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Supporting Information (Online Material) for

Plethora of Structural Transitions, Distortions and Modulations in Cu-doped $BiMn_7O_{12}$ Quadruple Perovskites

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Table S1. Structure parameters of $BiCu_{0.5}Mn_{6.5}O_{12}$ at 50 K, 300 K and 400 K from neutron powder diffraction data in the average models

Site	WP	*x*	*y*	*z*	*U* (Å^2)
		T = 50 K, space group *I*2/*m*			
Bi	2*a*	0	0	0	0.0498(16)
Mn1	2*c*	0.5	0	0	0.0208(18)
Mn2	2*d*	0.5	0.5	0	= *U*(Mn1)
Mn3	2*b*	0	0.5	0	= *U*(Mn1)
Mn4	4*e*	0.75	0.25	0.75	0.0109(8)
Mn5	4*f*	0.25	0.25	0.75	= *U*(Mn4)
O1	8*j*	0.0020(11)	0.1760(13)	0.6887(16)	0.0141(6)
O2	4*i*	0.6901(12)	0	0.8241(17)	= *U*(O1)
O3	4*i*	0.3119(13)	0	0.8202(19)	= *U*(O1)
O4	8*j*	0.1758(8)	0.6896(15)	0.0060(9)	= *U*(O1)
		T = 300 K, space group *I*2/*m*			
Bi	2*a*	0	0	0	0.0441(15)
Mn1	2*c*	0.5	0	0	0.0203(18)
Mn2	2*d*	0.5	0.5	0	= *U*(Mn1)
Mn3	2*b*	0	0.5	0	= *U*(Mn1)
Mn4	4*e*	0.75	0.25	0.75	0.0116(8)
Mn5	4*f*	0.25	0.25	0.75	= *U*(Mn4)
O1	8*j*	0.0030(7)	0.1751(10)	0.6887(9)	0.0156(6)
O2	4*i*	0.6913(9)	0	0.8251(10)	= *U*(O1)
O3	4*i*	0.3137(10)	0	0.8196(12)	= *U*(O1)
O4	8*j*	0.1766(7)	0.6898(12)	0.0073(6)	= *U*(O1)
		T = 400 K, space group *Im*-3			
Bi	2*a*	0	0	0	0.0460(15)
Mn1	6*b*	0	0.5	0.5	0.0206(18)
Mn2	8*c*	0.25	0.25	0.25	0.0138(8)
O	24*g*	0	0.31069(14)	0.17626(15)	0.0189(6)

WP: Wyckoff position. Octahedral sites are marked by bold, blue letters.

At 50 K: Space group $I2/m$ (No. 12, unique axis b, cell choice 3), Z = 2. g(Bi) = g(Mn4) = g(Mn5) = g(O1) = g(O2) = g(O3) = g(O4) = 1, and Mn1, Mn2, and Mn3 are occupied by 0.8333Mn+0.1667Cu. g is the occupation factor.

a = 7.42439(18) Å, b = 7.4431(2) Å, c = 7.4403(3) Å, β = 90.2709(18)°, and V = 411.15(2) Å^3; R_{wp} = 7.20 %, R_p = 5.73 %.

At 300 K: Space group $I2/m$ (No. 12, unique axis b, cell choice 3), Z = 2. g(Bi) = g(Mn4) = g(Mn5) = g(O1) = g(O2) = g(O3) = g(O4) = 1, and Mn1, Mn2, and Mn3 are occupied by 0.8333Mn+0.1667Cu. g is the occupation factor.

a = 7.43419(17) Å, b = 7.44493(14) Å, c = 7.44850(18) Å, β = 90.4203(15)°, and V = 412.241(16) Å^3; R_{wp} = 6.66 %, R_p = 5.46 %.

At 400 K: Space group Im-3 (No 204); Z = 2. g(Bi) = g(Mn2) = g(O) = 1, and Mn1 is occupied by 0.8333Mn+0.1667Cu. g is the occupation factor.

a = 7.44784(3) Å and V = 413.134(3) Å^3; R_{wp} = 7.26 %, R_p = 6.30 %.

Table S2. Bond lengths, bond-valence sum (BVS), and distortion parameters of MnO_6 (Δ) in $BiCu_{0.5}Mn_{6.5}O_{12}$ at 50 K, 300 K and 400 K

T = 50 K, space group $I2/m$			
Bi-O2 ×2	2.642(10)	Mn3-O4 ×4	1.923(9)
Bi-O1 ×4	2.661(11)	Mn3-O3 ×2	2.767(10)
Bi-O3 ×2	2.680(11)	Mn3-O2 ×2	2.788(10)
Bi-O4 ×4	2.654(10)	BVS(Mn3)	+2.83
BVS(Bi)	+2.58	**Mn4**-O4 ×2	1.947(7)
Mn1-O2 ×2	1.929(11)	**Mn4**-O2 ×2	1.992(4)
Mn1-O3 ×2	1.929(12)	**Mn4**-O1 ×2	2.005(9)
Mn1-O1 ×4	2.790(12)	BVS(Mn4)	+3.31
BVS(Mn1)	+2.78	Δ(Mn4)	1.6×10^{-4}
Mn2-O1 ×4	1.920(11)	**Mn5**-O1 ×2	1.973(9)
Mn2-O4 ×4	2.791(11)	**Mn5**-O3 ×2	1.986(4)
BVS(Mn2)	+2.84	**Mn5**-O4 ×2	2.036(7)
		BVS(Mn5)	+3.16
		Δ(Mn5)	1.8×10^{-4}
T = 300 K, space group $I2/m$			
Bi-O2 ×2	2.630(7)	Mn3-O4 ×4	1.929(7)
Bi-O1 ×4	2.660(7)	Mn3-O3 ×2	2.764(8)
Bi-O3 ×2	2.699(8)	Mn3-O2 ×2	2.801(8)
Bi-O4 ×4	2.657(8)	BVS(Mn3)	+2.79
BVS(Bi)	+2.57	**Mn4**-O4 ×2	1.937(5)
Mn1-O2 ×2	1.935(7)	**Mn4**-O2 ×2	1.993(3)
Mn1-O3 ×2	1.923(8)	**Mn4**-O1 ×2	2.017(6)
Mn1-O1 ×4	2.789(8)	BVS(Mn4)	+3.30
BVS(Mn1)	+2.78	Δ(Mn4)	2.9×10^{-4}
Mn2-O1 ×4	1.918(7)	**Mn5**-O1 ×2	1.970(6)
Mn2-O4 ×4	0.763(4)	**Mn5**-O3 ×2	1.988(3)
BVS(Mn2)	+2.86	**Mn5**-O4 ×2	2.046(5)
		BVS(Mn5)	+3.14
		Δ(Mn5)	2.6×10^{-4}
T = 400 K, space group Im-3			
Bi-O ×12	2.6604(10)	Mn1-O ×4	1.9264(11)
BVS(Bi)	+2.57	Mn1-O ×4	2.7932(11)
		BVS(Mn1)	+2.80
		Mn2-O ×6	1.9932(4)
		BVS(Mn2)	+3.19

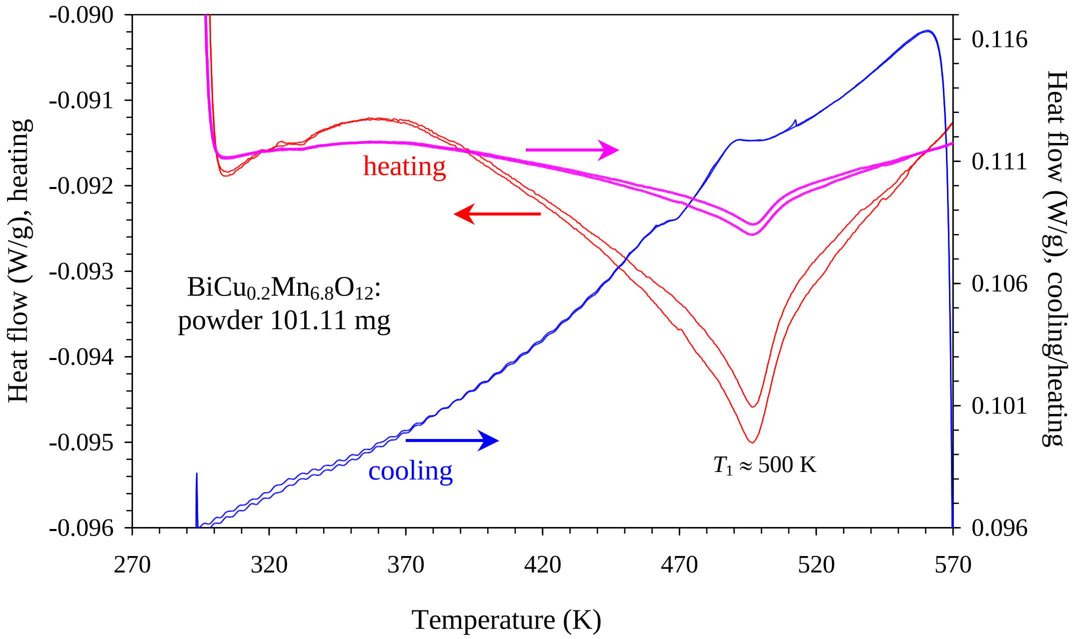

Figure S1a. DSC curves of $BiCu_{0.2}Mn_{6.8}O_{12}$ (two runs) on heating (red; left-hand axis) and cooling (blue; right-hand axis) at 10 K/min. Small bumps near 470 K on cooling curves are instrumental artifacts. Shifted (by +0.203 W/g) heating curves are also plotted (pink color) using the right-hand axis to show the heating-cooling curves on the same scale.

