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Magnetic Order in A Quenched-High-Temperature-Phase of Cu-Doped MnBi

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $Cu_xMn_{1-x}Bi$ at 150 (2) K. (U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor (Å^2))

$Cu_{0.03(2)}Mn_{0.97(2)}Bi_{0.99(1)}$:

Atom	Wyck.	Occ.	*x*	*y*	*z*	U_{eq}
Bi1	6*h*	1	0.2946 (1)	0.1473 (1)	¼	0.0129 (1)
Bi2	2*c*	0.843 (3)	$^1/_3$	$^2/_3$	¼	0.0102 (2)
Bi3	6*h*	0.036 (1)	0.2275 (5)	0.7725 (5)	¼	0.036 (1)
Mn1	6*g*	1	½	0	0	0.0134 (3)
Mn2	2*d*	0.67 (6)	$^2/_3$	$^1/_3$	¼	0.014 (1)
Cu1	2*d*	0.10 (6)	$^2/_3$	$^1/_3$	¼	0.014 (1)
Mn3	4*f*	0.1156	$^2/_3$	$^1/_3$	0.138 (4)	0.014 (1)

$Cu_{0.04(2)}Mn_{0.96(2)}Bi_{0.99(1)}$:

Atom	Wyck.	Occ.	*x*	*y*	*z*	U_{eq}
Bi1	6*h*	1	0.8527 (1)	0.1473 (1)	¼	0.0129 (2)
Bi2	2*c*	0.820 (4)	$^1/_3$	$^2/_3$	¼	0.0106 (3)
Bi3	6*h*	0.040 (1)	0.2280 (6)	0.7720 (6)	¼	0.0106 (5)
Mn1	6*g*	1	½	0	0	0.0138 (3)
Mn2	2*d*	0.49 (7)	$^2/_3$	$^1/_3$	¼	0.008 (2)
Cu1	2*d*	0.16 (7)	$^2/_3$	$^1/_3$	¼	0.008 (2)
Mn3	4*f*	0.176	$^2/_3$	$^1/_3$	0.152 (2)	0.008 (2)

$Cu_{0.08(2)}Mn_{0.92(2)}Bi_{0.99(1)}$:

Atom	Wyck.	Occ.	*x*	*y*	*z*	U_{eq}
Bi1	6*h*	1	0.7055 (1)	0.8527 (1)	¼	0.0140 (2)
Bi2	2*d*	0.820 (4)	$^1/_3$	$^2/_3$	¼	0.0118 (3)
Bi3	6*h*	0.0414 (13)	0.458 (1)	0.229 (1)	¼	0.0118 (3)
Mn1	6*g*	1	½	0	0	0.0143 (3)
Mn2	2*c*	0.41 (8)	$^2/_3$	$^1/_3$	¼	0.018 (2)
Cu1	2*c*	0.31 (8)	$^2/_3$	$^1/_3$	¼	0.018 (2)
Mn3	4*f*	0.1363	$^2/_3$	$^1/_3$	0.144 (4)	0.018 (2)

$Cu_{0.11(4)}Mn_{0.89(4)}Bi_{0.99(1)}$:

Atom	Wyck.	Occ.	*x*	*y*	*z*	U_{eq}
Bi1	6*h*	1	0.2947 (1)	0.1473 (1)	¼	0.0149 (2)
Bi2	2*c*	0.799 (3)	$^1/_3$	$^2/_3$	¼	0.0129 (2)
Bi3	6*h*	0.0489 (1)	0.5409 (7)	0.7705 (3)	¼	0.0129 (3)
Mn1	6*g*	0.92 (3)	½	0	0	0.0160 (4)
Cu1	6*g*	0.08 (3)	½	0	0	0.0160 (4)
Mn2	2*d*	0.43 (5)	$^2/_3$	$^1/_3$	¼	0.014 (1)
Cu2	2*d*	0.21 (5)	$^2/_3$	$^1/_3$	¼	0.014 (1)
Mn3	4*f*	0.1808	$^2/_3$	$^1/_3$	0.148 (2)	0.014 (1)

$Cu_{0.14(7)}Mn_{0.86(7)}Bi_{0.99(1)}$:

