$Ba_2\mathit{Ln}_{1-x}Mn_2Te_5$ (*Ln* = Pr, Gd, and Yb; *x* = *Ln* vacancy): syntheses, crystal structures, optical, resistivity, and electronic structure

Gopabandhu Panigrahi,[a] Subhendu Jana,[a] Mohd Ishtiyak,[a] S. Narayanswamy,[b] Pinaki P. Bhattacharjee,[b] K. V. Ramanujachary,[c] Manish Niranjan,[d] and Jai Prakash[a*]

[a]*Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana 502285, India*

[b]*Department of Materials Science & Metallurgical Engineering, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana 502285, India*

[c]*Department of Chemistry and Biochemistry, Rowan University, Glassboro, New Jersey 08028, USA*

[d]*Department of Physics, Indian Institute of Technology Hyderabad, Kandi, Sangareddy, Telangana 502285, India*

Electronic Supplementary Information (E.S.I.)

The following chemicals were used as received for the syntheses of polycrystalline $Ba_2\mathit{Ln}_{1-x}$ Mn_2Te_5: barium rod (Alfa Aesar 99+%), lanthanum (Alfa Aesar 99.9%), cerium (Alfa Aesar 99.9%), praseodymium (Alfa Aesar 99.9%), neodymium (Alfa Aesar 99.9%), gadolinium (Alfa Aesar 99.9%), ytterbium lumps (Alfa Aesar 99.9%), manganese pieces (Alfa Aesar 99.9%), and tellurium ingot (Sigma-Aldrich 99.999%). These chemicals were stored inside the argon-filled dry glove box due to their air and moisture sensitivity. All the chemical manipulations were hence performed inside the argon-filled glove box. The surface of praseodymium, neodymium, gadolinium, and ytterbium lumps was first shaved to remove the oxidized layer, and then small pieces of these metals were cut for the reactions.

Syntheses of polycrystalline $Ba_2\mathit{Ln}_{1-x}Mn_2Te_5$ (*Ln* = La, Ce, Pr, Nd, Sm, and Yb)

We have made attempts to synthesize the polycrystalline form of $Ba_2Ln_{1-x}Mn_2Te_5$ using the sealed tube solid-state method. A stoichiometric amount of Ba, *Ln*, Mn, and Te were loaded inside a carbon-coated fused silica tube having 10 mm inner diameter and 12 mm outer diameter inside an Argon filled glove box. The total mass of the reactants was about 400 mg in each reaction. The fused silica tube containing the reaction mixture was first evacuated (*ca*. 10^{-4} Torr) and sealed using a flame torch. The sealed ampoule was then placed inside a programmable muffle furnace, and the temperature was ramped up to 1273 K with a heating rate of ~78 K/h. The reaction mixture was annealed at 1273 K for 120 h. Then the furnace was switched off and allowed to cool to room temperature. The reaction tube was opened under ambient conditions to reveal a homogenous looking black product that was further ground into fine powder inside the argon-filled glove box. The Powder X-ray diffraction data of these black polycrystalline products were collected for phase identification. The PXRD patterns were analyzed by using *Match3!*[1] Software, and it was found that the reaction products contain the target phases in small amounts along with major secondary phases (binary and ternary compounds) (Fig SI 1).