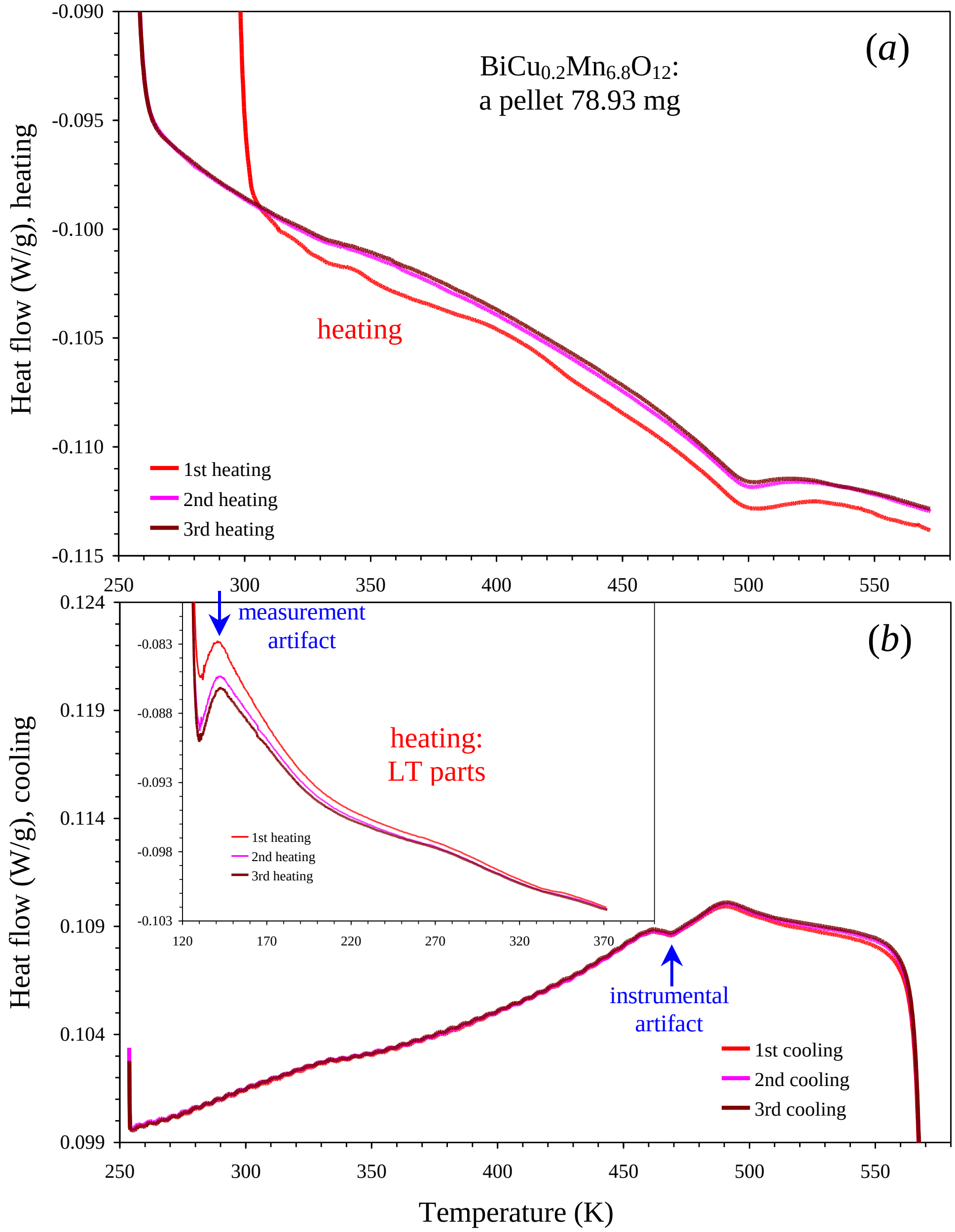

Figure S1b. DSC curves of $BiCu_{0.2}Mn_{6.8}O_{12}$ (three runs; a pellet of 78.93 mg) on (a) heating and (b) cooling at 10 K/min. Small bumps near 470 K on cooling curves are instrumental artifacts. Inset shows DSC curves from 123 K to 370 K on heating (three runs) to emphasize the absence of low-temperature DSC anomalies.

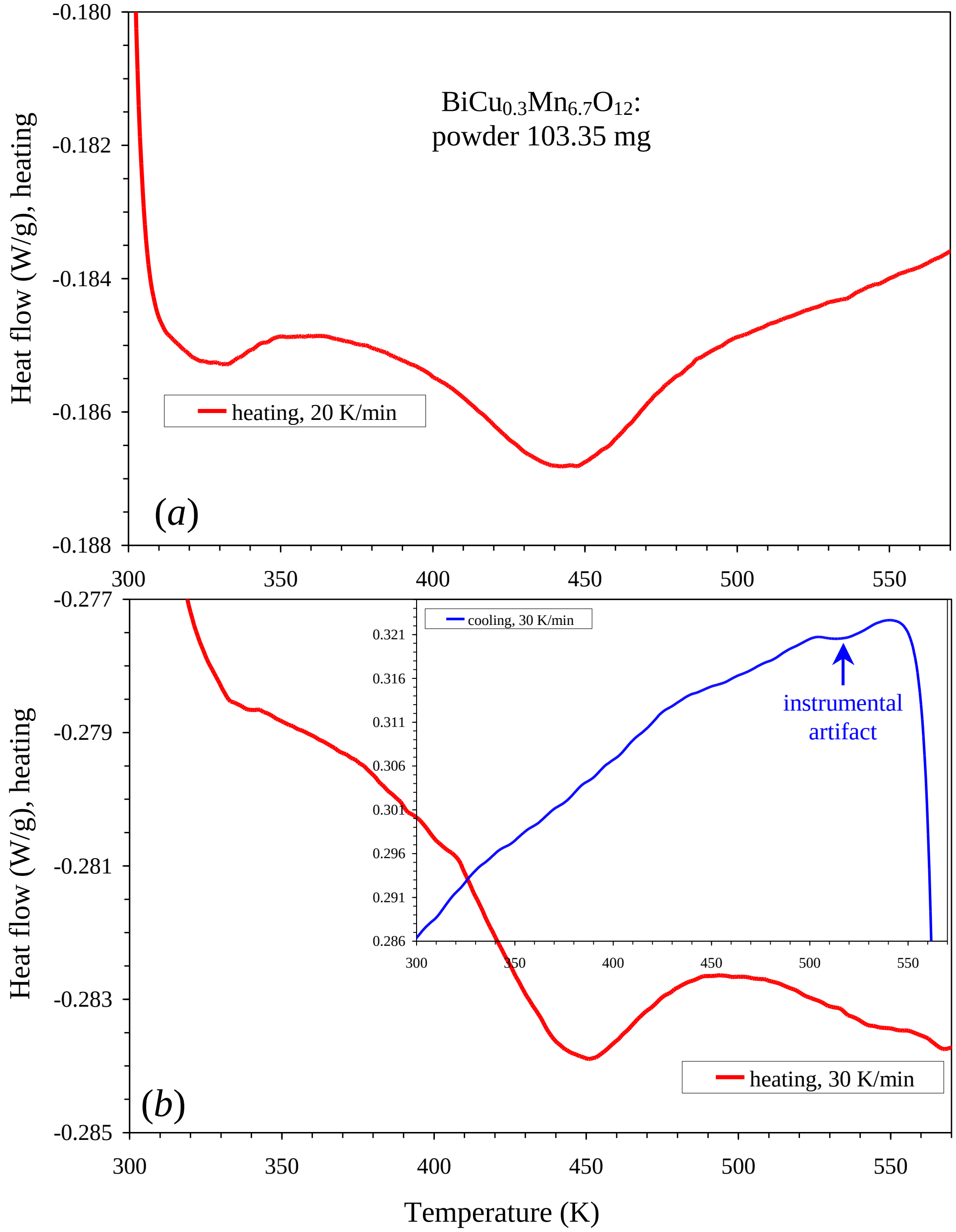

Figure S1c. DSC curves of $BiCu_{0.3}Mn_{6.7}O_{12}$ (powder sample of 103.35 mg) on (a) heating with 20 K/min and (b) on heating with 30 K/min. Inset shows a DSC curve on cooling with 30 K/min.

