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BaI_3O_9OH: A new alkaline-earth metal hydroxy iodates with two groups

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Supporting Information

Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$), and bond valence sum (BVS) calculations for BaI_3O_9H. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}	BVS
Ba (1)	6525(1)	2036(1)	5010(1)	13(1)	2.13
I (1)	9371(1)	2082(1)	7706(1)	12(1)	5.47
I (2)	4719(1)	105(1)	7691(1)	10(1)	5.23
I (3)	8211(1)	6705(1)	4675(1)	11(1)	5.47
O (1)	11640(7)	2944(7)	7635(5)	27(1)	1.78
O (2)	9865(6)	3245(6)	4521(4)	22(1)	1.92
O (3)	6804(6)	5554(6)	5420(4)	20(1)	2.13
O (4)	4460(6)	446(5)	3471(4)	15(1)	2.10
O (5)	8428(6)	4023(5)	8032(4)	22(1)	1.96
O (6)	6627(6)	1046(5)	8300(4)	15(1)	2.20
O (7)	4932(6)	-1882(5)	8304(4)	15(1)	2.06
O (8)	7310(6)	8717(6)	4874(4)	25(1)	2.33
O (9)	9041(6)	2163(6)	6420(4)	24(1)	2.24
H (1)	12160(100)	3260(100)	8140(70)	29	

Table S2. Bond lengths (Å) and angles (°) for BaI_3O_9H.

Ba (1)-O (2)	2.882(5)	I (1)-O (1)	1.902(5)
Ba (1)-O (3)	2.876(5)	I (1)-O (5)	1.784(4)
Ba (1)-O (3) #1	3.259(5)	I (1)-O (6)	2.466(5)
Ba (1)-O (4) #2	3.012(5)	I (1)-O (9)	1.781(5)
Ba (1)-O (4)	2.894(4)	I (2)-O (4) #2	1.808(5)
Ba (1)-O (5) #3	3.278(6)	I (2)-O (6)	1.830(4)
Ba (1)-O (6) #3	2.819(5)	I (2)-O (7)	1.804(4)
Ba (1)-O (7) #4	2.774(5)	I (3)-O (2) #6	1.819(5)
Ba (1)-O (8) #1	3.055(5)	I (3)-O (3)	1.791(5)
Ba (1)-O (8) #5	2.733(5)	I (3)-O (8)	1.782(5)
Ba (1)-O (9)	2.692(5)		
O (2)-Ba (1)-O (3) #1	118.42(13)	O (7) #4-Ba (1)-O (8) #1	65.02(14)
O (2)-Ba (1)-O (4)	116.76(14)	O (8) #5-Ba (1)-O (2)	95.93(15)
O (2)-Ba (1)-O (4) #2	130.29(13)	O (8) #5-Ba (1)-O (3) #1	137.75(14)
O (2)-Ba (1)-O (5) #3	56.18(13)	O (8) #5-Ba (1)-O (3)	161.65(15)
O (2)-Ba (1)-O (8) #1	166.36(14)	O (8) #1-Ba (1)-O (3) #1	50.00(12)
O (3)-Ba (1)-O (2)	69.97(14)	O (8) #5-Ba (1)-O (4)	68.90(14)
O (3)-Ba (1)-O (3) #1	60.56(15)	O (8) #5-Ba (1)-O (4) #2	58.17(15)
O (3)-Ba (1)-O (4)	127.44(13)	O (8) #1-Ba (1)-O (5) #3	118.30(13)
O (3)-Ba (1)-O (4) #2	121.85(14)	O (8) #5-Ba (1)-O (5) #3	65.19(15)
O (3)-Ba (1)-O (5) #3	112.55(13)	O (8) #5-Ba (1)-O (6) #3	117.12(16)
O (3) #1-Ba (1)-O (5) #3	112.86(12)	O (8) #5-Ba (1)-O (7) #4	117.54(15)
O (3)-Ba (1)-O (8) #1	104.31(13)	O (8) #5-Ba (1)-O (8) #1	91.92(14)
O (4) #2-Ba (1)-O (3) #1	106.83(12)	O (9)-Ba (1)-O (2)	61.62(13)
O (4)-Ba (1)-O (3) #1	73.68(12)	O (9)-Ba (1)-O (3)	77.08(14)