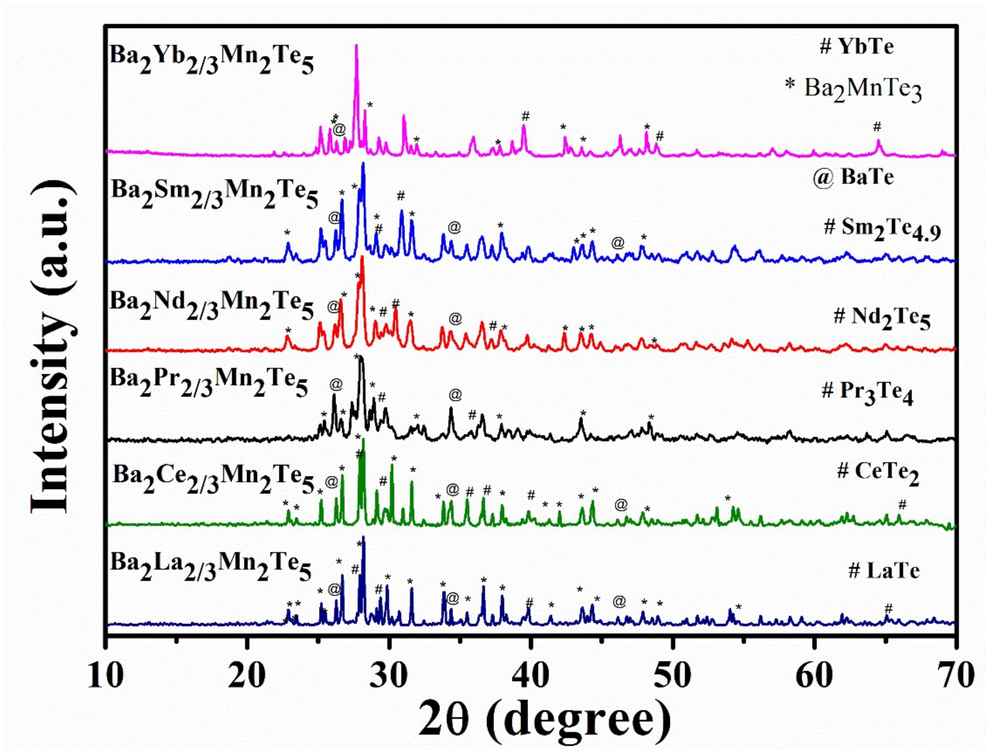

Fig SI 1. The PXRD patterns of the polycrystalline $Ba_2Ln_{1-x}Mn_2Te_5$ compounds. The JCPDS numbers of Binary and ternary phases shown in the figure are given in the parentheses. (# LaTe [96 - 900 - 8664], # CeTe2 [96 - 152 - 1987], # Pr3Te4 [96 - 153 - 8877] # Nd2Te5 [96 - 154 - 1086], # Sm2Te4.9 [96 - 412 -4105], @ BaTe [96 - 101 - 0424], * Ba2MnTe3 [96 - 722 - 1358], and # YbTe [96 - 101 - 0894]).

Table SI1: Atomic displacement parameters (Å²) for $Ba_2Ln_{1-x}Mn_2Te_5$

$Ba_2Pr_{2/3}□_{1/3}Mn_2Te_5$						
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0222 (3)	0.0183 (3)	0.0355 (3)	0.000	0.0102 (2)	0.000
Pr1	0.0218 (5)	0.0188 (4)	0.0194 (4)	0.000	0.0084 (4)	0.000
Mn1	0.0225 (7)	0.0186 (6)	0.0262 (6)	0.000	0.0137 (5)	0.000
Te1	0.0214 (3)	0.0129 (3)	0.0425 (4)	0.000	0.0161 (3)	0.000
Te2	0.0174 (3)	0.0203 (3)	0.0186 (3)	0.000	0.0060 (2)	0.000
Te3	0.0196 (4)	0.0228 (4)	0.0152 (3)	0.000	0.0086 (3)	0.000
$Ba_2Gd_{2/3}□_{1/3}Mn_2Te_5$						
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.0213(3)	0.0201(3)	0.0356 (4)	0.000	0.0101 (3)	0.000
Gd1	0.0199 5)	0.0188 5)	0.0191 (5)	0.000	0.0076 (4)	0.000
Mn1	0.0199(8)	0.0183(7)	0.0259 (8)	0.000	0.0128 (6)	0.000
Te1	0.0191(3)	0.0120 3)	0.0402 (4)	0.000	0.0150 (3)	0.000
Te2	0.0151(3)	0.0206 3)	0.0175 (3)	0.000	0.0056 (2)	0.000
Te3	0.0177(4)	0.0229(5)	0.0147 (4)	0.000	0.0081 (3)	0.000
$Ba_2Yb_{0.74(1)}Mn_2Te_5$						
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba01	0.0176 (2)	0.0166 (2)	0.0279 (2)	0.000	0.00859 (16)	0.000
Yb01	0.0207 (3)	0.0196 (3)	0.0173 (3)	0.000	0.0078 (2)	0.000
Mn01	0.0185 (5)	0.0177 (5)	0.0226 (5)	0.000	0.0099 (4)	0.000
Te01	0.0191 (2)	0.0149 (2)	0.0370 (3)	0.000	0.0137 (2)	0.000
Te02	0.0170 (2)	0.0231 (2)	0.0178 (2)	0.000	0.00522 (16)	0.000
Te03	0.0191 (3)	0.0231 (3)	0.0147 (3)	0.000	0.0076 (2)	0.000

