Five coordinated Mn in $Ba_4Mn_2Si_2Te_9$: synthesis, crystal structure, physical properties, and electronic structure

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Electronic Supplementary Information (E.S.I.)

Table SI1: The computed fractional atomic coordinates (x,y,z) of atoms in $Ba_4Mn_2Si_2Te_9$. The position vector is given as $\vec{r} = x\vec{a} + y\vec{b} + z\vec{c}$.

	x		*y*		*z*	
	Cal.	**Exp.**	**Cal.**	**Exp.**	**Cal.**	**Exp.**
Ba(1)	0.18216	0.17871	0.61438	0.61493	0.26152	0.26159
Mn(1)	0.02873	0.03115	0.16967	0.17500	0.55274	0.50000
Mn(2)	-0.00504	0.00000	-0.00792	0.00000	0.35101	0.35170
Si(1)	0.06761	0.06968	0.06946	0.07880	-0.00452	0.00000
Te(1)	0.05965	0.06236	0.23313	0.24474	0.20302	0.20542
Te(2)	0.16056	0.16709	0.93685	0.92455	0.49579	0.50000
Te(3)	0.21754	0.21454	0.89941	0.90113	-0.00213	0.00000
Te(4)	0.01067	0.00000	0.47341	0.50000	0.49779	0.50000

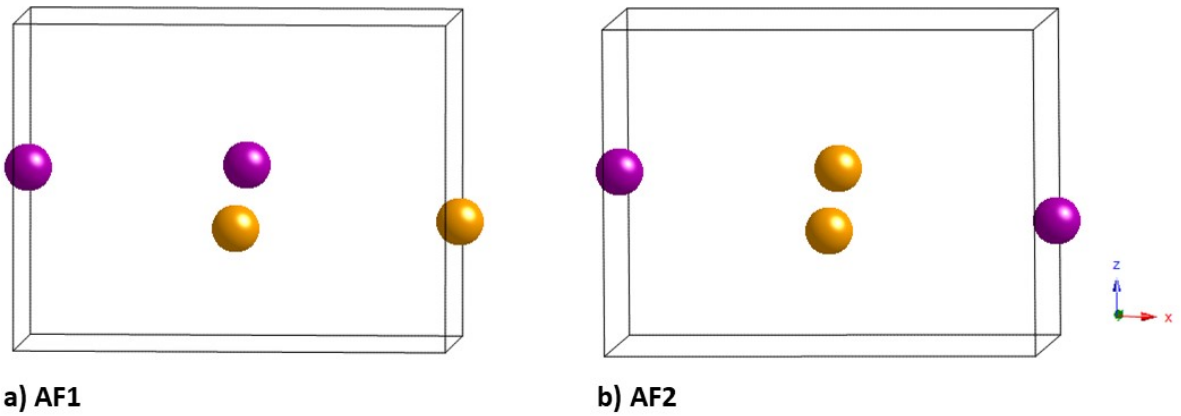

Fig. SI1: The orientations of magnetic moments of Mn atoms in $Ba_4Mn_2Si_2Te_9$ with (a) AF1 and (b) AF2 antiferromagnetic configurations. The yellow and purple balls indicate Mn atoms with spin-up and spin-down orientations, respectively. (Only Mn atoms are shown in the unit cell).

Table SI2: Atomic displacement parameters (Å^2) for $Ba_4Mn_2Si_2Te_9$ structure.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba(1)	0.01707(14)	0.01661(15)	0.01646(15)	0.00102(11)	0.00139(11)	0.00069(12)
Si(1)	0.0114(9)	0.0121(9)	0.0212(10)	0.0013(7)	0.000	0.000
Mn(1)	0.0212(12)	0.0175(12)	0.0326(14)	0.0029(10)	0.000	0.000
Mn(2)	0.0203(11)	0.0241(12)	0.0183(12)	-0.0005(10)	0.000	0.000
Te(1)	0.01611(16)	0.01556(16)	0.02095(18)	-0.00107(12)	0.00253(13)	-0.00127(14)
Te(2)	0.0175(2)	0.0177(2)	0.0168(2)	-0.00032(18)	0.000	0.000
Te(3)	0.0143(2)	0.0136(2)	0.0163(2)	0.00262(17)	0.000	0.000
Te(4)	0.0216(3)	0.0203(3)	0.0123(3)	-0.0062(3)	0.000	0.000

Table SI3: Bond distances (Å) and angles (º) for $Ba_4Mn_2Si_2Te_9$ structure.

