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Supporting information for article:

Synthesis and crystal structure of $Ba_2Y_{0.87(1)}Mn_{1.71(1)}Te_5$

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Synthesis of polycrystalline $Ba_2Y_{0.87}Mn_{1.71}Te_5$ sample

We attempted to synthesize a pure-phase polycrystalline sample with the loaded composition of $Ba_2Y_{0.87}Mn_{1.71}Te_5$ for physical property measurements. Multiple reactions with diverse temperature profiles were loaded to optimize the conditions to obtain a pure phase $Ba_2Y_{0.87}Mn_{1.71}Te_5$ sample. Regrettably, all the products of these reactions were multiphasic. We have got the best quality sample using the following synthesis procedure: the reactants Ba (253.8 mg, 1.848 mmol), Y (55.1 mg, 0.619 mmol), Mn (101.5 mg, 1.846 mmol), and Te (589.6 mg, 4.621 mmol) were weighed inside the glove box. The reactants were loaded into a fused silica tube inside the Ar-filled glove box and then vacuum sealed (*ca*. 10^{-4} Torr) using the flame torch. The reaction tube was heated in two segments inside the programmable muffle furnace. Firstly, the furnace's temperature was increased to 1273 K in 24 h and dwelled there for 168 h. It was then cooled to 1073 K in 12 h, where it was kept for 96 h before turning off the furnace. The reaction tube was then broken to obtain a reddish-black colored lump, which was then homogenized into a fine powder inside the Ar-filled glove box. The powder was pelletized and then vacuum-sealed inside the fused silica tube using a high-pressure hydraulic press. The tube was heated at 1223 K in 18 h and annealed there for 168 h before shutting off the furnace. The obtained pellet was then homogenized into a fine powder for phase analysis using the powder X-ray diffraction method. The same sample was used to collect optical absorption dataset.

Powder X-ray diffraction (PXRD) study

The phase purities of the polycrystalline samples were evaluated by the PXRD studies. The finely ground samples of $Ba_2Y_{0.87}Mn_{1.71}Te_5$ were used to collect the PXRD data at room temperature using a PAN analytical empyrean diffractometer with a Cu-*Kα* radiation source (λ = 1.5406 Å). The PXRD data were recorded using a θ-2θ geometry over a 2θ range of 10° to 70° with a working voltage and current of 40 kV and 30 mA, respectively. The phase analyses of the products were done using *Match3!* Software (New Match! version 3.13).

UV-visible-near infrared (UV-vis-NIR) absorption study

An optical bandgap study of the mixed-phase polycrystalline sample with the loaded composition of $Ba_2Y_{0.87}Mn_{1.71}Te_5$ was carried out at room temperature (298(2) K) using a JASCO V-770 UV-vis-NIR spectrophotometer. A dried $BaSO_4$ powder was used as a standard reference for the absorption study, and the dataset was collected in the diffuse reflectance mode over the wavelength range of 2400 nm (0.51 eV) to 340 nm (3.6 eV). Later, the Kubelka–Munk equation, $\alpha/S = (1 - R)\ 2\ /2R$, was used to transform the reflectance data into absorption data (G. Kortüm, 1969). Here α, *S*, and *R* are the absorption coefficient, scattering coefficient, and reflectance, respectively. The direct optical band gap was calculated using the Tauc method, as shown in Fig. S1.

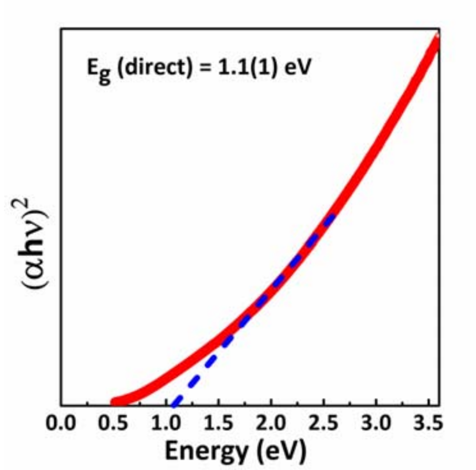

Fig. S1: The Tauc plot for the polycrystalline sample with the loaded composition of $Ba_2Y_{0.87}Mn_{1.71}Te_5$. The Ba_2MnTe_3 phase is present as the major phase in the sample.