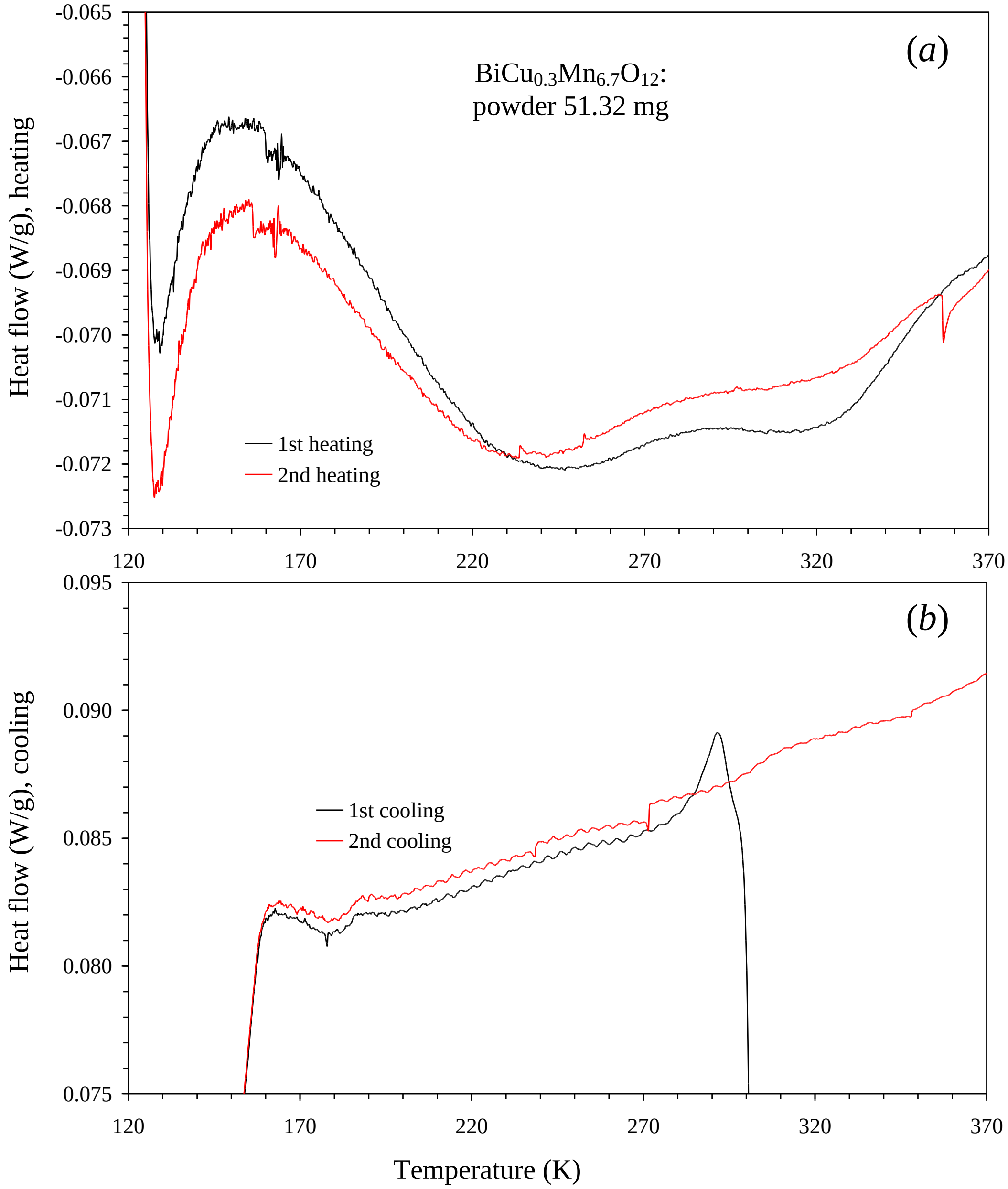

Figure S1d. DSC curves of $BiCu_{0.3}Mn_{6.7}O_{12}$ (two runs, powder sample of 51.32 mg) on (a) heating and (b) cooling with 10 K/min in low-temperature regions.

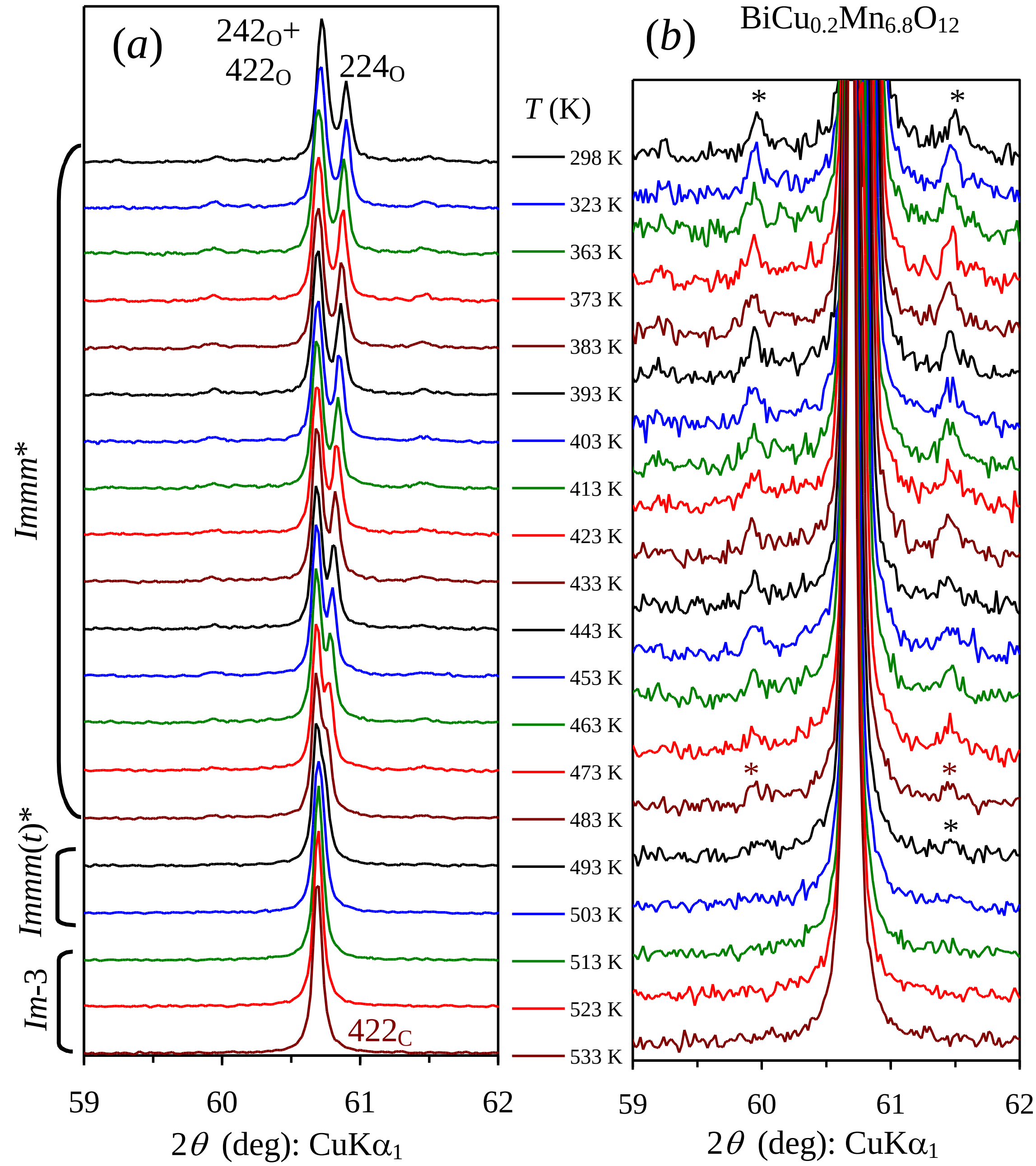

Figure S2. High-temperature laboratory X-ray powder diffraction patterns of $BiCu_{0.2}Mn_{6.8}O_{12}$. Fragments of diffraction patterns near the *422* cubic reflection are shown. Reflection indexes for the *Immm* orthorhombic (O) and *Im*-3 cubic (C) space groups are given. The panel (b) shows the zoomed part of panel (a) to emphasize the incommensurately modulated reflections (marked by the stars). Very weak incommensurately modulated reflections were still observed at 493 K, where the a_O and b_O lattice parameters already merge. Measurements were performed on heating.