Ba1—Te1^{i}	3.5151(5)	Si1—Te1	2.5151(13)
Ba1—Te3^{ii}	3.5204(5)	Mn1—Mn2	2.170(3)
Ba1—Te4	3.5335(3)	Mn1—Mn2^{viii}	2.170(3)
Ba1—Te2^{ii}	3.5719(5)	Mn1—Te2^{ix}	2.808(3)
Ba1—Te2	3.6062(5)	Mn1—Te2^{vi}	2.851(3)
Ba1—Te1	3.6329(5)	Mn1—Te4	2.865(3)
Ba1—Te3	3.6485(5)	Mn1—Te1	3.0381(8)
Ba1—Te1^{iii}	3.7096(5)	Mn1—Te1^{iv}	3.0381(8)
Ba1—Ba1^{iii}	4.7652(3)	Mn1—Mn1^{viii}	3.166(5)
Ba1—Ba1^{ii}	4.7653(3)	Mn2—Te1^{x}	2.7207(14)
Ba1—Ba1^{iv}	4.7696(7)	Mn2—Te1	2.7207 (14)
Si1—Si1^{v}	2.327(4)	Mn2—Te2^{vi}	2.7749 (15)
Si1—Te3^{vi}	2.492(2)	Mn2—Te2^{ix}	2.7749 (15)
Si1—Te1^{vii}	2.5151(13)	Mn2—Mn2^{viii}	2.968(5)
Te1^{i}—Ba1—Te3^{ii}	116.289(13)	Mn1—Mn2—Mn1^{viii}	93.71(14)
Te1^{i}—Ba1—Te4	65.007(8)	Mn1—Mn2—Te1^{x}	168.34(10)
Te3^{ii}—Ba1—Te4	129.022(12)	Mn1^{viii}—Mn2—Te1^{x}	75.88(5)

Te1^{i}—Ba1—Te2^{ii}	143.679(13)	Mn1—Mn2—Te1	75.88(5)
Te3^{ii}—Ba1—Te2^{ii}	90.717(11)	Mn1^{viii}—Mn2—Te1	168.34(10)
Te4—Ba1—Te2^{ii}	79.256(10)	Te1^{x}—Mn2—Te1	114.95(9)
Te1^{i}—Ba1—Te2	78.748(12)	Mn1—Mn2—Te2^{vi}	69.17(8)
Te3^{ii}—Ba1—Te2	154.958(15)	Mn1^{viii}—Mn2—Te2^{vi}	67.93(8)
Te4—Ba1—Te2	74.726(10)	Te1^{x}—Mn2—Te2^{vi}	110.598(13)
Te2^{ii}—Ba1—Te2	86.093(10)	Te1—Mn2—Te2^{vi}	102.900(12)
Te1^{i}—Ba1—Te1	83.472(11)	Mn1—Mn2—Te2^{ix}	67.93(8)
Te3^{ii}—Ba1—Te1	65.818(11)	Mn1^{viii}—Mn2—Te2^{ix}	69.17(8)
Te4—Ba1—Te1	63.794(8)	Te1^{x}—Mn2—Te2^{ix}	102.901(12)
Te2^{ii}—Ba1—Te1	86.611(13)	Te1—Mn2—Te2^{ix}	110.598(13)
Te2—Ba1—Te1	138.519(13)	Te2^{vi}—Mn2—Te2^{ix}	115.34(9)
Te1^{i}—Ba1—Te3	76.660(12)	Mn1—Mn2—Mn2^{viii}	46.85 (7)
Te3^{ii}—Ba1—Te3	77.014(8)	Mn1^{viii}—Mn2—Mn2^{viii}	46.85(7)
Te4—Ba1—Te3	140.198(12)	Te1^{x}—Mn2—Mn2^{viii}	122.53(5)
Te2^{ii}—Ba1—Te3	136.057(14)	Te1—Mn2—Mn2^{viii}	122.53(5)
Te2—Ba1—Te3	88.148(11)	Te2^{vi}—Mn2—Mn2^{viii}	57.67(5)
Te1—Ba1—Te3	123.657(13)	Te2^{ix}—Mn2—Mn2^{viii}	57.67(5)
Te1^{i}—Ba1—Te1^{iii}	137.554(11)	Si1—Te1—Mn2	90.00(6)
Te3^{ii}—Ba1—Te1^{iii}	70.431(11)	Si1—Te1—Mn1	133.05 (6)
Te4—Ba1—Te1^{iii}	146.022(12)	Mn2—Te1—Mn1	43.84(7)
Te2^{ii}—Ba1—Te1^{iii}	72.324(11)	Si1—Te1—Ba1^{i}	111.54(5)
Te2—Ba1—Te1^{iii}	84.976(12)	Mn2—Te1—Ba1^{i}	84.382(12)
Te1—Ba1—Te1^{iii}	130.798(13)	Mn1—Te1—Ba1^{i}	77.69(5)
Te3—Ba1—Te1^{iii}	63.780(11)	Si1—Te1—Ba1	128.38(4)
Te1^{i}—Ba1—Ba1^{iii}	93.071(9)	Mn2—Te1—Ba1	138.36(5)
Te3^{ii}—Ba1—Ba1^{iii}	108.676(11)	Mn1—Te1—Ba1	95.02(5)
Te4—Ba1—Ba1^{iii}	122.287(7)	Ba1^{i}—Te1—Ba1	93.682(11)
Te2^{ii}—Ba1—Ba1^{iii}	101.019(12)	Si1—Te1—Ba1^{ii}	84.91(5)
Te2—Ba1—Ba1^{iii}	48.098(8)	Mn2—Te1—Ba1^{ii}	88.241(13)
Te1—Ba1—Ba1^{iii}	170.854(8)	Mn1—Te1—Ba1^{ii}	85.53(5)
Te3—Ba1—Ba1^{iii}	47.198(8)	Ba1^{i}—Te1—Ba1^{ii}	161.891(16)
Te1^{iii}—Ba1—Ba1^{iii}	48.836(9)	Ba1—Te1—Ba1^{ii}	80.926(8)
Te1^{i}—Ba1—Ba1^{ii}	133.704(11)	Mn2^{xi}—Te2—Mn2^{ix}	64.66(9)
Te3^{ii}—Ba1—Ba1^{ii}	49.502(8)	Mn2^{xi}—Te2—Mn1^{ix}	45.74(5)
Te4—Ba1—Ba1^{ii}	90.852(6)	Mn2^{ix}—Te2—Mn1^{ix}	45.74(5)
Te2^{ii}—Ba1—Ba1^{ii}	48.714(9)	Mn2^{xi}—Te2—Mn1^{xi}	45.35(5)