O (4)-Ba (1)-O (4) #2	93.98(13)	O (9)-Ba (1)-O (3) #1	130.70(14)
O (4)-Ba (1)-O (5) #3	62.14(13)	O (9)-Ba (1)-O (4)	154.72(14)
O (4) #2-Ba (1)-O (5) #3	123.29(12)	O (9)-Ba (1)-O (4) #2	73.94(14)
O (4) #2-Ba (1)-O (8) #1	63.34(13)	O (9)-Ba (1)-O (5) #3	105.60(14)
O (4)-Ba (1)-O (8) #1	56.16(15)	O (9)-Ba (1)-O (6) #3	122.33(14)
O (6) #3-Ba (1)-O (2)	63.83(13)	O (9)-Ba (1)-O (7) #4	72.28(15)
O (6) #3-Ba (1)-O (3) #1	65.19(13)	O (9)-Ba (1)-O (8) #1	130.31(16)
O (6) #3-Ba (1)-O (3)	68.08(14)	O (6) #3-Ba (1)-O (3)	68.08(14)
O (6) #3-Ba (1)-O (4)	70.28(13)	O (1)-I (1)-O (6)	163.6(2)
O (6) #3-Ba (1)-O (4) #2	163.61(13)	O (5)-I (1)-O (1)	95.3(2)
O (6) #3-Ba (1)-O (5) #3	53.97(12)	O (5)-I (1)-O (6)	80.6(2)
O (6) #3-Ba (1)-O (8) #1	102.63(14)	O (9)-I (1)-O (1)	91.4(2)
O (7) #4-Ba (1)-O (2)	120.08(14)	O (9)-I (1)-O (5)	100.3(2)
O (7) #4-Ba (1)-O (3) #1	67.31(13)	O (9)-I (1)-O (6)	104.9(2)
O (7) #4-Ba (1)-O (3)	63.92(14)	O (4) #2-I (2)-O (6)	101.1(2)
O (7) #4-Ba (1)-O (4) #2	59.64(12)	O (7)-I (2)-O (4) #2	99.9(2)
O (7) #4-Ba (1)-O (4)	121.13(14)	O (7)-I (2)-O (6)	95.4(2)
O (7) #4-Ba (1)-O (5) #3	176.07(12)	O (3)-I (3)-O (2) #6	99.8(2)
O (7) #4-Ba (1)-O (6) #3	124.12(13)	O (8)-I (3)-O (2) #6	101.8(2)
O (9)-Ba (1)-O (8) #5	85.95(16)	O (8)-I (3)-O (3)	96.9(2)

Symmetry transformations used to generate equivalent atoms:

#1 x, y−1, z	#2 −x+1, y+1/2, −z+3/2	#3 x, −y+1/2, z−1/2
#4 −x+1, −y, −z+1	#5 −x+1, −y+1, −z+1	#6 −x+2, −y+1, −z+1
#7 x, −y+1/2, z+1/2	#8 −x+1, y−1/2, −z+3/2	#9 x, y+1, z

Table S3. Anisotropic displacement parameters ($Å^2$) for BaI_3O_9H.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba (1)	14(1)	13(1)	11(1)	1(1)	1(1)	-2(1)
I (1)	12(1)	14(1)	10(1)	1(1)	0(1)	0(1)
I (2)	9(1)	11(1)	10(1)	-1(1)	0(1)	1(1)
I (3)	11(1)	13(1)	9(1)	0(1)	2(1)	-1(1)
O (1)	16(3)	37(3)	27(4)	2(3)	1(3)	-10(2)
O (2)	19(3)	33(3)	12(3)	4(2)	-6(2)	-6(2)
O (3)	27(3)	17(2)	16(3)	1(2)	6(2)	-9(2)
O (4)	19(3)	15(2)	10(3)	-2(2)	0(2)	1(2)
O (5)	19(3)	19(2)	28(3)	-8(2)	-3(3)	7(2)
O (6)	12(2)	18(2)	15(3)	-1(2)	1(2)	-4(2)
O (7)	22(3)	11(2)	13(3)	1(2)	2(2)	-1(2)
O (8)	25(3)	16(3)	34(4)	-4(2)	11(3)	2(2)
O (9)	20(3)	42(3)	11(3)	1(2)	-1(2)	0(2)

Table S4. Hydrogen bond lengths [Å] and angles [deg.] for BaI_3O_9H. D, hydrogen bond donor; A, hydrogen bond acceptor.