Atom	Wyck.	Occ.	*x*	*y*	*z*	U_{eq}
Bi1	6*h*	1	0.2960 (1)	0.1480 (1)	¼	0.0151 (3)
Bi2	2*c*	0.738 (5)	$^1/_3$	$^2/_3$	¼	0.0143 (4)
Bi3	6*h*	0.074 (2)	0.5389 (9)	0.7694 (5)	¼	0.0143 (6)
Mn1	6*g*	0.88 (6)	½	0	0	0.0165 (8)
Cu1	6*g*	0.12 (6)	½	0	0	0.0165 (8)
Mn2	2*d*	0.25 (9)	$^2/_3$	$^1/_3$	¼	0.017 (5)
Cu2	2*d*	0.20 (9)	$^2/_3$	$^1/_3$	¼	0.017 (5)
Mn3	4*f*	0.2754	$^2/_3$	$^1/_3$	0.154 (3)	0.017 (5)

Table S2. Anisotropic thermal displacement parameters for $Cu_xMn_{1-x}Bi$ at 150 (2) K.

$Cu_{0.03(2)}Mn_{0.97(2)}Bi_{0.99(1)}$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1	0.0101 (2)	0.0128 (2)	0.0148 (2)	-0.0000 (1)	0	0.0050 (1)
Bi2	0.0091 (2)	0.0091 (2)	0.0123 (3)	0	0	0.0046 (1)
Bi3	0.0091 (5)	0.0091 (5)	0.0123 (2)	0	0	0.0046 (3)
Mn1	0.0148 (6)	0.0167 (6)	0.0094 (5)	0.0021 (4)	0.0006 (4)	0.0083 (5)
Mn2	0.0095 (8)	0.0095 (8)	0.024 (2)	0	0	0.0048 (4)
Cu1	0.0095 (8)	0.0095 (8)	0.024 (2)	0	0	0.0048 (4)
Mn3	0.0095 (8)	0.0095 (8)	0.024 (2)	0	0	0.0048 (4)

$Cu_{0.04(2)}Mn_{0.96(2)}Bi_{0.99(1)}$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1	0.0118 (2)	0.0118 (2)	0.0173 (2)	0.0000 (1)	0.0000 (1)	0.0075 (2)
Bi2	0.0076 (3)	0.0076 (3)	0.0165 (4)	0	0	0.0038 (2)
Bi3	0.0076 (6)	0.0076 (6)	0.0165 (3)	0	0	0.0038 (3)
Mn1	0.0135 (7)	0.0161 (7)	0.0127 (7)	0.0019 (5)	0.0012 (5)	0.0081 (6)
Mn2	0.009 (1)	0.009 (1)	0.008 (3)	0	0	0.0042 (5)
Cu1	0.009 (1)	0.009 (1)	0.008 (3)	0	0	0.0042 (5)
Mn3	0.009 (1)	0.009 (1)	0.008 (3)	0	0	0.0042 (5)

$Cu_{0.08(2)}Mn_{0.92(2)}Bi_{0.99(1)}$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1	0.0100 (2)	0.0134 (2)	0.0175 (3)	0.0001 (1)	0	0.0050 (1)
Bi2	0.0091 (3)	0.0091 (3)	0.0172 (4)	0	0	0.0045 (2)
Bi3	0.0091 (7)	0.0091 (7)	0.0172 (3)	0	0	0.0045 (3)
Mn1	0.0140 (7)	0.0170 (8)	0.0130 (8)	-0.0022 (5)	-0.0009 (5)	0.0087 (6)
Mn2	0.010 (1)	0.010 (1)	0.034 (3)	0	0	0.0051 (6)
Cu1	0.010 (1)	0.010 (1)	0.034 (3)	0	0	0.0051 (6)
Mn3	0.010 (1)	0.010 (1)	0.034 (3)	0	0	0.0051 (6)