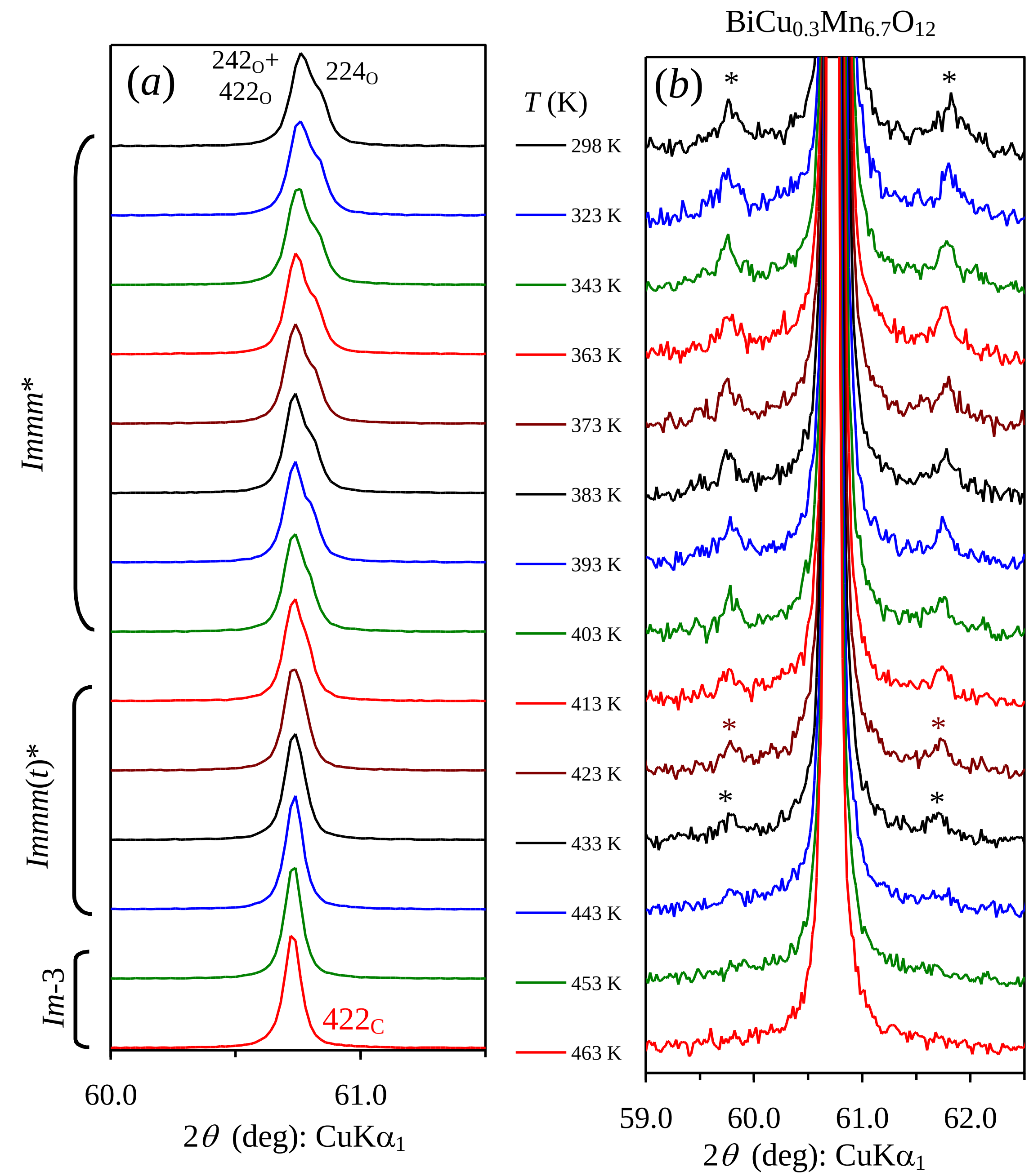

Figure S3. High-temperature laboratory X-ray powder diffraction patterns of $BiCu_{0.3}Mn_{6.7}O_{12}$. Fragments of diffraction patterns near the *422* cubic reflection are shown. Reflection indexes for the *Immm* orthorhombic (O) and *Im*-3 cubic (C) space groups are given. The panel (b) shows the zoomed part of panel (a) to emphasize the incommensurately modulated reflections (marked by the stars). Weak incommensurately modulated reflections were still observed at 413-443 K, where the a_O and b_O lattice parameters already merge. Measurements were performed on heating.

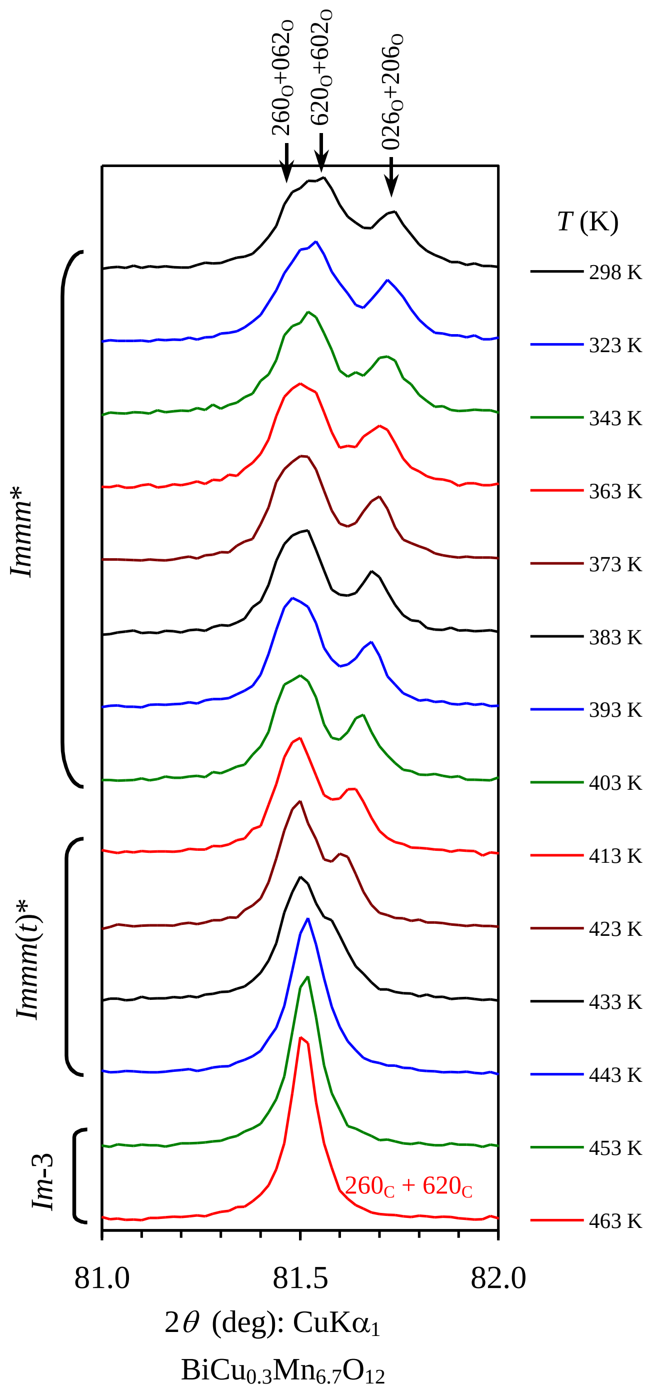

Figure S4. High-temperature laboratory X-ray powder diffraction patterns of $BiCu_{0.3}Mn_{6.7}O_{12}$. Fragments of diffraction patterns near the *260* and *620* cubic reflections are shown. Reflection indexes for the *Immm* orthorhombic (O) and *Im*-3 cubic (C) space groups are given. Measurements were performed on heating. This figure illustrates that a_O, b_O and c_O are different in the *Immm** phase, but a_O and b_O merge in the *Immm*(*t*)* phase, and all a_O, b_O and c_O merge in the cubic *Im*-3 phase.

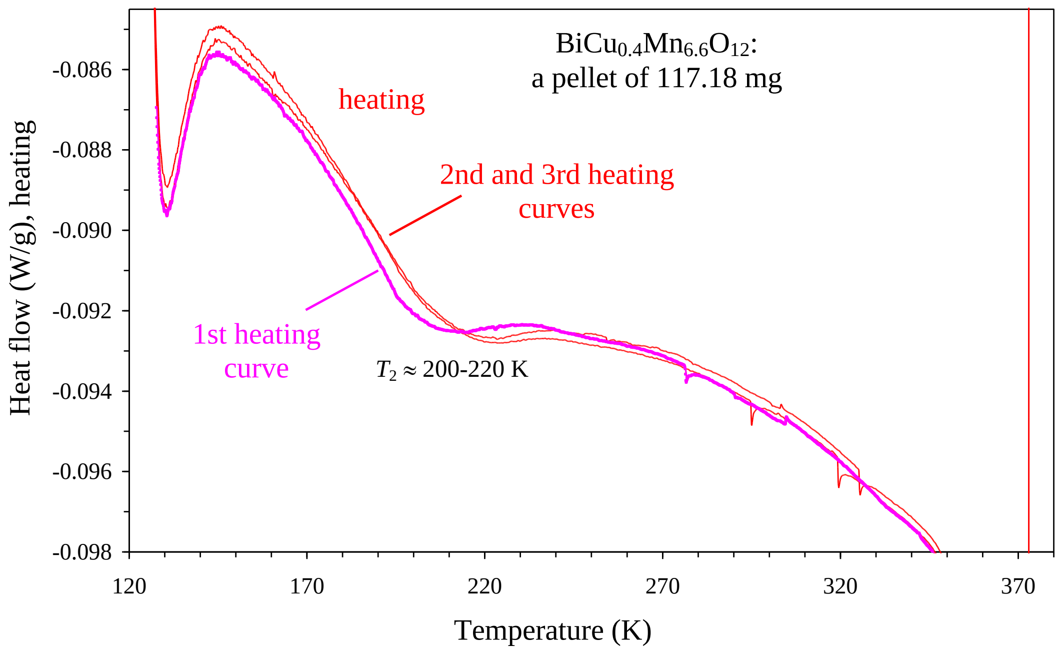

Figure S5. Details of the DSC curves of $BiCu_{0.4}Mn_{6.6}O_{12}$ (three runs) on heating in a low-temperature region.

