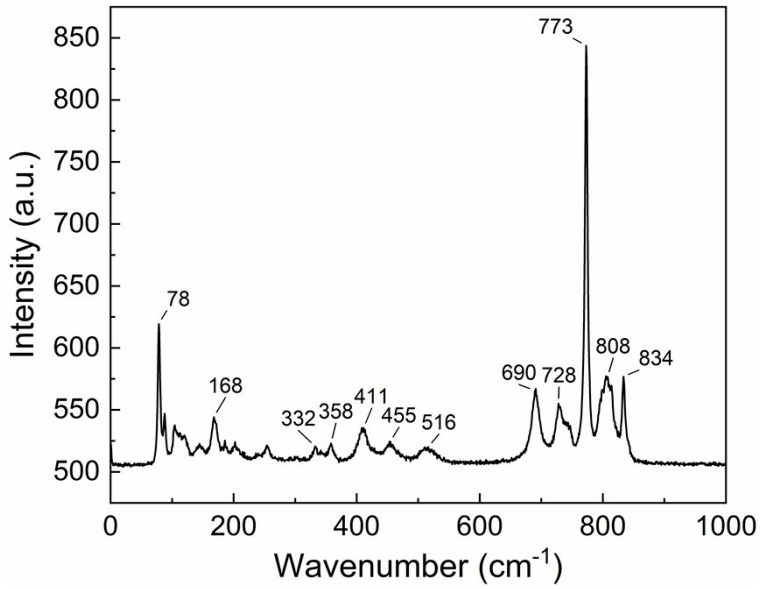

Figure S5. The Raman spectrum of $NaGaI_3O_9F$.

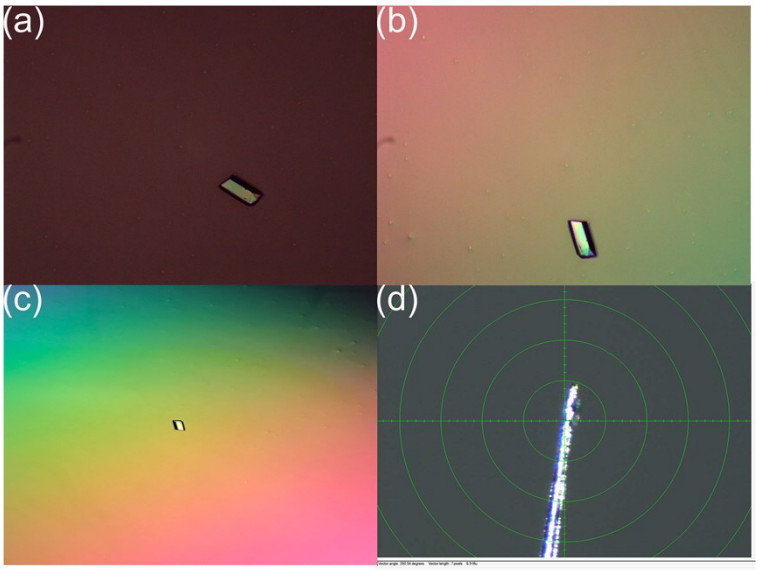

Figure S6. Birefringence measurement of $NaGaI_3O_9F$; (a) the original crystal; (b) the crystal in the extinction state; (c) the crystal interference color observed under the microscope and (d) the photographs of crystal thickness.