$Cu_{0.11(4)}Mn_{0.89(4)}Bi_{0.99(1)}$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1	0.0109 (2)	0.0148 (1)	0.0176 (2)	0.0000 (1)	0	0.0055 (1)
Bi2	0.0101 (2)	0.0101 (2)	0.0185 (3)	0	0	0.0051 (1)
Bi3	0.0101 (4)	0.0101 (4)	0.0185 (2)	0	0	0.0051 (2)
Mn1	0.0164 (6)	0.0193 (6)	0.0137 (6)	0.0023 (4)	0.0013 (4)	0.0099 (4)
Cu1	0.0164 (6)	0.0193 (6)	0.0137 (6)	0.0023 (4)	0.0013 (4)	0.0099 (4)
Mn2	0.0103 (7)	0.0103 (7)	0.020 (2)	0	0	0.0052 (4)
Cu2	0.0103 (7)	0.0103 (7)	0.020 (2)	0	0	0.0052 (4)
Mn3	0.0103 (7)	0.0103 (7)	0.020 (2)	0	0	0.0052 (4)

$Cu_{0.14(7)}Mn_{0.86(7)}Bi_{0.99(1)}$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Bi1	0.0088 (4)	0.0135 (3)	0.0214 (4)	-0.0001 (2)	0	0.0044 (2)
Bi2	0.0090 (5)	0.0090 (5)	0.0251 (7)	0	0	0.0045 (3)
Bi3	0.0090 (5)	0.0090 (5)	0.0251 (7)	0	0	0.0045 (3)
Mn1	0.016 (1)	0.020 (1)	0.016 (1)	0.004 (1)	0.002 (1)	0.011 (1)
Cu1	0.016 (1)	0.020 (1)	0.016 (1)	0.004 (1)	0.002 (1)	0.011 (1)
Mn2	0.009 (2)	0.009 (2)	0.033 (16)	0	0	0.003 (1)
Cu2	0.009 (2)	0.009 (2)	0.033 (16)	0	0	0.003 (1)
Mn3	0.009 (2)	0.009 (2)	0.033 (16)	0	0	0.003 (1)

Figure S1. Single crystal X-ray diffraction patterns from (0kl), (h0l) and (hk0) planes for $Cu_{0.03(2)}Mn_{0.97(2)}Bi_{0.99(1)}$.

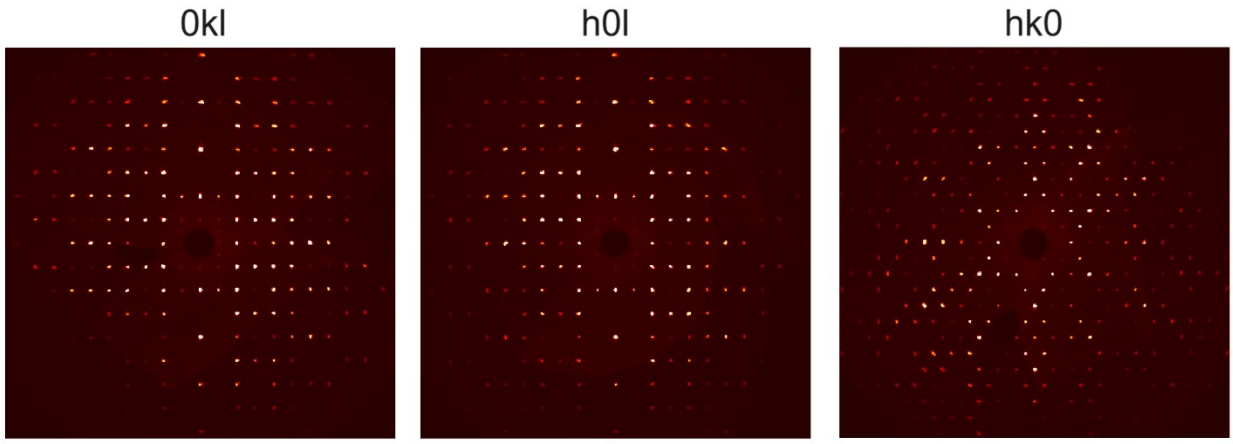

Figure S2. Single crystal X-ray diffraction patterns from (0kl), (h0l) and (hk0) planes for $Cu_{0.04(2)}Mn_{0.96(2)}Bi_{0.99(1)}$.