Table S1 Atomic displacement parameters (Å^2) for the $Ba_2Y_{0.87(1)}Mn_{1.71(1)}Te_5$.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.02203(17)	0.01482(15)	0.03531(19)	0.000	0.00659(14)	0.000
Y1	0.0221(5)	0.0235(5)	0.0247(5)	0.000	0.0091(3)	0.000
Mn1	0.0215(5)	0.0175(5)	0.0286(5)	0.000	0.0124(4)	0.000
Te1	0.02063(18)	0.01460(16)	0.03142(19)	0.000	0.01026(14)	0.000
Te2	0.01764(17)	0.01892(16)	0.01930(15)	0.000	0.00761(12)	0.000
Te3	0.0190(2)	0.0204(2)	0.0179(2)	0.000	0.00628(17)	0.000

Table S2 Geometric parameters (Å, °) for the $Ba_2Y_{0.87(1)}Mn_{1.71(1)}Te_5$.

Ba1−Te3^{i}	3.4808 (3)	Y1−Te1	3.0683 (4)

Ba1—Te3	3.4808 (3)	Y1—Te2^{vii}	3.1125 (3)
Ba1—Te1^{ii}	3.5262 (4)	Y1—Te2^{viii}	3.1125 (3)
Ba1—Te1^{iii}	3.5262 (4)	Y1—Te2^{ix}	3.1125 (3)
Ba1—Te2^{iv}	3.5602 (5)	Y1—Te2^{x}	3.1125 (3)
Ba1—Te2^{ii}	3.6181 (4)	Mn1—Te3^{xi}	2.6784 (10)
Ba1—Te2^{iii}	3.6181 (4)	Mn1—Te1^{xii}	2.7070 (6)
Ba1—Ba1^{i}	4.5782 (3)	Mn1—Te1^{xi}	2.7070 (6)
Ba1—Ba1^{v}	4.5782 (3)	Mn1—Te2	2.7531 (11)
Y1—Te1^{vi}	3.0683 (4)		
Te3^{i}—Ba1—Te3	82.239 (9)	Te2^{viii}—Y1—Te2^{x}	85.307 (10)
Te3^{i}—Ba1—Te1^{ii}	135.294 (14)	Te2^{ix}—Y1—Te2^{x}	180.000 (12)
Te3—Ba1—Te1^{ii}	81.772 (8)	Te3^{xi}—Mn1—Te1^{xii}	111.46 (3)
Te3^{i}—Ba1—Te1^{iii}	81.772 (8)	Te3^{xi}—Mn1—Te1^{xi}	111.46 (3)
Te3—Ba1—Te1^{iii}	135.294 (14)	Te1^{xii}—Mn1—Te1^{xi}	115.48 (4)
Te1^{ii}—Ba1—Te1^{iii}	80.958 (12)	Te3^{xi}—Mn1—Te2	100.29 (3)
Te3^{i}—Ba1—Te2^{iv}	137.957 (5)	Te1^{xii}—Mn1—Te2	108.49 (3)
Te3—Ba1—Te2^{iv}	137.957 (5)	Te1^{xi}—Mn1—Te2	108.49 (3)
Te1^{ii}—Ba1—Te2^{iv}	74.903 (10)	Mn1^{viii}—Te1—Mn1^{ix}	115.48 (4)
Te1^{iii}—Ba1—Te2^{iv}	74.903 (10)	Mn1^{viii}—Te1—Y1	79.20 (2)
Te3^{i}—Ba1—Te2^{ii}	121.448 (12)	Mn1^{ix}—Te1—Y1	79.20 (2)
Te3—Ba1—Te2^{ii}	71.916 (8)	Mn1^{viii}—Te1—Ba1^{ii}	161.81 (2)
Te1^{ii}—Ba1—Te2^{ii}	92.276 (8)	Mn1^{ix}—Te1—Ba1^{ii}	81.497 (19)
Te1^{iii}—Ba1—Te2^{ii}	149.445 (13)	Y1—Te1—Ba1^{ii}	98.816 (11)