Table SI2: Geometric parameters (º) for $Ba_2Pr_{2/3}□_{1/3}Mn_2Te_5$

$Te03^{i}$—Ba01—Te03	81.45 (3)	$Te02^{viii}$—Pr01—$Te02^{x}$	87.36 (2)
$Te03^{i}$—Ba01—$Te01^{ii}$	133.50 (2)	$Te02^{ix}$—Pr01—$Te02^{x}$	180.000 (18)
Te03—Ba01—$Te01^{ii}$	80.93 (2)	$Te03^{xi}$—Mn01—$Te01^{xii}$	110.62 (4)
$Te03^{i}$—Ba01—$Te01^{iii}$	80.93 (2)	$Te03^{xi}$—Mn01—$Te01^{xi}$	110.62 (4)
Te03—Ba01—$Te01^{iii}$	133.50 (2)	$Te01^{xii}$—Mn01—$Te01^{xi}$	113.94 (6)

Te01^{ii}—Ba01—Te01^{iii}	80.85 (2)	Te03^{xi}—Mn01—Te02	99.56 (5)
Te03^{i}—Ba01—Te02^{iv}	138.111 (16)	Te01^{xii}—Mn01—Te02	110.60 (4)
Te03—Ba01—Te02^{iv}	138.111 (16)	Te01^{xi}—Mn01—Te02	110.60 (4)
Te01^{ii}—Ba01—Te02^{iv}	77.45 (2)	Mn01^{viii}—Te01—Mn01^{ix}	113.94 (6)
Te01^{iii}—Ba01—Te02^{iv}	77.45 (2)	Mn01^{viii}—Te01—Pr01	77.75 (4)
Te03^{i}—Ba01—Te02^{ii}	121.22 (2)	Mn01^{ix}—Te01—Pr01	77.75 (4)
Te03—Ba01—Te02^{ii}	71.70 (2)	Mn01^{viii}—Te01—Ba01^{ii}	161.18 (3)
Te01^{ii}—Ba01—Te02^{ii}	92.97 (2)	Mn01^{ix}—Te01—Ba01^{ii}	81.91 (3)
Te01^{iii}—Ba01—Te02^{ii}	151.52 (3)	Pr01—Te01—Ba01^{ii}	96.89 (3)
Te02^{iv}—Ba01—Te02^{ii}	74.07 (2)	Mn01^{viii}—Te01—Ba01^{iii}	81.91 (3)
Te03^{i}—Ba01—Te02^{iii}	71.70 (2)	Mn01^{ix}—Te01—Ba01^{iii}	161.18 (3)
Te03—Ba01—Te02^{iii}	121.22 (2)	Pr01—Te01—Ba01^{iii}	96.89 (3)
Te01^{ii}—Ba01—Te02^{iii}	151.52 (3)	Ba01^{ii}—Te01—Ba01^{iii}	80.85 (2)
Te01^{iii}—Ba01—Te02^{iii}	92.97 (2)	Mn01—Te02—Pr01^{xii}	77.55 (3)
Te02^{iv}—Ba01—Te02^{iii}	74.07 (2)	Mn01—Te02—Pr01^{xi}	77.55 (3)