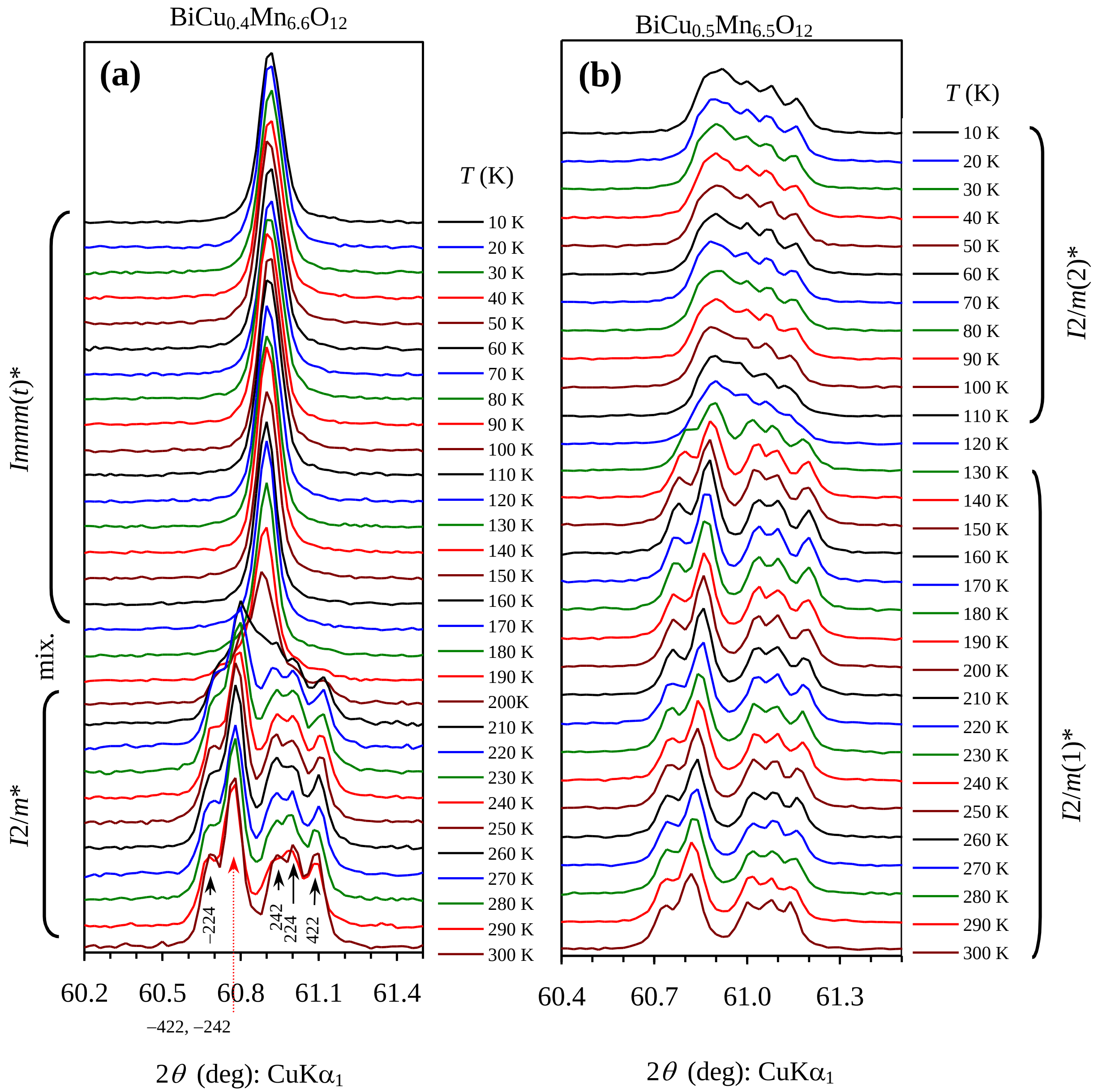

Figure S6. Low-temperature laboratory X-ray powder diffraction patterns of (a) $BiCu_{0.4}Mn_{6.6}O_{12}$ and (b) $BiCu_{0.5}Mn_{6.5}O_{12}$ between 10 K and 300 K with a step of 10 K. Fragments of diffraction patterns near the *422* cubic reflection are shown. Reflection indexes for the monoclinic *I*2/*m* space group are given. Measurements were performed on heating.

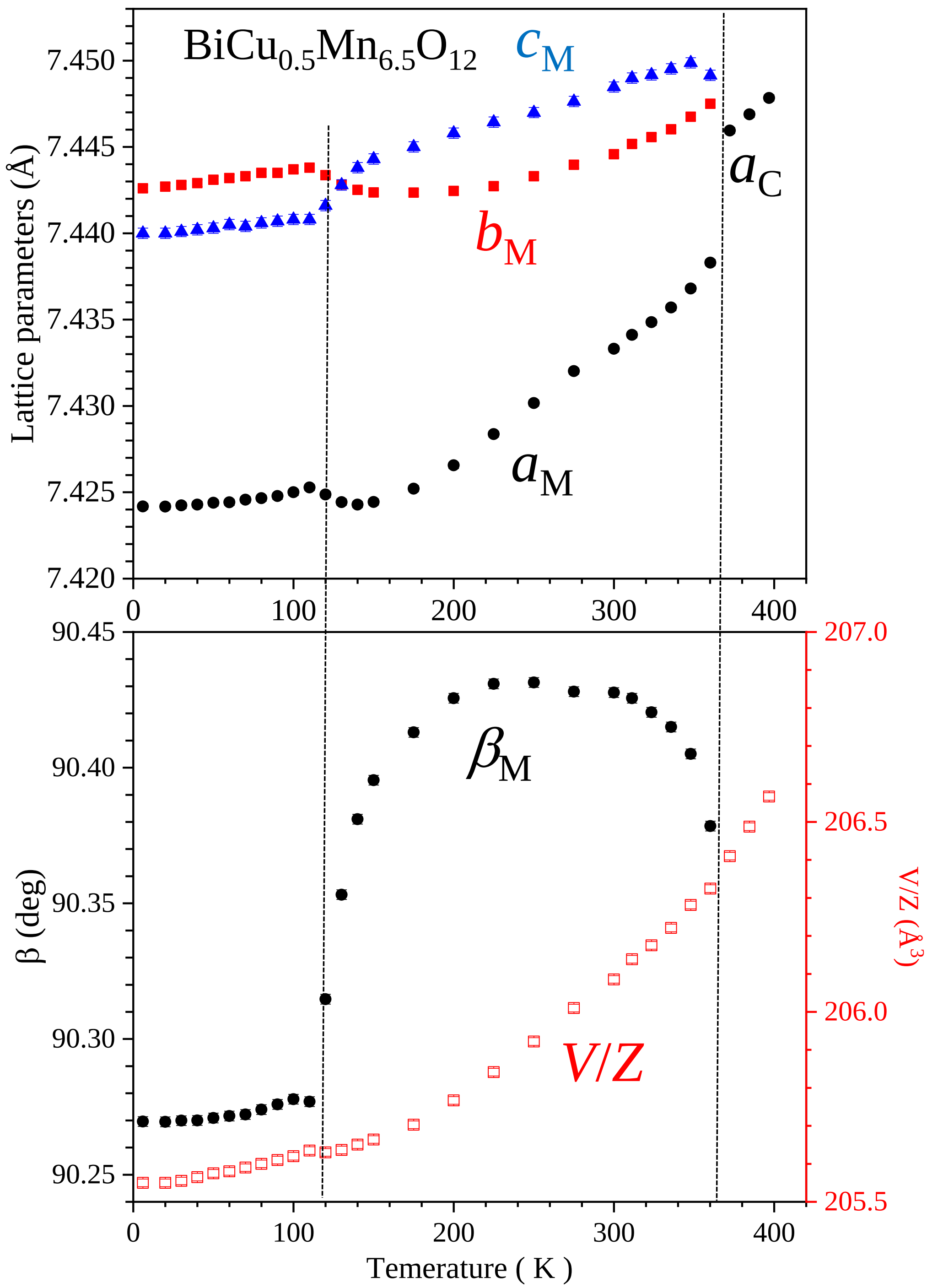

Figure S7. Temperature dependence of (a) the lattice parameters and (b) monoclinic *β* angle (left-hand axis) and the normalized unit-cell volume (*V*/Z) (right-hand axis) in $BiCu_{0.5}Mn_{6.5}O_{12}$ from neutron diffraction data. Measurements were performed on heating.