Te2—Ba1—Ba1^{ii}	134.655(9)	Mn2^{ix}—Te2—Mn1^{xi}	45.35(5)
Te1—Ba1—Ba1^{ii}	50.238(7)	Mn1^{ix}—Te2—Mn1^{xi}	68.05(9)
Te3—Ba1—Ba1^{ii}	124.950(10)	Mn2^{xi}—Te2—Ba1^{xii}	135.92(3)
Te1^{iii}—Ba1—Ba1^{ii}	84.286(11)	Mn2^{ix}—Te2—Ba1^{xii}	90.24(4)
Ba1^{iii}—Ba1—Ba1^{ii}	132.467(14)	Mn1^{ix}—Te2—Ba1^{xii}	134.17(2)
Te1^{i}—Ba1—Ba1^{iv}	99.201(8)	Mn1^{xi}—Te2—Ba1^{xii}	90.98(4)
Te3^{ii}—Ba1—Ba1^{iv}	138.015(8)	Mn2^{xi}—Te2—Ba1^{iii}	90.24(4)
Te4—Ba1—Ba1^{iv}	47.554(5)	Mn2^{ix}—Te2—Ba1^{iii}	135.92(3)
Te2^{ii}—Ba1—Ba1^{iv}	48.113(8)	Mn1^{ix}—Te2—Ba1^{iii}	134.17(2)
Te2—Ba1—Ba1^{iv}	48.601(8)	Mn1^{xi}—Te2—Ba1^{iii}	90.98(4)
Te1—Ba1—Ba1^{iv}	98.899(8)	Ba1^{xii}—Te2—Ba1^{iii}	83.773(15)
Te3—Ba1—Ba1^{iv}	135.825(8)	Mn2^{xi}—Te2—Ba1	81.90(3)
Te1^{iii}—Ba1—Ba1^{iv}	98.713(8)	Mn2^{ix}—Te2—Ba1	124.50(3)
Ba1^{iii}—Ba1—Ba1^{iv}	90.0	Mn1^{ix}—Te2—Ba1	79.03 (4)
Ba1^{ii}—Ba1—Ba1^{iv}	90.0	Mn1^{xi}—Te2—Ba1	127.00 (3)
Si1^{v}—Si1—Te3^{vi}	105.31(12)	Ba1^{xii}—Te2—Ba1	139.857(16)
Si1^{v}—Si1—Te1^{vii}	107.96(7)	Ba1^{iii}—Te2—Ba1	83.188(9)
Te3^{vi}—Si1—Te1^{vii}	112.87(5)	Mn2^{xi}—Te2—Ba1^{iv}	124.50(3)
Si1^{v}—Si1—Te1	107.96(7)	Mn2^{ix}—Te2—Ba1^{iv}	81.90(3)
Te3^{vi}—Si1—Te1	112.87(5)	Mn1^{ix}—Te2—Ba1^{iv}	79.03(4)
Te1^{vii}—Si1—Te1	109.57(8)	Mn1^{xi}—Te2—Ba1^{iv}	127.00(3)
Mn2—Mn1—Mn2^{viii}	86.29(14)	Ba1^{xii}—Te2—Ba1^{iv}	83.188(9)
Mn2—Mn1—Te2^{ix}	66.33(7)	Ba1^{iii}—Te2—Ba1^{iv}	139.856(16)
Mn2^{viii}—Mn1—Te2^{ix}	66.33(7)	Ba1—Te2—Ba1^{iv}	82.799(16)
Mn2—Mn1—Te2^{vi}	65.48(7)	Si1^{xi}—Te3—Ba1^{iii}	89.44(3)
Mn2^{viii}—Mn1—Te2^{vi}	65.48(7)	Si1^{xi}—Te3—Ba1^{xiii}	89.44(3)
Te2^{ix}—Mn1—Te2^{vi}	111.95(9)	Ba1^{iii}—Te3—Ba1^{xiii}	96.033(16)
Mn2—Mn1—Te4	131.88(8)	Si1^{xi}—Te3—Ba1	108.79(3)
Mn2^{viii}—Mn1—Te4	131.88(8)	Ba1^{iii}—Te3—Ba1	83.300(9)
Te2^{ix}—Mn1—Te4	99.60(8)	Ba1^{xiii}—Te3—Ba1	161.731(16)
Te2^{vi}—Mn1—Te4	148.45(10)	Si1^{xi}—Te3—Ba1^{vii}	108.79(3)
Mn2—Mn1—Te1	60.28(5)	Ba1^{iii}—Te3—Ba1^{vii}	161.730(16)
Mn2^{viii}—Mn1—Te1	146.19(11)	Ba1^{xiii}—Te3—Ba1^{vii}	83.300(9)
Te2^{ix}—Mn1—Te1	101.16(5)	Ba1—Te3—Ba1^{vii}	91.650(15)
Te2^{vi}—Mn1—Te1	93.70(5)	Mn1^{ix}—Te4—Mn1	180.0
Te4—Mn1—Te1	79.76(5)	Mn1^{ix}—Te4—Ba1	79.58(4)
Mn2—Mn1—Te1^{iv}	146.19(11)	Mn1—Te4—Ba1	100.42(4)