Te02^{ii}—Ba01—Te02^{iii}	79.27 (2)	Pr01^{xii}—Te02—Pr01^{xi}	92.64 (2)
Te03^{i}—Ba01—Ba01^{i}	49.277 (16)	Mn01—Te02—Ba01^{xiii}	170.22 (4)
Te03—Ba01—Ba01^{i}	130.724 (15)	Pr01^{xii}—Te02—Ba01^{xiii}	95.79 (2)
Te01^{ii}—Ba01—Ba01^{i}	130.423 (12)	Pr01^{xi}—Te02—Ba01^{xiii}	95.79 (2)
Te01^{iii}—Ba01—Ba01^{i}	49.577 (12)	Mn01—Te02—Ba01^{ii}	81.48 (3)
Te02^{iv}—Ba01—Ba01^{i}	90.0	Pr01^{xii}—Te02—Ba01^{ii}	90.149 (18)
Te02^{ii}—Ba01—Ba01^{i}	129.635 (12)	Pr01^{xi}—Te02—Ba01^{ii}	157.71 (2)
Te02^{iii}—Ba01—Ba01^{i}	50.365 (12)	Ba01^{xiii}—Te02—Ba01^{ii}	105.93 (2)
Te03^{i}—Ba01—Ba01^{v}	130.724 (15)	Mn01—Te02—Ba01^{iii}	81.48 (3)
Te03—Ba01—Ba01^{v}	49.277 (15)	Pr01^{xii}—Te02—Ba01^{iii}	157.71 (2)
Te01^{ii}—Ba01—Ba01^{v}	49.577 (12)	Pr01^{xi}—Te02—Ba01^{iii}	90.149 (19)
Te01^{iii}—Ba01—Ba01^{v}	130.423 (12)	Ba01^{xiii}—Te02—Ba01^{iii}	105.93 (2)
Te02^{iv}—Ba01—Ba01^{v}	90.0	Ba01^{ii}—Te02—Ba01^{iii}	79.27 (2)
Te02^{ii}—Ba01—Ba01^{v}	50.365 (12)	Mn01^{ii}—Te03—Mn01^{ix}	180.0
Te02^{iii}—Ba01—Ba01^{v}	129.635 (12)	Mn01^{ii}—Te03—Ba01	83.53 (3)
Ba01^{i}—Ba01—Ba01^{v}	180.0	Mn01^{ix}—Te03—Ba01	96.47 (3)
Te01^{vi}—Pr01—Te01	180.0	Mn01^{ii}—Te03—Ba01^{xiv}	96.47 (3)
Te01^{vi}—Pr01—Te02^{vii}	90.62 (2)	Mn01^{ix}—Te03—Ba01^{xiv}	83.53 (3)
Te01—Pr01—Te02^{vii}	89.38 (2)	Ba01—Te03—Ba01^{xiv}	98.55 (3)
Te01^{vi}—Pr01—Te02^{viii}	89.38 (2)	Mn01^{ii}—Te03—Ba01^{v}	83.53 (3)
Te01—Pr01—Te02^{viii}	90.62 (2)	Mn01^{ix}—Te03—Ba01^{v}	96.47 (3)
Te02^{vii}—Pr01—Te02^{viii}	180.000 (18)	Ba01—Te03—Ba01^{v}	81.45 (3)