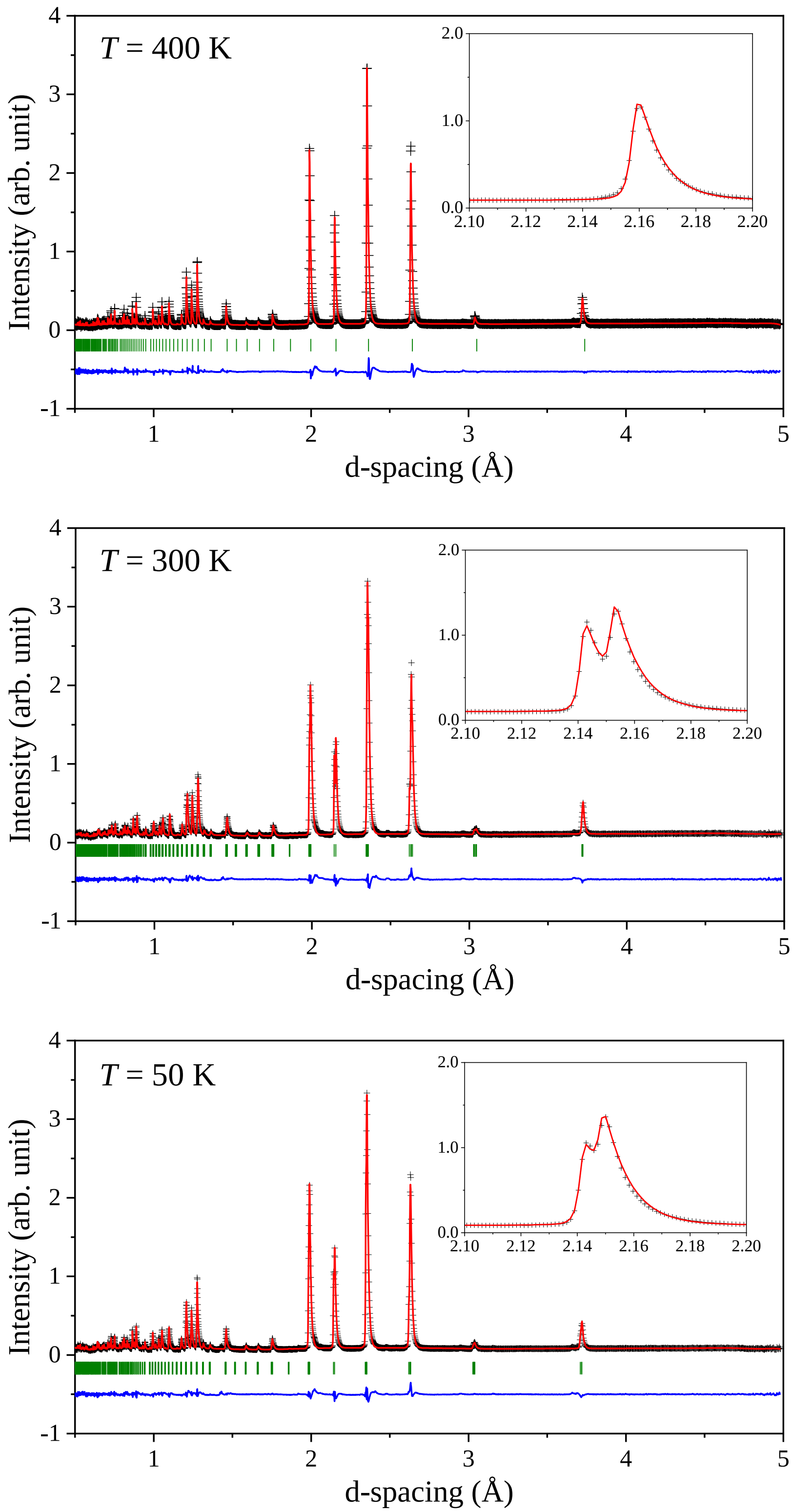

Figure S8. Experimental (crosses), calculated (red lines), and difference neutron diffraction patterns of $BiCu_{0.5}Mn_{6.5}O_{12}$ at 50 K (bottom, space group *I*2/*m*), 300 K (middle, space group *I*2/*m*), and 400 K (top, space group *Im*-3) after the Rietveld analysis (see Tables S1 and S2 for the refined structural parameters). Insets show zoomed details.

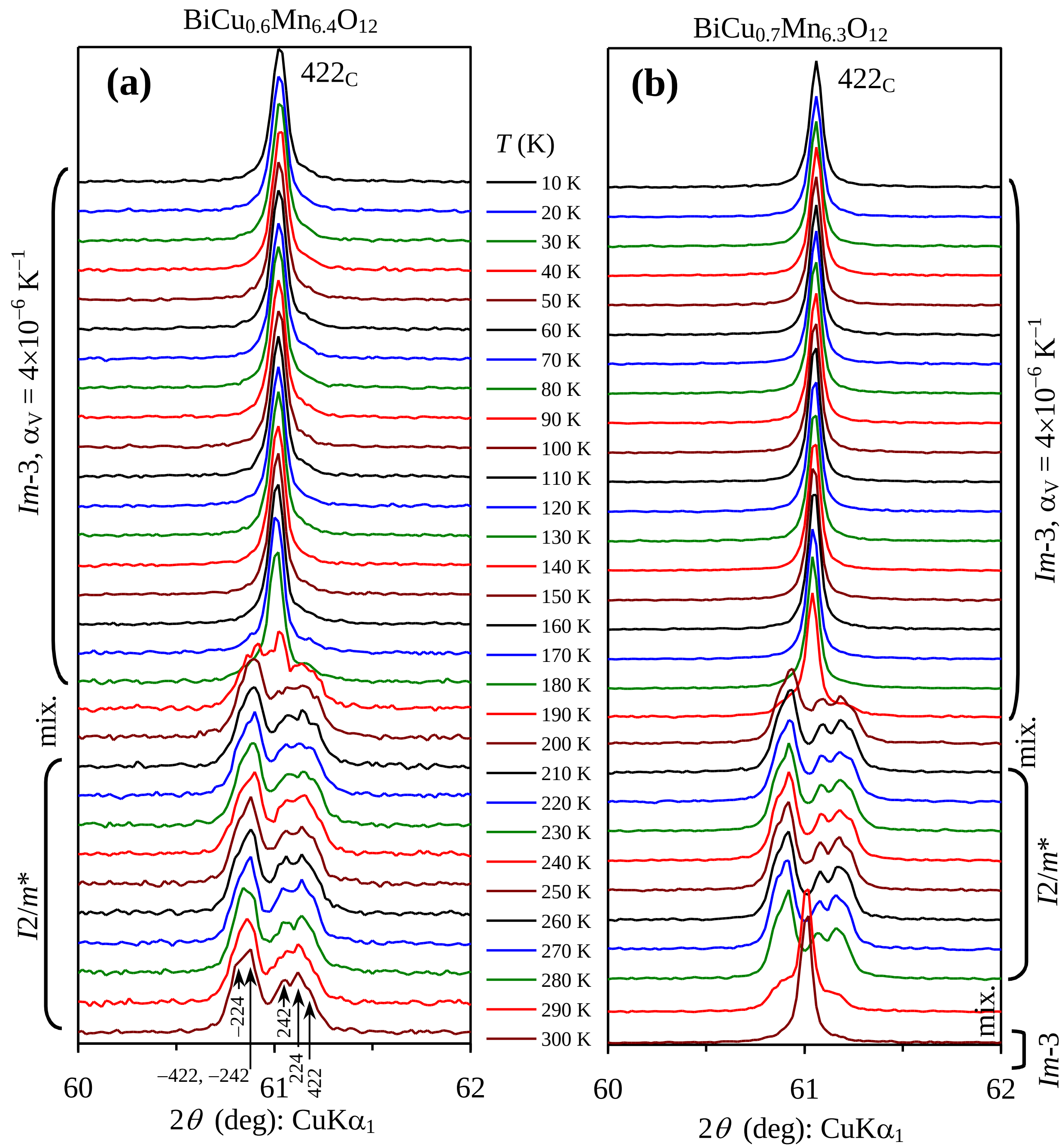

Figure S9. Low-temperature laboratory X-ray powder diffraction patterns of (a) $BiCu_{0.6}Mn_{6.4}O_{12}$ and (b) $BiCu_{0.7}Mn_{6.3}O_{12}$ between 10 K and 300 K with a step of 10 K. Fragments of diffraction patterns near the *422* cubic reflection (422_C) are shown. Reflection indexes for the monoclinic *I*2/*m* space group are given. Measurements were performed on heating.

α_V (= (1/V)*ΔV/ΔT) is the volumetric coefficient of thermal expansion for the low-temperature *Im*-3 cubic phase.