D–H···A	d (D–H)	d (H···A)	d (D···A)	< (D–H···A)
O1–H1···O4[1]	0.83(8)	2.10(8)	2.748(7)	135(8)

Table S5. The investigation of the reported some large birefringent alkali earth iodates.

compound	band gap (eV)	Δn @1064 nm	refs.
$Ba_2[FeF_4(IO_3)_2]IO_3$	3.9	0.125	1
$Ba[InF_3(IO_3)_2]$	4.35	0.172	2
$Mg(H_2O)_6[(IO_2(OH))_2(IO_3)]_2$	4.10	0.230	3
$Sr(IO_3)_2$	4.14	0.093	4
$Ba(IO_2F_2)_2$	4.34	0.092	4

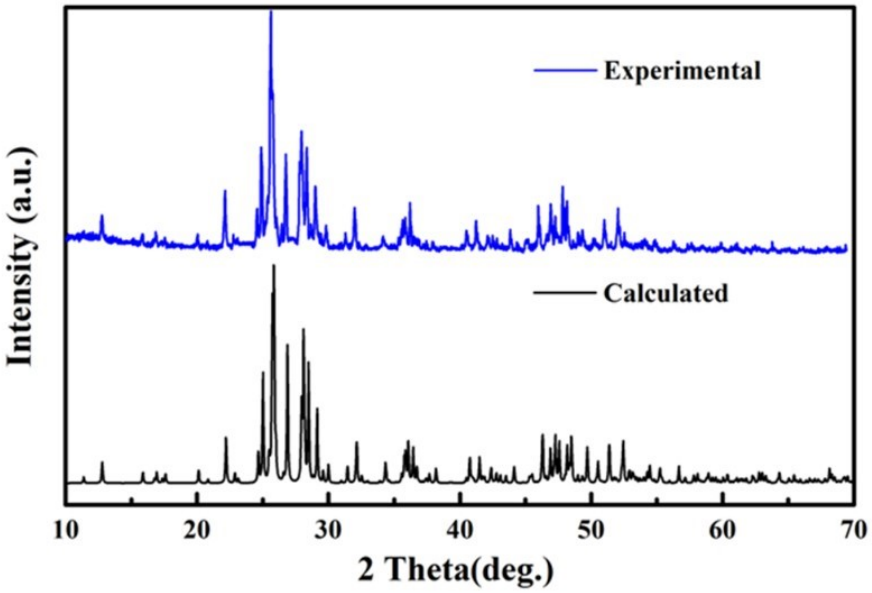

Figure S1. Experimental and calculated powder XRD pattern of BaI_3O_9H.

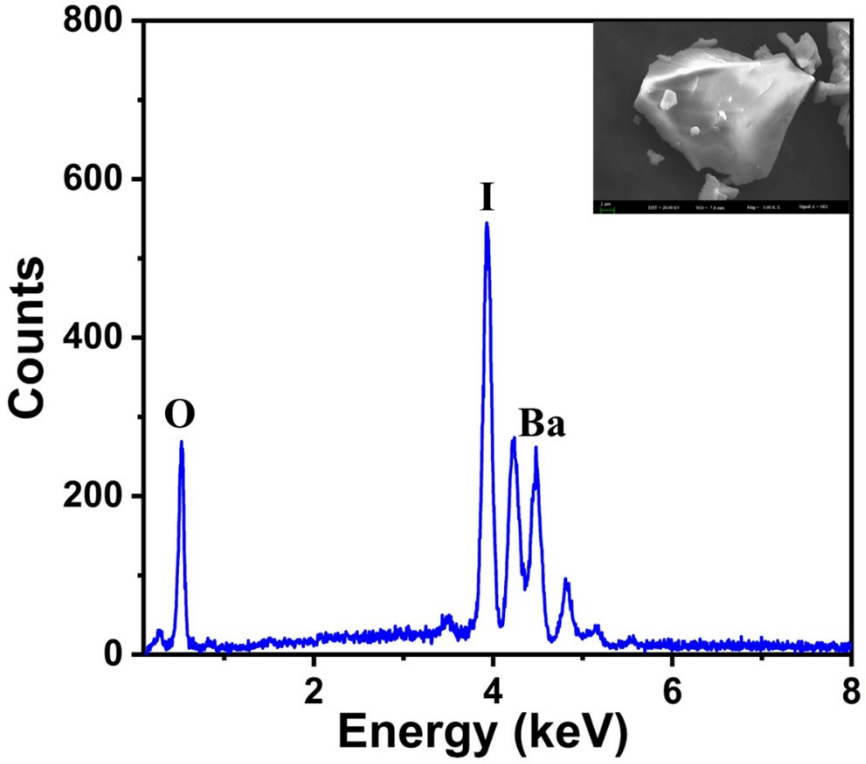

Figure S2. The energy dispersive X-ray spectroscope (EDS) for BaI_3O_9H.

