Supporting Information for

Ba_2HgTe_5: A Hg-based Telluride with Giant Birefringence Induced by Linear [$HgTe_2$] units

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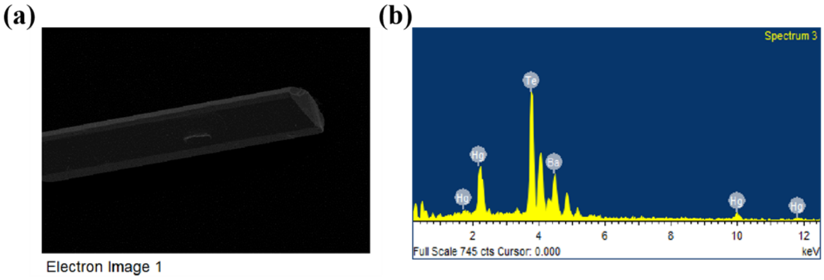
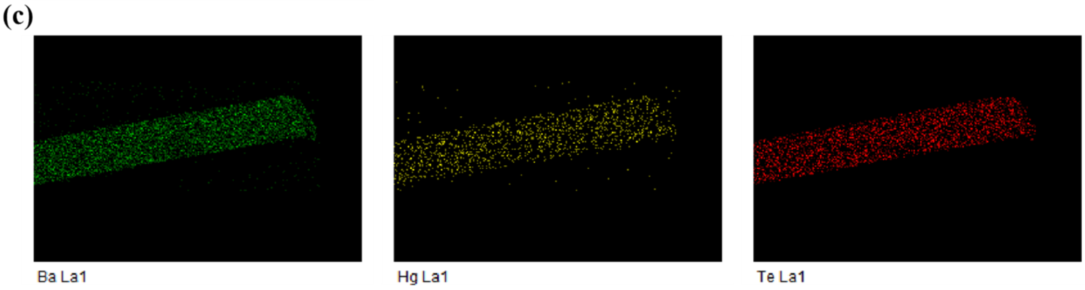
1. Figure S1