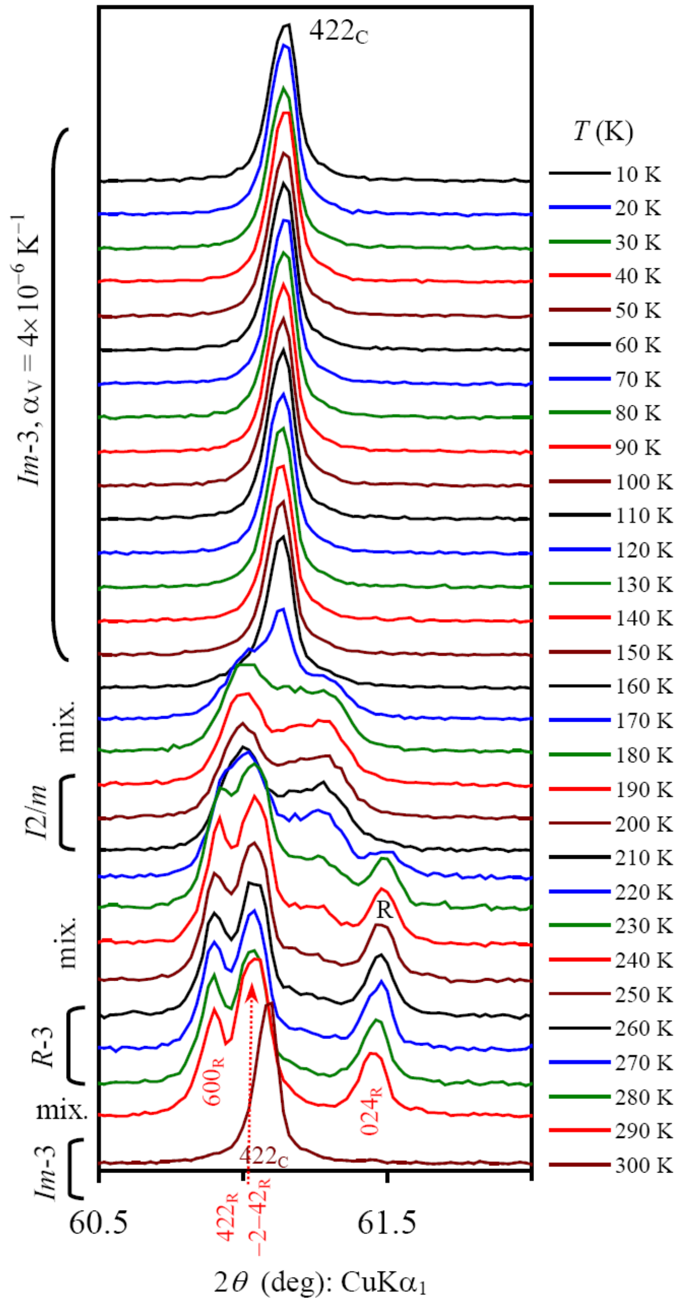

Figure S10. Low-temperature laboratory X-ray powder diffraction patterns of $BiCu_{0.8}Mn_{6.2}O_{12}$ between 10 K and 300 K with a step of 10 K. Fragments of diffraction patterns near the *422* cubic reflection (422_C) are shown. R denotes a characteristic reflection from the *R*-3 phase. Indexes of reflections for the *R*-3 phase are given. Measurements were performed on heating.

α_V (= (1/V)*ΔV/ΔT) is the volumetric coefficient of thermal expansion for the low-temperature *Im*-3 cubic phase.

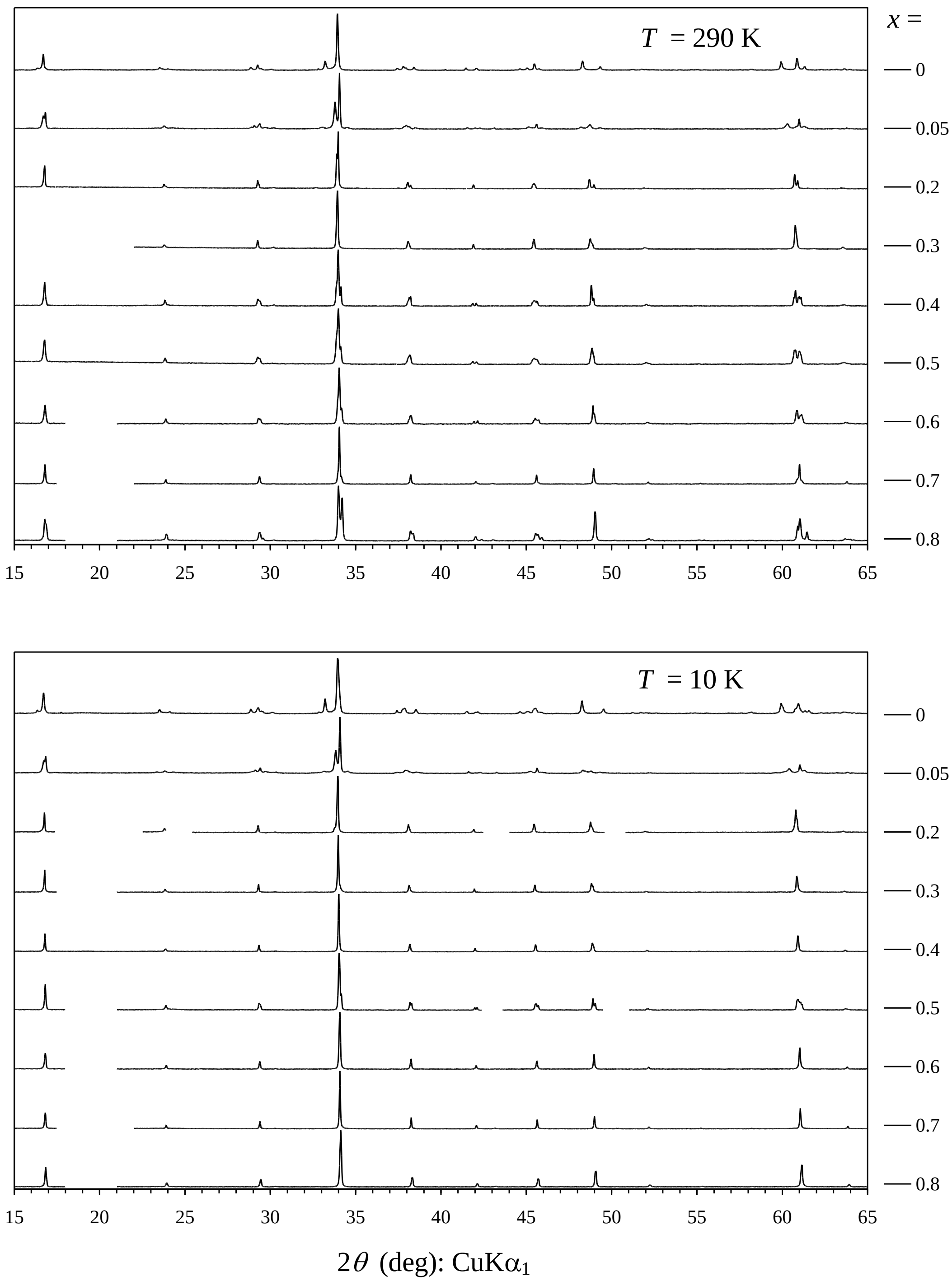

Figure S11a. Laboratory X-ray powder diffraction patterns of $BiCu_xMn_{7-x}O_{12}$ (a) at 290 K and (b) at 10 K. Regions containing artifact reflections (from grease and/or Cu holder) were removed.