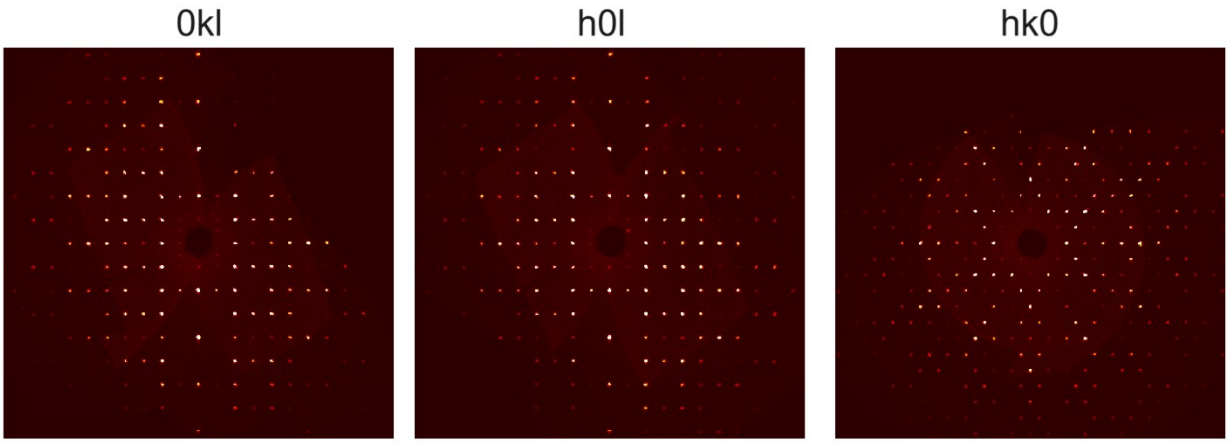

Figure S3. Single crystal X-ray diffraction patterns from (0kl), (h0l) and (hk0) planes for $Cu_{0.08(2)}Mn_{0.92(2)}Bi_{0.99(1)}$.

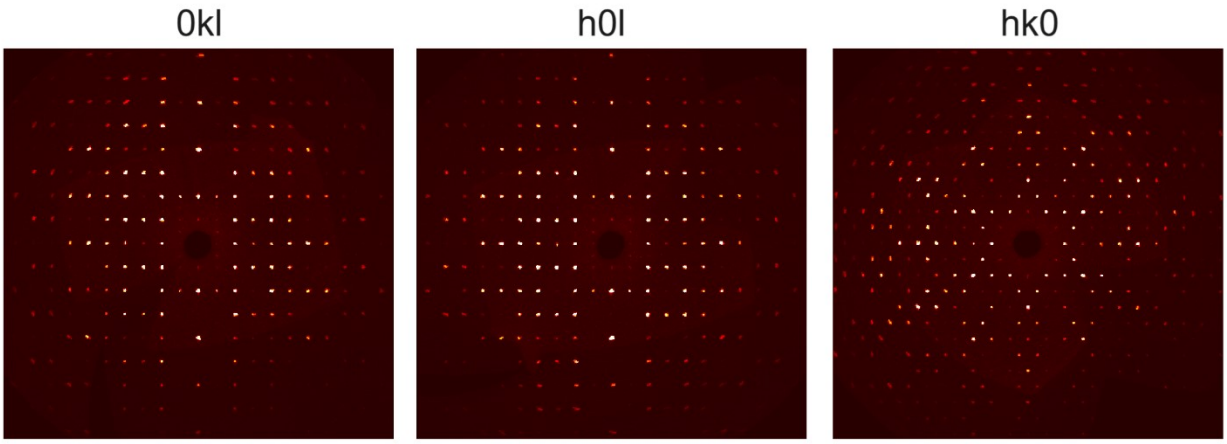

Figure S4. Single crystal X-ray diffraction patterns from (0kl), (h0l) and (hk0) planes for $Cu_{0.11(4)}Mn_{0.89(4)}Bi_{0.99(1)}$.