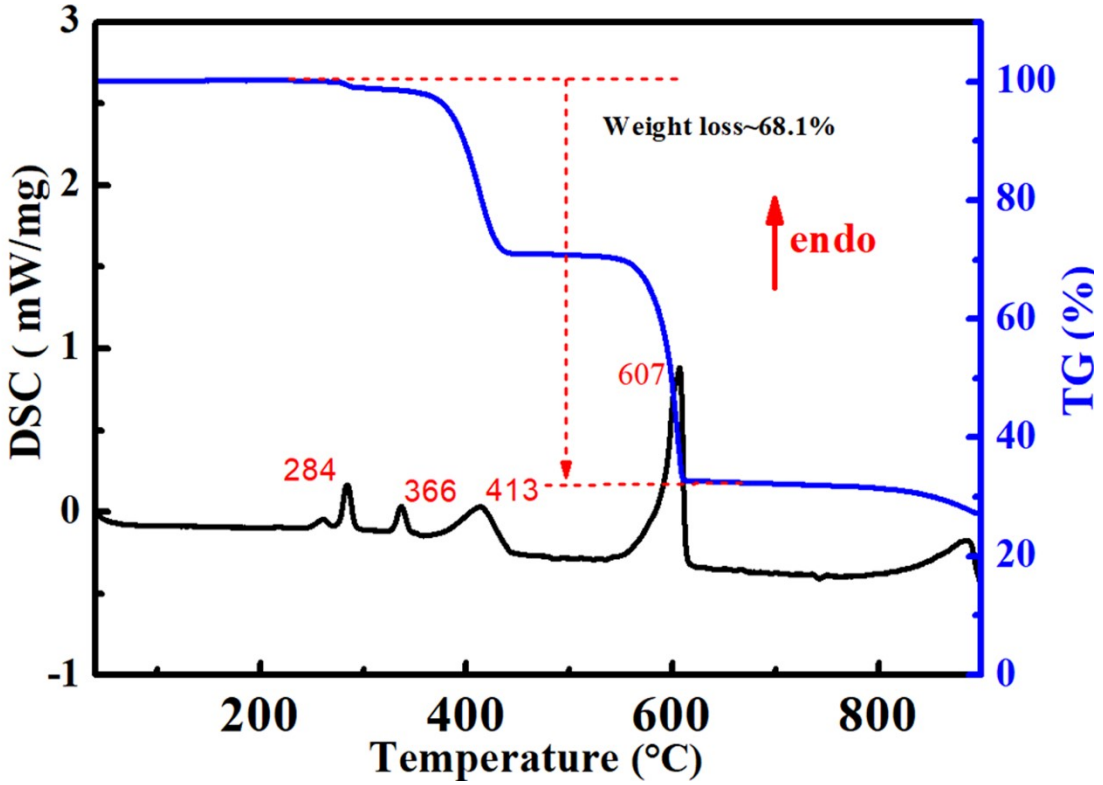

Figure S3. DSC and TG curves of BaI_3O_9H. It is speculated that the decomposition of BaI_3O_9H follows the following equation: $4BaI_3O_9H = 4BaO + 6I_2\uparrow + 15O_2\uparrow + 2H_2O\uparrow$. The calculated weight loss of gas is about 68.1 %, which is close to experimental value.

References

1. Q. M. Huang, C. L. Hu, B. P. Yang, Z. Fang, Y. Huang, J. G. Mao, *Chem. Commun.*, 2021, **57**, 11525–11528.

2. X. Q. Jiang, H. P. Wu, H. W. Yu, Z. G. Hu, J. Y. Wang, Y. C. Wu, *Cryst. Growth Des.*, 2021, **21**, 4005–4012.

3. Y. Li, K. M. Ok, *J*. *Mater*. *Chem*. *C*, 2022, DOI: 10.1039/D2TC01638A.

4. M. Q. Gai, T. H. Tong, Y. Wang, Z. H. Yang, S. L. Pan, *Chem*. *Mater*., 2020, 32, 5723-5728.