Mn2^{viii}—Mn1—Te1^{iv}	60.28(5)	Mn1^{ix}—Te4—Ba1^{iv}	79.58(4)
Te2^{ix}—Mn1—Te1^{iv}	101.16(5)	Mn1—Te4—Ba1^{iv}	100.42(4)
Te2^{vi}—Mn1—Te1^{iv}	93.70(5)	Ba1—Te4—Ba1^{iv}	84.893(11)
Te4—Mn1—Te1^{iv}	79.76(5)	Mn1^{ix}—Te4—Ba1^{i}	100.42(4)
Te1—Mn1—Te1^{iv}	151.83(10)	Mn1—Te4—Ba1^{i}	79.58(4)
Mn2—Mn1—Mn1^{viii}	43.15(7)	Ba1—Te4—Ba1^{i}	95.107(11)
Mn2^{viii}—Mn1—Mn1^{viii}	43.15(7)	Ba1^{iv}—Te4—Ba1^{i}	180.0
Te2^{ix}—Mn1—Mn1^{viii}	56.62(8)	Mn1^{ix}—Te4—Ba1^{ix}	100.42(4)
Te2^{vi}—Mn1—Mn1^{viii}	55.33(8)	Mn1—Te4—Ba1^{ix}	79.58(4)
Te4—Mn1—Mn1^{viii}	156.21(14)	Ba1—Te4—Ba1^{ix}	180.0
Te1—Mn1—Mn1^{viii}	103.28(5)	Ba1^{iv}—Te4—Ba1^{ix}	95.107(11)
Te1^{iv}—Mn1—Mn1^{viii}	103.28(5)	Ba1^{i}—Te4—Ba1^{ix}	84.893(11)

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