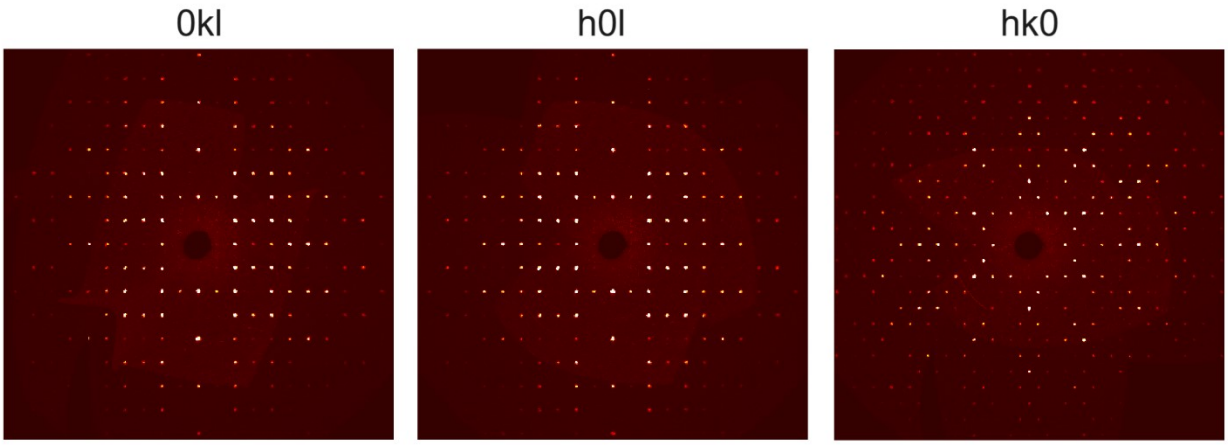

Figure S5. Single crystal X-ray diffraction patterns from (0kl), (h0l) and (hk0) planes for $Cu_{0.14(7)}Mn_{0.86(7)}Bi_{0.99(1)}$.

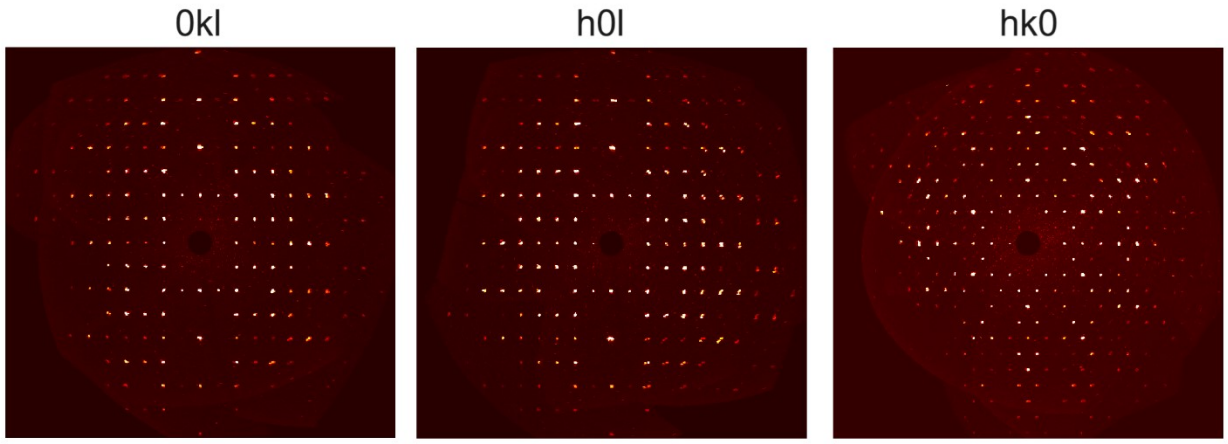

Figure S6. Comparison of powder XRD patterns for $Cu_xMn_{1-x}Bi$ and reported QHTP-MnBi.