Te01^{vi}—Pr01—Te02^{ix}	89.38 (2)	Ba01^{xiv}—Te03—Ba01^{v}	180.00 (2)
Te01—Pr01—Te02^{ix}	90.62 (2)	Mn01^{ii}—Te03—Ba01^{xv}	96.47 (3)
Te02^{vii}—Pr01—Te02^{ix}	87.36 (2)	Mn01^{ix}—Te03—Ba01^{xv}	83.53 (3)
Te02^{viii}—Pr01—Te02^{ix}	92.64 (2)	Ba01—Te03—Ba01^{xv}	180.0
Te01^{vi}—Pr01—Te02^{x}	90.62 (2)	Ba01^{xiv}—Te03—Ba01^{xv}	81.45 (3)
Te01—Pr01—Te02^{x}	89.38 (2)	Ba01^{v}—Te03—Ba01^{xv}	98.55 (3)
Te02^{vii}—Pr01—Te02^{x}	92.64 (2)		

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.

Table SI3: Geometric parameters (°) for $Ba_2Gd_{2/3}\square_{1/3}Mn_2Te_5$

Te3^{i}—Ba1—Te3	81.01 (3)	Te2^{viii}—Gd1—Te2^{x}	86.65 (2)
Te3^{i}—Ba1—Te1^{ii}	133.30 (3)	Te2^{ix}—Gd1—Te2^{x}	180.00 (2)
Te3—Ba1—Te1^{ii}	81.17 (2)	Te3^{xi}—Mn1—Te1^{xii}	111.51 (4)
Te3^{i}—Ba1—Te1^{iii}	81.17 (2)	Te3^{xi}—Mn1—Te1^{xi}	111.51 (4)
Te3—Ba1—Te1^{iii}	133.30 (3)	Te1^{xii}—Mn1—Te1^{xi}	113.39 (6)
Te1^{ii}—Ba1—Te1^{iii}	80.51 (3)	Te3^{xi}—Mn1—Te2	100.01 (6)
Te3^{i}—Ba1—Te2^{iv}	138.651 (17)	Te1^{xii}—Mn1—Te2	109.81 (4)
Te3—Ba1—Te2^{iv}	138.651 (17)	Te1^{xi}—Mn1—Te2	109.81 (4)
Te1^{ii}—Ba1—Te2^{iv}	76.24 (3)	Mn1^{viii}—Te1—Mn1^{ix}	113.39 (6)
Te1^{iii}—Ba1—Te2^{iv}	76.24 (3)	Mn1^{viii}—Te1—Gd1	78.12 (4)
Te3^{i}—Ba1—Te2^{ii}	121.14 (3)	Mn1^{ix}—Te1—Gd1	78.12 (4)
Te3—Ba1—Te2^{ii}	72.04 (2)	Mn1^{viii}—Te1—Ba1^{ii}	161.82 (4)
Te1^{ii}—Ba1—Te2^{ii}	93.25 (2)	Mn1^{ix}—Te1—Ba1^{ii}	82.53 (3)
Te1^{iii}—Ba1—Te2^{ii}	151.39 (3)	Gd1—Te1—Ba1^{ii}	97.68 (3)
Te2^{iv}—Ba1—Te2^{ii}	75.16 (2)	Mn1^{viii}—Te1—Ba1^{iii}	82.53 (3)
Te3^{i}—Ba1—Te2^{iii}	72.04 (2)	Mn1^{ix}—Te1—Ba1^{iii}	161.82 (4)
Te3—Ba1—Te2^{iii}	121.14 (3)	Gd1—Te1—Ba1^{iii}	97.68 (3)
Te1^{ii}—Ba1—Te2^{iii}	151.39 (3)	Ba1^{ii}—Te1—Ba1^{iii}	80.51 (3)
Te1^{iii}—Ba1—Te2^{iii}	93.25 (2)	Mn1—Te2—Gd1^{xii}	77.84 (3)
Te2^{iv}—Ba1—Te2^{iii}	75.16 (2)	Mn1—Te2—Gd1^{xi}	77.84 (3)