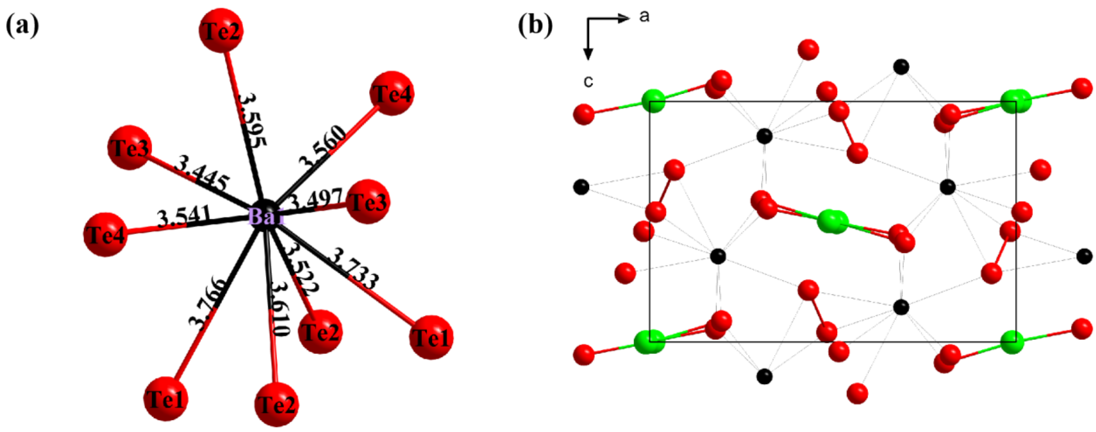


Element	Atomic%
Ba	26.18
Hg	12.68
Te	61.15
Totals	100.00



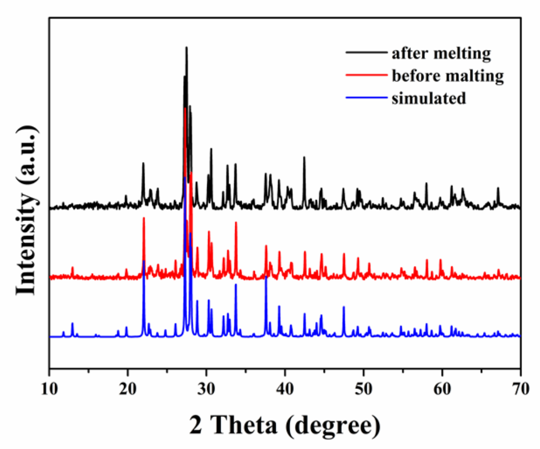
(a) Scanning electron microscopy (SEM) image of Ba_2HgTe_5; (b) Elemental analysis of Ba_2HgTe_5 by EDX spectroscopy. (c) Elemental distribution of the as-grown crystal.

2. Figure S2



(a) Coordination mode of Ba atom and (b) $[BaTe_9]$ polyhedra in the unit cell of Ba_2HgTe_5.

3. Figure S3



The PXRD of Ba_2HgTe_5 before and after DSC measurements.

4. **Table S1** Atomic coordinates (×10[4]), equivalent isotropic displacement parameters (Å[2]×10[3]), and wyckoff sites for Ba_2HgTe_5.

Atom	**Wyckoff site**	**x**	**y**	**z**	U_{eq}
Ba1	8d	31340(8)	49284(13)	14401(13)	367(4)
Hg1	4c	48939(10)	7500	49840(17)	544(4)
Te1	4c	51624(14)	2500	403(2)	388(5)
Te2	8d	56700(9)	48275(14)	21475(15)	393(4)
Te3	4c	30412(14)	7500	4133(2)	380(5)
Te4	4c	67949(14)	7500	5545(2)	388(5)

5. **Table S2** Selected bond lengths (Å) and angles (°) for Ba_2HgTe_5.

Lengths(Å)			
Hg1−Te3	2.642(2)	Te1−Te2	2.8053(18)
Hg1−Te4	2.644(2)	Te1−Te2^5	2.8053(18)
Angles(°)			
Te3−Hg1−Te4	174.20(9)	Te2−Te1− Te2^5	105.00(8)

Symmetry transformations used to generate equivalent atoms:

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

^{5} x,-y+1/2,z ^{6} -x+1/2,-y+1,z+1/2 ^{7} -x+1,y-1/2,-z ^{8} x+1/2,y,-z+1/2

^{9} x,-y+3/2,z ^{10} -x+1/2,y+1/2,z+1/2 ^{11} x+1/2,-y+3/2,-z+1/2 ^{12} -x+1,y+1/2,-z+1

6. Table S3 Comparison of the birefringence of the title compound and some known Hg-based chalcogenides.

Compound	S.G.	Hg polyhedra	△n	SHG intensity	Refs.
Ba_2HgTe_5	*Pnma*	$HgTe_2$	0.643	/	**This work**
$BaHgGeSe_4$	*Ama*2	$HgSe_4$	0.27	4.7 × AGS	1
$EuHgGeS_4$	*Ama*2	HgS_4	0.25	0.9 × AGS	2
$BaHgSe_2$	$Pmc2_1$	$HgSe_3$, $HgSe_2$	0.1473	1.5 × AGS	3
$CuHgPS_4$	$Pna2_1$	HgS_4	0.11	6.5 × AGS	4
$AgHgPS_4$	*Pn*	HgS_4	0.11	5.09 × AGS	5
Hg_2GeSe_4	I- 4	$HgSe_4$	0.11	2.1 × AGS	6
$BaHgSnS_4$	*Ama*2	HgS_4	0.1	2.8 × AGS	7
$BaHgSnSe_4$	*Fdd*2	$HgSe_4$	0.1	5.1 × AGS	7
$HgGa_2S_4$	I- 4	HgS_4	0.078	2-3 × AGS	8
$KHg_4Ga_5Se_{12}$	*R*3	$HgSe_4$	0.072	20 × AGS	9
$BaHgS_2$	$Pmc2_1$	HgS_4, HgS_2	0.07	6.5 × AGS	10
$Hg_3P_2S_8$	*Aba*2	HgS_4	0.05	4.2 × AGS	11-12

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