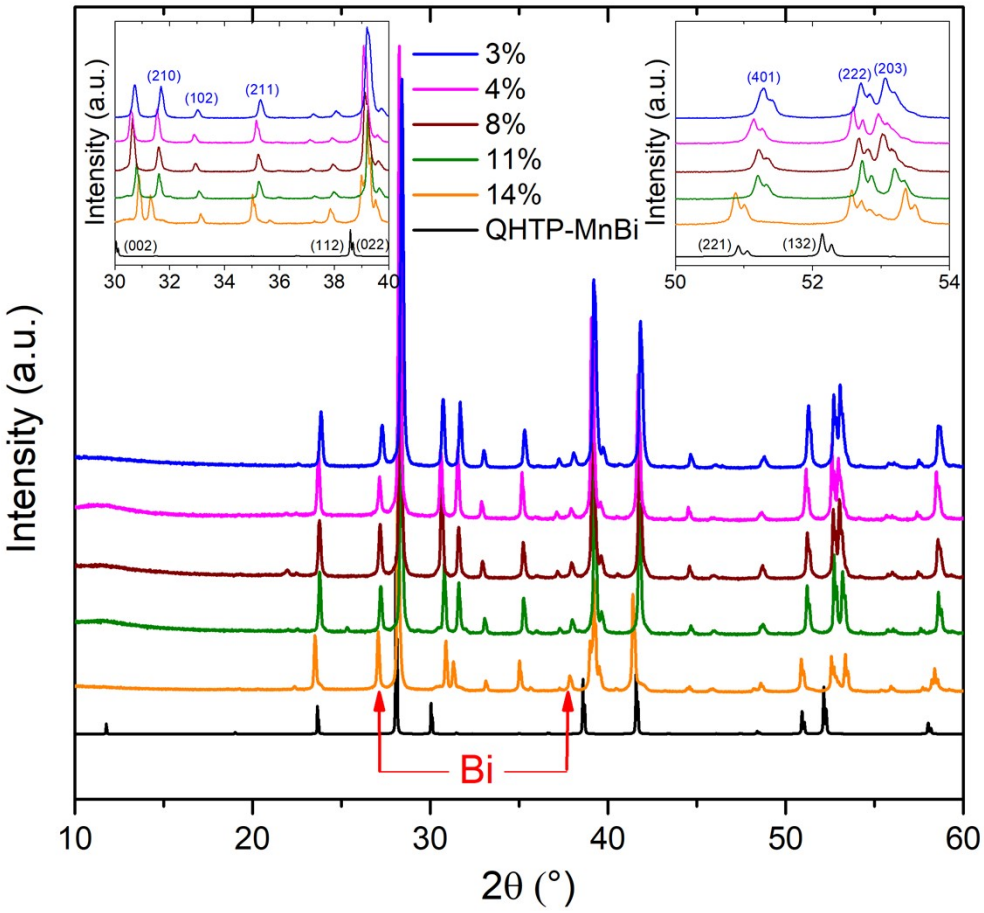

Figure S7. Temperature-dependent heat capacity (C_p) of $Cu_{0.04}Mn_{0.96}Bi_{0.99}$.

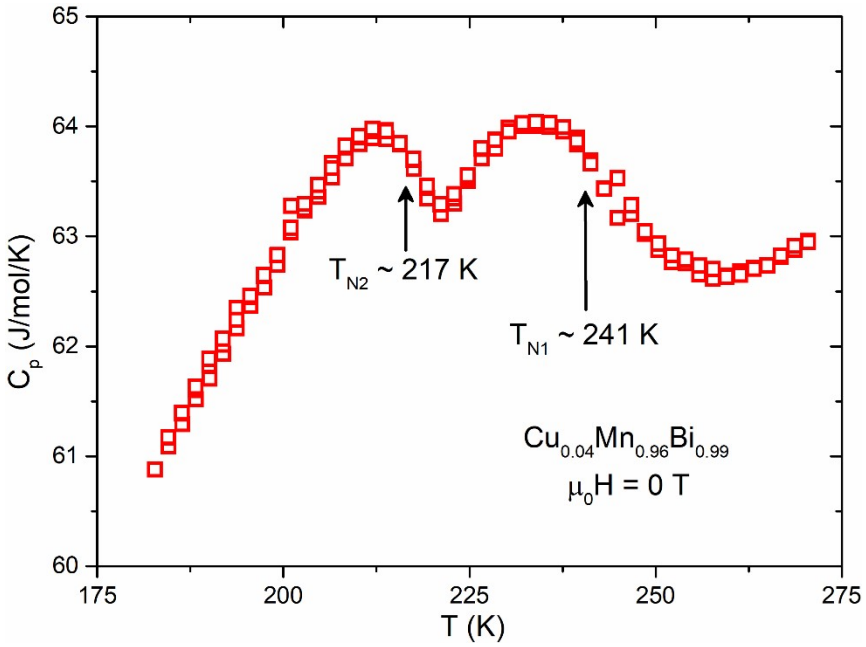

Figure S8. The first derivative of χT vs T curves for **(a)** $Cu_{0.11(4)}Mn_{0.89(4)}Bi_{0.99(1)}$ and **(b)** $Cu_{0.14(7)}Mn_{0.86(7)}Bi_{0.99(1)}$.