Te2^{ii}—Ba1—Te2^{iii}	78.91 (3)	Gd1^{xii}—Te2—Gd1^{xi}	93.35 (2)
Te3^{i}—Ba1—Ba1^{i}	49.495 (16)	Mn1—Te2—Ba1^{xiii}	171.99 (4)
Te3—Ba1—Ba1^{i}	130.506 (16)	Gd1^{xii}—Te2—Ba1^{xiii}	96.75 (2)

Te1^{ii}—Ba1—Ba1^{i}	130.255 (13)	Gd1^{xi}—Te2—Ba1^{xiii}	96.75 (2)
Te1^{iii}—Ba1—Ba1^{i}	49.744 (13)	Mn1—Te2—Ba1^{ii}	81.25 (3)
Te2^{iv}—Ba1—Ba1^{i}	90.0	Gd1^{xii}—Te2—Ba1^{ii}	89.999 (19)
Te2^{ii}—Ba1—Ba1^{i}	129.455 (13)	Gd1^{xi}—Te2—Ba1^{ii}	157.60 (3)
Te2^{iii}—Ba1—Ba1^{i}	50.545 (13)	Ba1^{xiii}—Te2—Ba1^{ii}	104.84 (2)
Te3^{i}—Ba1—Ba1^{v}	130.506 (16)	Mn1—Te2—Ba1^{iii}	81.25 (3)
Te3—Ba1—Ba1^{v}	49.495 (16)	Gd1^{xii}—Te2—Ba1^{iii}	157.60 (3)
Te1^{ii}—Ba1—Ba1^{v}	49.744 (13)	Gd1^{xi}—Te2—Ba1^{iii}	89.999 (19)
Te1^{iii}—Ba1—Ba1^{v}	130.255 (13)	Ba1^{xiii}—Te2—Ba1^{iii}	104.84 (2)
Te2^{iv}—Ba1—Ba1^{v}	90.0	Ba1^{ii}—Te2—Ba1^{iii}	78.91 (3)
Te2^{ii}—Ba1—Ba1^{v}	50.545 (13)	Mn1^{ii}—Te3—Mn1^{ix}	180.0
Te2^{iii}—Ba1—Ba1^{v}	129.455 (13)	Mn1^{ii}—Te3—Ba1	83.26 (3)
Ba1^{i}—Ba1—Ba1^{v}	180.0	Mn1^{ix}—Te3—Ba1	96.74 (3)
Te1—Gd1—Te1^{vi}	180.0	Mn1^{ii}—Te3—Ba1^{xiv}	96.74 (3)
Te1—Gd1—Te2^{vii}	88.77 (2)	Mn1^{ix}—Te3—Ba1^{xiv}	83.26 (3)
Te1^{vi}—Gd1—Te2^{vii}	91.23 (2)	Ba1—Te3—Ba1^{xiv}	98.99 (3)
Te1—Gd1—Te2^{viii}	91.23 (2)	Mn1^{ii}—Te3—Ba1^{v}	83.26 (3)
Te1^{vi}—Gd1—Te2^{viii}	88.77 (2)	Mn1^{ix}—Te3—Ba1^{v}	96.74 (3)
Te2^{vii}—Gd1—Te2^{viii}	180.0	Ba1—Te3—Ba1^{v}	81.01 (3)
Te1—Gd1—Te2^{ix}	91.23 (2)	Ba1^{xiv}—Te3—Ba1^{v}	180.0
Te1^{vi}—Gd1—Te2^{ix}	88.77 (2)	Mn1^{ii}—Te3—Ba1^{xv}	96.74 (3)
Te2^{vii}—Gd1—Te2^{ix}	86.65 (2)	Mn1^{ix}—Te3—Ba1^{xv}	83.26 (3)
Te2^{viii}—Gd1—Te2^{ix}	93.35 (2)	Ba1—Te3—Ba1^{xv}	180.0
Te1—Gd1—Te2^{x}	88.77 (2)	Ba1^{xiv}—Te3—Ba1^{xv}	81.01 (3)
Te1^{vi}—Gd1—Te2^{x}	91.23 (2)	Ba1^{v}—Te3—Ba1^{xv}	98.99 (3)
Te2^{vii}—Gd1—Te2^{x}	93.35 (2)		

