High temperature monoclinic *Cc* phase with reduced *c*/*a* ratio in Bi-based perovskite compound $Bi_2ZnTi_{1-x}Mn_xO_6$

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Figure S1

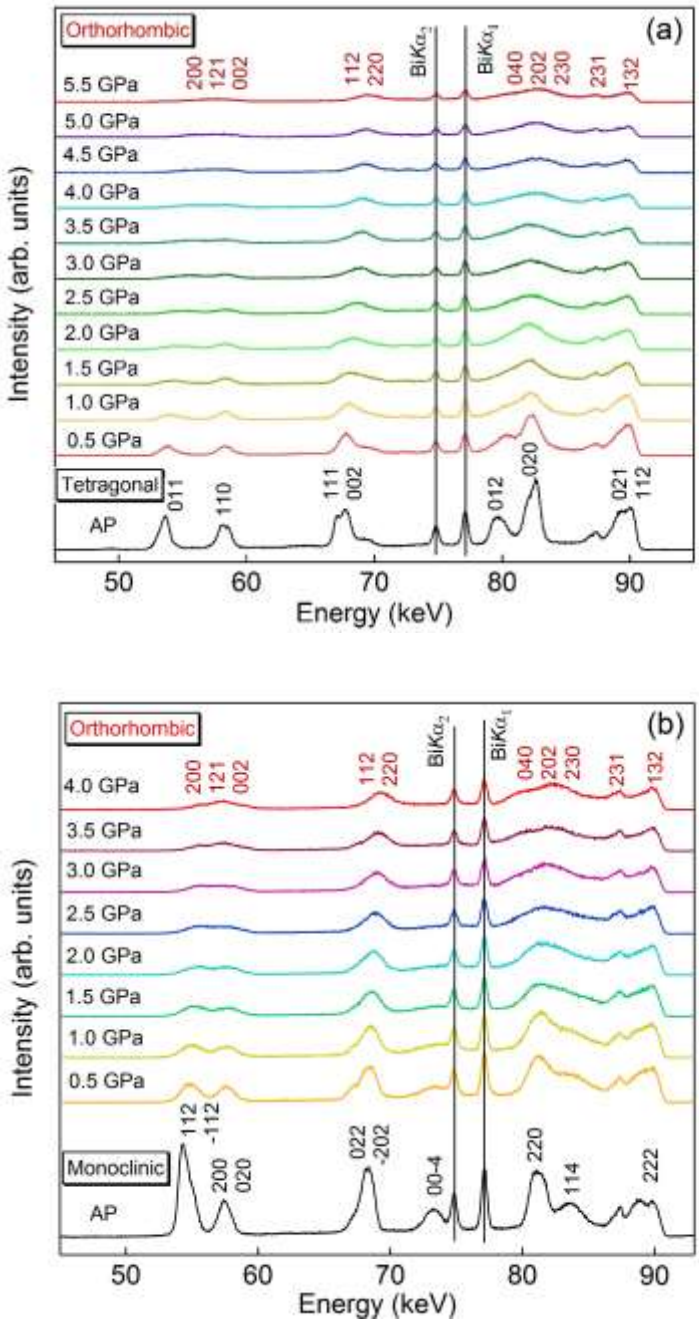

Figure S1 (a) Energy-dispersive SXRD patterns of Bi_2ZnTiO_6 under different pressure. (b) Energy-dispersive SXRD patterns of $Bi_2ZnTi_{0.8}Mn_{0.2}O_6$ under different pressure.

Table S1. Comparison of the atomic displacements in BO_6 octahedron for $Bi_2ZnTi_{0.6}Mn_{0.4}O_6$ (BZTM) and $PbTi_{0.48}Zr_{0.52}O_3$ (PZT).[a]

	Shift x (BZTM)	Shift x (PZT)	Shift z (BZTM)	Shift z (PZT)
B site (×4)	-0.04681	-0.02301	-0.03005	0.0356
O1(×4)	-0.07185	-0.03699	-0.06778	0.0453
O2(×4)	0.06302	-0.01501	0.1264	0.0636
O3(×4)	-0.10074	-0.04901	-0.04778	0. 0545

[a] The shift x and shift z are the atomic position displacements along x and z directions.

Table S2 Crystallographic parameters of $Bi_2ZnTi_{0.6}Mn_{0.4}O_6$ at 900 K.[b]

Site	Wyckoff position	x	y	z	U_{iso}(Å^2)	g
Bi	1a	0	0	0	0.0637(0)	1.0
Zn	1b	0.5	0.5	0.5615(7)	0.0348(6)	0.5
Ti	1b	0.5	0.5	0.5615(7)	0.0348(6)	0.3
Mn	1b	0.5	0.5	0.5615(7)	0.0348(6)	0.2
O1	1b	0.5	0.5	-0.1521(3)	0.0126(7)	1.0
O2	2c	0.5	0	0. 3062(4)	0.0126(7)	1.0

[b] Parameters: wavelength λ = 0.419736 Å, space group *P4mm* (No. 99), Z = 1, a = 3.8862(3) Å, c = 4.2876(0) Å, V = 64.75 Å^3. Occupation factors of all of the sites are unity. R values (%): R_{wp} = 7.36, R_p = 4.72. Occupation factors of all of the sites are fixed to the unity.