Te2^{iv}—Ba1—Te2^{ii}	74.567 (11)	Mn1^{viii}—Te1—Ba1^{iii}	81.497 (19)
Te3^{i}—Ba1—Te2^{iii}	71.916 (8)	Mn1^{ix}—Te1—Ba1^{iii}	161.81 (2)
Te3—Ba1—Te2^{iii}	121.448 (12)	Y1—Te1—Ba1^{iii}	98.816 (11)
Te1^{ii}—Ba1—Te2^{iii}	149.445 (13)	Ba1^{ii}—Te1—Ba1^{iii}	80.958 (12)
Te1^{iii}—Ba1—Te2^{iii}	92.276 (8)	Mn1—Te2—Y1^{xii}	77.746 (16)
Te2^{iv}—Ba1—Te2^{iii}	74.567 (10)	Mn1—Te2—Y1^{xi}	77.746 (16)
Te2^{ii}—Ba1—Te2^{iii}	78.496 (12)	Y1^{xii}—Te2—Y1^{xi}	94.693 (10)
Te3^{i}—Ba1—Ba1^{i}	48.880 (5)	Mn1—Te2—Ba1^{xiii}	172.50 (3)
Te3—Ba1—Ba1^{i}	131.120 (4)	Y1^{xii}—Te2—Ba1^{xiii}	97.265 (9)
Te1^{ii}—Ba1—Ba1^{i}	130.479 (6)	Y1^{xi}—Te2—Ba1^{xiii}	97.265 (9)
Te1^{iii}—Ba1—Ba1^{i}	49.521 (6)	Mn1—Te2—Ba1^{ii}	80.273 (19)
Te2^{iv}—Ba1—Ba1^{i}	90.0	Y1^{xii}—Te2—Ba1^{ii}	89.148 (7)
Te2^{ii}—Ba1—Ba1^{i}	129.248 (6)	Y1^{xi}—Te2—Ba1^{ii}	156.314 (12)
Te2^{iii}—Ba1—Ba1^{i}	50.752 (6)	Ba1^{xiii}—Te2—Ba1^{ii}	105.434 (11)
Te3^{i}—Ba1—Ba1^{v}	131.120 (5)	Mn1—Te2—Ba1^{iii}	80.273 (19)
Te3—Ba1—Ba1^{v}	48.880 (5)	Y1^{xii}—Te2—Ba1^{iii}	156.314 (12)
Te1^{ii}—Ba1—Ba1^{v}	49.521 (6)	Y1^{xi}—Te2—Ba1^{iii}	89.148 (6)
Te1^{iii}—Ba1—Ba1^{v}	130.479 (6)	Ba1^{xiii}—Te2—Ba1^{iii}	105.434 (11)
Te2^{iv}—Ba1—Ba1^{v}	90.0	Ba1^{ii}—Te2—Ba1^{iii}	78.496 (11)
Te2^{ii}—Ba1—Ba1^{v}	50.752 (6)	Mn1^{ii}—Te3—Mn1^{ix}	180.0
Te2^{iii}—Ba1—Ba1^{v}	129.248 (6)	Mn1^{ii}—Te3—Ba1^{v}	83.888 (18)
Ba1^{i}—Ba1—Ba1^{v}	180.0	Mn1^{ix}—Te3—Ba1^{v}	96.112 (18)
Te1^{vi}—Y1—Te1	180.0	Mn1^{ii}—Te3—Ba1^{xiv}	96.112 (18)
Te1^{vi}—Y1—Te2^{vii}	91.596 (9)	Mn1^{ix}—Te3—Ba1^{xiv}	83.888 (18)

Te1−Y1−Te2^{vii}	88.404 (9)	Ba1^{v}−Te3−Ba1^{xiv}	180.0
Te1^{vi}−Y1−Te2^{viii}	88.404 (9)	Mn1^{ii}−Te3−Ba1^{xv}	96.112 (18)
Te1−Y1−Te2^{viii}	91.596 (9)	Mn1^{ix}−Te3−Ba1^{xv}	83.888 (18)
Te2^{vii}−Y1−Te2^{viii}	180.000 (12)	Ba1^{v}−Te3−Ba1^{xv}	97.761 (9)
Te1^{vi}−Y1−Te2^{ix}	88.404 (8)	Ba1^{xiv}−Te3−Ba1^{xv}	82.239 (9)
Te1−Y1−Te2^{ix}	91.596 (8)	Mn1^{ii}−Te3−Ba1	83.888 (18)
Te2^{vii}−Y1−Te2^{ix}	85.307 (10)	Mn1^{ix}−Te3−Ba1	96.112 (18)
Te2^{viii}−Y1−Te2^{ix}	94.693 (10)	Ba1^{v}−Te3−Ba1	82.239 (9)
Te1^{vi}−Y1−Te2^{x}	91.596 (8)	Ba1^{xiv}−Te3−Ba1	97.761 (9)
Te1−Y1−Te2^{x}	88.404 (8)	Ba1^{xv}−Te3−Ba1	180.0
Te2^{vii}−Y1−Te2^{x}	94.693 (10)		

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) -*x*+1/2, -*y*+1/2, -*z*+1; (iii) -*x*+1/2, -*y*-1/2, -*z*+1; (iv) *x*, *y*, *z*+1; (v) *x*, *y*+1, *z*; (vi) -*x*, -*y*, -*z*; (vii) -*x*+1/2, -*y*+1/2, -*z*; (viii) *x*-1/2, *y*-1/2, *z*; (ix) *x*-1/2, *y*+1/2, *z*; (x) -*x*+1/2, -*y*-1/2, -*z*; (xi) *x*+1/2, *y*-1/2, *z*; (xii) *x*+1/2, *y*+1/2, *z*; (xiii) *x*, *y*, *z*-1; (xiv) -*x*, -*y*, -*z*+1; (xv) -*x*, -*y*+1, -*z*+1.

References

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