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.

Table SI4: Geometric parameters (º) for $Ba_2Yb_{0.74(1)}Mn_2Te_5$

$Te03^{i}$—Ba01—Te03	80.97 (3)	$Te01^{x}$—Yb01—$Mn01^{vi}$	46.34 (2)
$Te03^{i}$—Ba01—$Te01^{ii}$	133.227 (19)	Te01—Yb01—$Mn01^{vi}$	133.658 (19)
Te03—Ba01—$Te01^{ii}$	81.05 (2)	$Mn01^{ix}$—Yb01—$Mn01^{vi}$	102.93 (3)
$Te03^{i}$—Ba01—$Te01^{iii}$	81.05 (2)	$Mn01^{viii}$—Yb01—$Mn01^{vi}$	77.07 (3)
Te03—Ba01—$Te01^{iii}$	133.227 (19)	$Te02^{vi}$—Yb01—$Mn01^{vii}$	133.75 (3)
$Te01^{ii}$—Ba01—$Te01^{iii}$	80.67 (2)	$Te02^{vii}$—Yb01—$Mn01^{vii}$	46.25 (3)
$Te03^{i}$—Ba01—$Te02^{iv}$	138.534 (16)	$Te02^{viii}$—Yb01—$Mn01^{vii}$	77.64 (2)
Te03—Ba01—$Te02^{iv}$	138.534 (16)	$Te02^{ix}$—Yb01—$Mn01^{vii}$	102.36 (2)
$Te01^{ii}$—Ba01—$Te02^{iv}$	76.89 (2)	$Te01^{x}$—Yb01—$Mn01^{vii}$	133.658 (19)
$Te01^{iii}$—Ba01—$Te02^{iv}$	76.89 (2)	Te01—Yb01—$Mn01^{vii}$	46.342 (19)
$Te03^{i}$—Ba01—$Te02^{ii}$	121.046 (19)	$Mn01^{ix}$—Yb01—$Mn01^{vii}$	77.07 (3)
Te03—Ba01—$Te02^{ii}$	71.62 (2)	$Mn01^{viii}$—Yb01—$Mn01^{vii}$	102.93 (3)
$Te01^{ii}$—Ba01—$Te02^{ii}$	93.06 (2)	$Mn01^{vi}$—Yb01—$Mn01^{vii}$	180.00 (4)
$Te01^{iii}$—Ba01—$Te02^{ii}$	151.86 (2)	$Te03^{xi}$—Mn01—Te02	99.68 (4)
$Te02^{iv}$—Ba01—$Te02^{ii}$	74.967 (19)	$Te03^{xi}$—Mn01—$Te01^{xii}$	109.80 (3)
$Te03^{i}$—Ba01—$Te02^{iii}$	71.62 (2)	Te02—Mn01—$Te01^{xii}$	111.30 (3)
Te03—Ba01—$Te02^{iii}$	121.046 (19)	$Te03^{xi}$—Mn01—$Te01^{xi}$	109.80 (3)
$Te01^{ii}$—Ba01—$Te02^{iii}$	151.86 (2)	Te02—Mn01—$Te01^{xi}$	111.30 (3)
$Te01^{iii}$—Ba01—$Te02^{iii}$	93.058 (19)	$Te01^{xii}$—Mn01—$Te01^{xi}$	114.02 (5)
$Te02^{iv}$—Ba01—$Te02^{iii}$	74.967 (19)	$Te03^{xi}$—Mn01—$Yb01^{xi}$	129.88 (3)
$Te02^{ii}$—Ba01—$Te02^{iii}$	79.57 (2)	Te02—Mn01—$Yb01^{xi}$	56.67 (3)
$Te03^{i}$—Ba01—$Ba01^{i}$	49.514 (15)	$Te01^{xii}$—Mn01—$Yb01^{xi}$	119.76 (4)
Te03—Ba01—$Ba01^{i}$	130.486 (15)	$Te01^{xi}$—Mn01—$Yb01^{xi}$	56.73 (3)
$Te01^{ii}$—Ba01—$Ba01^{i}$	130.337 (11)	$Te03^{xi}$—Mn01—$Yb01^{xii}$	129.88 (3)
$Te01^{iii}$—Ba01—$Ba01^{i}$	49.662 (10)	Te02—Mn01—$Yb01^{xii}$	56.67 (3)
$Te02^{iv}$—Ba01—$Ba01^{i}$	90.0	$Te01^{xii}$—Mn01—$Yb01^{xii}$	56.73 (3)
$Te02^{ii}$—Ba01—$Ba01^{i}$	129.787 (11)	$Te01^{xi}$—Mn01—$Yb01^{xii}$	119.76 (4)
$Te02^{iii}$—Ba01—$Ba01^{i}$	50.213 (10)	$Yb01^{xi}$—Mn01—$Yb01^{xii}$	77.07 (3)
$Te03^{i}$—Ba01—$Ba01^{v}$	130.486 (14)	$Mn01^{vii}$—Te01—$Mn01^{ix}$	114.02 (5)
Te03—Ba01—$Ba01^{v}$	49.514 (14)	$Mn01^{vii}$—Te01—Yb01	76.93 (3)
$Te01^{ii}$—Ba01—$Ba01^{v}$	49.662 (11)	$Mn01^{ix}$—Te01—Yb01	76.93 (3)
$Te01^{iii}$—Ba01—$Ba01^{v}$	130.337 (11)	$Mn01^{vii}$—Te01—$Ba01^{ii}$	160.62 (3)
$Te02^{iv}$—Ba01—$Ba01^{v}$	90.0	$Mn01^{ix}$—Te01—$Ba01^{ii}$	81.80 (3)

