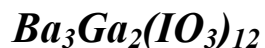


Electronic Supplementary Information

Synthesis and Structure of a new Mixed Metal Iodate



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Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $\text{Ba}_3\text{Ga}_2(\text{IO}_3)_{12}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
I1	775.1(5)	3540.4(6)	5582.3(5)	9.6(2)
Ga1	3333	6667	6667	10.2(5)
Ba1	0	0	6554.9(16)	28.4(4)
O1	2523(7)	5052(7)	5606(7)	19.5(14)
O2	957(7)	2747(8)	6928(6)	18.9(14)
O3	1187(7)	2650(7)	4481(6)	17.4(13)

Table S2. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $\text{Ba}_3\text{Ga}_2(\text{IO}_3)_{12}$. The Anisotropic displacement factor exponent takes the form: -

$$2\pi^2[h^2a^2U_{11}+2hka^*b^*U_{12}+\dots].$$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	10.3(3)	11.6(3)	8.1(3)	-0.31(17)	0.40(17)	6.4(2)
Ga1	10.9(7)	10.9(7)	8.7(10)	0	0	5.4(3)
Ba1	25.0(5)	25.0(5)	35.2(9)	0	0	12.5(2)
O1	15(3)	13(3)	22(4)	-5(3)	5(3)	1(3)
O2	19(3)	28(4)	11(3)	3(3)	-3(2)	13(3)
O3	17(3)	18(3)	21(3)	-5(3)	2(3)	10(3)

Table S3. Selected Bond Lengths [Å] for Ba₃Ga₂(IO₃)₁₂.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	O1	1.848(7)	Ba1	O1 ¹⁰	3.104(8)
I1	O2	1.817(7)	Ba1	O1 ¹¹	3.104(8)
I1	O3	1.791(7)	Ba1	O1 ¹²	3.104(8)
Ga1	O1 ³	1.972(7)	Ba1	O2 ¹³	2.748(8)
Ga1	O1 ⁴	1.972(7)	Ba1	O2 ⁸	2.748(8)
Ga1	O1	1.972(7)	Ba1	O2	2.748(8)
Ga1	O1 ⁵	1.972(7)	Ba1	O3 ¹⁴	2.835(7)
Ga1	O1 ⁶	1.972(7)	Ba1	O3 ¹⁵	2.835(7)
Ga1	O1 ⁷	1.972(7)	Ba1	O3 ⁹	2.835(7)

¹1/3+X,2/3+Y,-1/3+Z; ²1/3-X,2/3-Y,5/3-Z; ³1-Y,1+X-Y,+Z; ⁴-1/3+Y,1/3-X+Y,4/3-Z; ⁵2/3-X,4/3-Y,4/3-Z; ⁶2/3-Y+X,1/3+X,4/3-Z; ⁷+Y-X,1-X,+Z; ⁸-Y,+X-Y,+Z; ⁹-X,-Y,1-Z; ¹⁰-1/3+Y-X,1/3-X,1/3+Z; ¹¹2/3-Y,1/3+X-Y,1/3+Z; ¹²-1/3+X,-2/3+Y,1/3+Z; ¹³+Y-X,-X,+Z; ¹⁴+Y,-X+Y,1-Z; ¹⁵-Y+X,+X,1-Z.