Te02^{ii}—Ba01—Ba01^{v}	50.213 (10)	Yb01—Te01—Ba01^{ii}	97.05 (2)
Te02^{iii}—Ba01—Ba01^{v}	129.787 (10)	Mn01^{vii}—Te01—Ba01^{iii}	81.80 (3)
Ba01^{i}—Ba01—Ba01^{v}	180.0	Mn01^{ix}—Te01—Ba01^{iii}	160.61 (3)
Te02^{vi}—Yb01—Te02^{vii}	180.000 (14)	Yb01—Te01—Ba01^{iii}	97.05 (2)
Te02^{vi}—Yb01—Te02^{viii}	93.23 (2)	Ba01^{ii}—Te01—Ba01^{iii}	80.68 (2)
Te02^{vii}—Yb01—Te02^{viii}	86.77 (2)	Mn01—Te02—Yb01^{xii}	77.08 (2)
Te02^{vi}—Yb01—Te02^{ix}	86.77 (2)	Mn01—Te02—Yb01^{xi}	77.08 (2)
Te02^{vii}—Yb01—Te02^{ix}	93.23 (2)	Yb01^{xii}—Te02—Yb01^{xi}	93.23 (2)
Te02^{viii}—Yb01—Te02^{ix}	180.000 (14)	Mn01—Te02—Ba01^{xiii}	170.72 (3)
Te02^{vi}—Yb01—Te01^{x}	91.144 (19)	Yb01^{xii}—Te02—Ba01^{xiii}	96.650 (18)
Te02^{vii}—Yb01—Te01^{x}	88.856 (19)	Yb01^{xi}—Te02—Ba01^{xiii}	96.650 (18)
Te02^{viii}—Yb01—Te01^{x}	91.144 (18)	Mn01—Te02—Ba01^{ii}	81.99 (3)
Te02^{ix}—Yb01—Te01^{x}	88.856 (18)	Yb01^{xii}—Te02—Ba01^{ii}	89.691 (18)
Te02^{vi}—Yb01—Te01	88.855 (19)	Yb01^{xi}—Te02—Ba01^{ii}	157.634 (19)
Te02^{vii}—Yb01—Te01	91.145 (19)	Ba01^{xiii}—Te02—Ba01^{ii}	105.034 (18)
Te02^{viii}—Yb01—Te01	88.855 (19)	Mn01—Te02—Ba01^{iii}	81.99 (3)
Te02^{ix}—Yb01—Te01	91.145 (19)	Yb01^{xii}—Te02—Ba01^{iii}	157.634 (19)
Te01^{x}—Yb01—Te01	180.0	Yb01^{xi}—Te02—Ba01^{iii}	89.691 (18)
Te02^{vi}—Yb01—Mn01^{ix}	77.64 (2)	Ba01^{xiii}—Te02—Ba01^{iii}	105.034 (19)
Te02^{vii}—Yb01—Mn01^{ix}	102.36 (2)	Ba01^{ii}—Te02—Ba01^{iii}	79.57 (2)
Te02^{viii}—Yb01—Mn01^{ix}	133.75 (3)	Mn01^{ii}—Te03—Mn01^{ix}	180.0
Te02^{ix}—Yb01—Mn01^{ix}	46.25 (3)	Mn01^{ii}—Te03—Ba01	83.08 (2)
Te01^{x}—Yb01—Mn01^{ix}	133.658 (19)	Mn01^{ix}—Te03—Ba01	96.92 (2)
Te01—Yb01—Mn01^{ix}	46.34 (2)	Mn01^{ii}—Te03—Ba01^{xiv}	96.92 (3)
Te02^{vi}—Yb01—Mn01^{viii}	102.36 (2)	Mn01^{ix}—Te03—Ba01^{xiv}	83.08 (3)
Te02^{vii}—Yb01—Mn01^{viii}	77.64 (2)	Ba01—Te03—Ba01^{xiv}	99.03 (3)
Te02^{viii}—Yb01—Mn01^{viii}	46.25 (3)	Mn01^{ii}—Te03—Ba01^{v}	83.08 (3)
Te02^{ix}—Yb01—Mn01^{viii}	133.75 (3)	Mn01^{ix}—Te03—Ba01^{v}	96.92 (3)
Te01^{x}—Yb01—Mn01^{viii}	46.342 (19)	Ba01—Te03—Ba01^{v}	80.97 (3)
Te01—Yb01—Mn01^{viii}	133.658 (19)	Ba01^{xiv}—Te03—Ba01^{v}	180.000 (15)
Mn01^{ix}—Yb01—Mn01^{viii}	180.00 (4)	Mn01^{ii}—Te03—Ba01^{xv}	96.92 (3)
Te02^{vi}—Yb01—Mn01^{vi}	46.25 (3)	Mn01^{ix}—Te03—Ba01^{xv}	83.08 (3)
Te02^{vii}—Yb01—Mn01^{vi}	133.75 (3)	Ba01—Te03—Ba01^{xv}	180.0
Te02^{viii}—Yb01—Mn01^{vi}	102.36 (2)	Ba01^{xiv}—Te03—Ba01^{xv}	80.97 (3)
Te02^{ix}—Yb01—Mn01^{vi}	77.64 (2)	Ba01^{v}—Te03—Ba01^{xv}	99.03 (3)

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*+1/2, -*y*+1/2, -*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*, -*y*, -*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.

Table SI5 The computed lattices parameters and volume of $Ba_2Gd_{2/3}\square_{1/3}Mn_2Te_5$.

	a	***b***	***c***	α	β	γ	***Volume***
Cal.	15.283	4.556	10.284	89.993	114.9	90.013	649.73
Exp.	15.246	4.548	10.688	90.0	117.2	90.0	659.14

Reference:

1 Match! - Phase Analysis using Powder Diffraction, https://www.crystalimpact.de/match/, (accessed February 16, 2021).