Table S4. Selected Bond Angles (°) for Ba₃Ga₂(IO₃)₁₂.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	I1	O1	96.3(3)	O2	Ba1	O1 ¹²	63.0(2)
O3	I1	O1	94.1(3)	O2 ⁸	Ba1	O1 ¹²	72.4(2)
O3	I1	O2	100.1(3)	O2 ⁸	Ba1	O1 ¹¹	111.2(2)
O1 ⁴	Ga1	O1	87.4(3)	O2	Ba1	O1 ¹¹	72.4(2)
O1 ⁶	Ga1	O1 ⁵	87.4(3)	O2 ¹³	Ba1	O1 ¹¹	63.0(2)
O1 ⁶	Ga1	O1 ⁴	180.0	O2 ¹³	Ba1	O1 ¹²	111.2(2)
O1 ⁷	Ga1	O1 ⁶	87.3(3)	O2 ⁸	Ba1	O1 ¹⁰	63.0(2)
O1 ³	Ga1	O1 ⁷	92.6(3)	O2	Ba1	O1 ¹⁰	111.2(2)
O1 ⁷	Ga1	O1 ⁴	92.6(3)	O2 ¹³	Ba1	O1 ¹⁰	72.4(2)
O1 ⁴	Ga1	O1 ⁵	92.6(3)	O2 ¹³	Ba1	O2	117.72(7)
O1 ³	Ga1	O1 ⁵	180.0	O2 ¹³	Ba1	O2 ⁸	117.72(7)
O1 ⁶	Ga1	O1	92.6(3)	O2	Ba1	O2 ⁸	117.72(7)
O1 ³	Ga1	O1 ⁴	87.4(3)	O2 ⁸	Ba1	O3 ¹⁴	72.7(2)
O1 ³	Ga1	O1	87.4(3)	O2 ⁸	Ba1	O3 ¹⁵	163.4(2)
O1 ⁷	Ga1	O1	180.0	O2	Ba1	O3 ¹⁵	72.7(2)
O1 ³	Ga1	O1 ⁶	92.6(3)	O2 ¹³	Ba1	O3 ¹⁵	61.7(2)
O1 ⁷	Ga1	O1 ⁵	87.4(3)	O2	Ba1	O3 ¹⁴	61.7(2)
O1 ⁵	Ga1	O1	92.7(3)	O2 ¹³	Ba1	O3 ⁹	72.7(2)
O1 ¹¹	Ba1	O1 ¹²	52.0(2)	O2 ¹³	Ba1	O3 ¹⁴	163.4(2)
O1 ¹¹	Ba1	O1 ¹⁰	52.0(2)	O2 ⁸	Ba1	O3 ⁹	61.7(2)
O1 ¹⁰	Ba1	O1 ¹²	52.0(2)	O2	Ba1	O3 ⁹	163.4(2)
O3 ⁹	Ba1	O1 ¹¹	124.0(2)	O3 ⁹	Ba1	O1 ¹²	127.5(2)
O3 ¹⁴	Ba1	O1 ¹²	83.8(2)	O3 ¹⁵	Ba1	O1 ¹¹	83.8(2)
O3 ¹⁴	Ba1	O1 ¹¹	127.5(2)	O3 ¹⁴	Ba1	O1 ¹⁰	124.0(2)
O3 ⁹	Ba1	O3 ¹⁴	104.36(18)	O3 ¹⁵	Ba1	O1 ¹⁰	127.5(2)
O3 ⁹	Ba1	O3 ¹⁵	104.36(18)	O3 ¹⁵	Ba1	O1 ¹²	124.0(2)
O3 ¹⁵	Ba1	O3 ¹⁴	104.36(18)	O3 ⁹	Ba1	O1 ¹⁰	83.8(2)

¹1/3-X,2/3-Y,5/3-Z; ²1/3+X,2/3+Y,-1/3+Z; ³+Y-X,1-X,+Z; ⁴1-Y,1+X-Y,+Z; ⁵2/3-Y+X,1/3+X,4/3-Z; ⁶-1/3+Y,1/3-X+Y,4/3-Z; ⁷2/3-X,4/3-Y,4/3-Z; ⁸-Y,+X-Y,+Z; ⁹-X,-Y,1-Z; ¹⁰-1/3+X,-2/3+Y,1/3+Z; ¹¹2/3-Y,1/3+X-Y,1/3+Z; ¹²-1/3+Y-X,1/3-X,1/3+Z; ¹³+Y-X,-X,+Z; ¹⁴-Y+X,+X,1-Z; ¹⁵+Y,-X+Y,1-Z