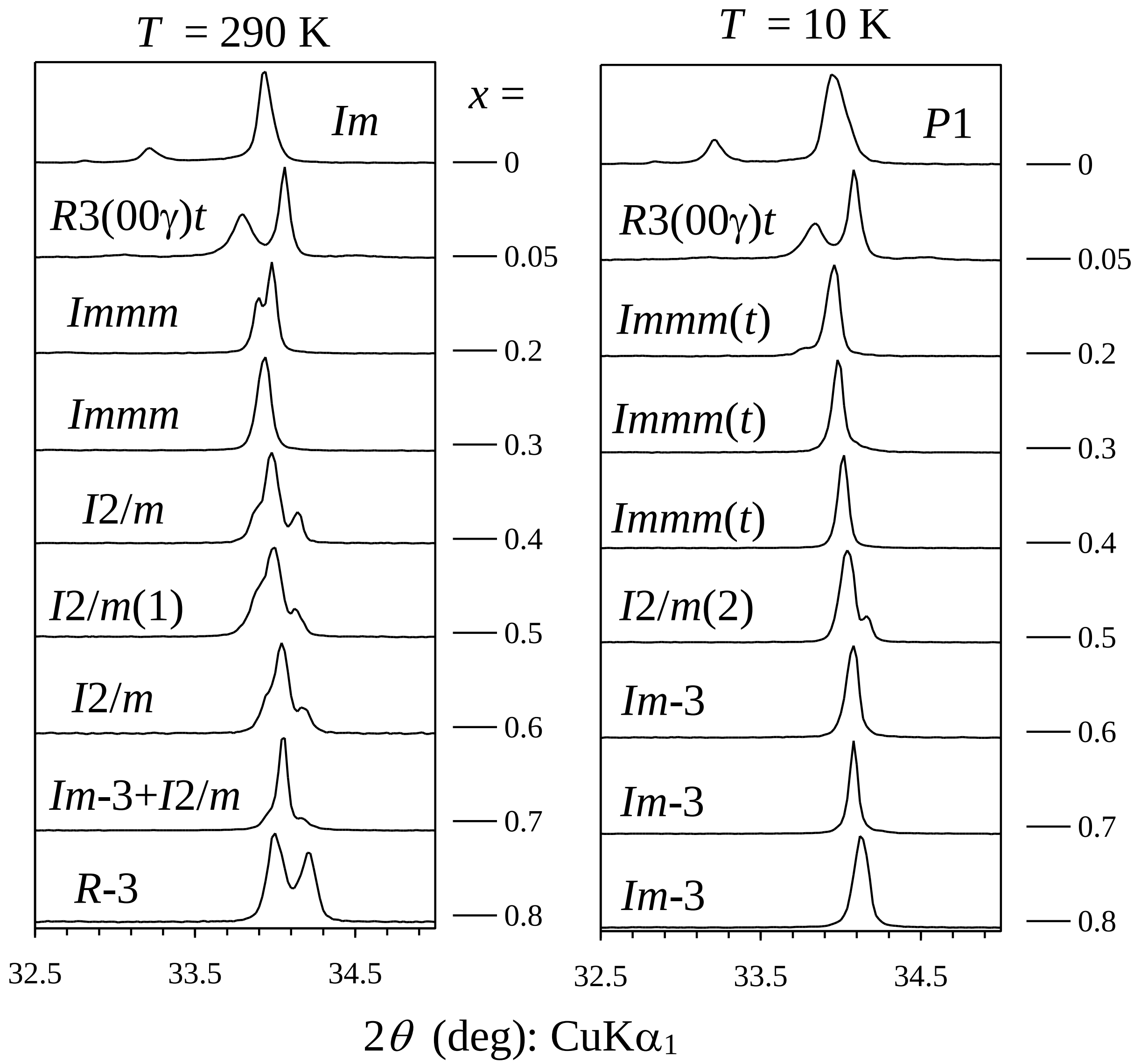

Figure S11b. Fragments of laboratory X-ray powder diffraction patterns of $BiCu_xMn_{7-x}O_{12}$ at 290 K (left) and at 10 K (right) near the strongest reflections.

Table S3 Temperature dependence of the lattice parameters in

$BiCu_{0.2}Mn_{6.8}O_{12}$ (space group *Immm*) from laboratory X-ray diffraction

T (K)	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
4	7.4524	7.4560	7.4385	413.323
10	7.4523	7.4548	7.4380	413.224
20	7.4516	7.4544	7.4377	413.144
30	7.4526	7.4559	7.4388	413.336
40	7.4528	7.4558	7.4387	413.342
50	7.4529	7.4556	7.4388	413.345
60	7.4522	7.4553	7.4383	413.260
70	7.4532	7.4558	7.4391	413.388
80	7.4537	7.4569	7.4396	413.507
90	7.4528	7.4551	7.4384	413.284
100	7.4539	7.4548	7.4390	413.362
110	7.4545	7.4554	7.4391	413.436
120	7.4534	7.4562	7.4388	413.405
130	7.4543	7.4575	7.4398	413.582
140	7.4538	7.4574	7.4394	413.531
150	7.4547	7.4573	7.4397	413.589
160	7.4552	7.4589	7.4401	413.724
170	7.4560	7.4601	7.4407	413.866
180	7.4560	7.4585	7.4399	413.733
190	7.4558	7.4588	7.4397	413.730
200	7.4562	7.4602	7.4397	413.831
210	7.4577	7.4620	7.4402	414.038
220	7.4578	7.4622	7.4394	414.019
230	7.4587	7.4634	7.4392	414.123
240	7.4592	7.4639	7.4379	414.097
250	7.4585	7.4628	7.4357	413.878
260	7.4599	7.4651	7.4353	414.062
270	7.4606	7.4655	7.4338	414.039
280	7.4616	7.4671	7.4330	414.139
290	7.4622	7.4685	7.4323	414.218
300	7.4618	7.4682	7.4300	414.046

$BiCu_{0.2}Mn_{6.8}O_{12}$ (space group *Immm* and *Im*-3) from laboratory X-ray diffraction

T (K)	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)	a_C (Å)	V_C (Å^3)
298	7.4642	7.4702	7.4293	414.245		
323	7.4655	7.4725	7.4284	414.400		
343	7.4663	7.4733	7.4291	414.529		
353	7.4665	7.4736	7.4298	414.593		
363	7.4667	7.4737	7.4307	414.660		
373	7.4669	7.4736	7.4317	414.726		
383	7.4672	7.4735	7.4329	414.800		
393	7.4672	7.4736	7.4342	414.879		
403	7.4673	7.4732	7.4356	414.943		
413	7.4676	7.4731	7.4374	415.054		
423	7.4674	7.4728	7.4388	415.102		
433	7.4674	7.4723	7.4404	415.163		

443	7.4677	7.4717	7.4425	415.269		
453	7.4677	7.4710	7.4444	415.335		
463	7.4676	7.4705	7.4466	415.421		
473	7.4678	7.4693	7.4489	415.489		
483	7.4678	7.4684	7.4517	415.598		
493	7.4673	7.4674	7.4543	415.663		
503	7.4663	7.4662	7.4579	415.740		
513	7.4643	7.4641	7.4632	415.807	7.4639	415.809
523					7.4643	415.873
533					7.4647	415.948
543					7.4651	416.015
553					7.4656	416.098
563					7.4661	416.177
573					7.4665	416.247
583					7.4670	416.331
593					7.4676	416.428
603					7.4680	416.501
613					7.4686	416.600
623					7.4691	416.680

$BiCu_{0.3}Mn_{6.7}O_{12}$ (space group *Immm*) from laboratory X-ray diffraction

T (K)	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å^3)
10	7.4518	7.4503	7.4461	413.391
20	7.4507	7.4501	7.4460	413.315
30	7.4504	7.4504	7.4458	413.301
40	7.4508	7.4520	7.4462	413.435
50	7.4510	7.4510	7.4462	413.392
60	7.4511	7.4510	7.4467	413.425
70	7.4519	7.4510	7.4469	413.486
80	7.4513	7.4516	7.4468	413.472
90	7.4522	7.4517	7.4470	413.540
100	7.4515	7.4513	7.4463	413.446
110	7.4518	7.4527	7.4470	413.573
120	7.4520	7.4520	7.4472	413.566
130	7.4532	7.4517	7.4475	413.628
140	7.4526	7.4525	7.4476	413.644
150	7.4524	7.4523	7.4472	413.597
160	7.4531	7.4527	7.4472	413.657
170	7.4518	7.4545	7.4481	413.736
180	7.4528	7.4542	7.4475	413.746
190	7.4532	7.4543	7.4478	413.792
200	7.4534	7.4542	7.4474	413.772
210	7.4535	7.4550	7.4475	413.826
220	7.4545	7.4559	7.4480	413.959
230	7.4542	7.4565	7.4475	413.951
240	7.4539	7.4578	7.4470	413.979
250	7.4548	7.4591	7.4465	414.070
260	7.4555	7.4605	7.4461	414.161
270	7.4566	7.4616	7.4459	414.273
280	7.4570	7.4620	7.4452	414.279

290	7.4566	7.4629	7.4441	414.248

$BiCu_{0.3}Mn_{6.7}O_{12}$ (space group *Immm* and *Im*-3) from laboratory X-ray diffraction

T (K)	a (Å)	b (Å)	c (Å)	V (Å^3)	a_C (Å)	V_C (Å^3)
303	7.4576	7.4643	7.4433	414.334		
313	7.4582	7.4645	7.4437	414.401		
323	7.4586	7.4649	7.4440	414.464		
333	7.4590	7.4651	7.4443	414.517		
343	7.4598	7.4655	7.4447	414.601		
353	7.4601	7.4655	7.4451	414.647		
363	7.4606	7.4656	7.4457	414.707		
373	7.4613	7.4657	7.4463	414.790		
383	7.4616	7.4655	7.4470	414.838		
393	7.4622	7.4651	7.4480	414.901		
403	7.4627	7.4650	7.4496	415.011		
413	7.4633	7.4638	7.4510	415.051		
423	7.4630	7.4635	7.4530	415.133		
428	7.4629	7.4631	7.4539	415.160		
433	7.4626	7.4628	7.4550	415.184		
438	7.4623	7.4624	7.4566	415.225		
443	7.4614	7.4616	7.4584	415.238		
448	7.4607	7.4607	7.4607	415.278	7.4607	415.274
453					7.4610	415.326
458					7.4611	415.340
463					7.4613	415.371
473					7.4617	415.441
483					7.4618	415.465
493					7.4622	415.532
503					7.4627	415.612
513					7.4630	415.654
523					7.4634	415.720
533					7.4637	415.771
543					7.4641	415.837
553					7.4646	415.928
563					7.4650	415.988
573					7.4655	416.077

$BiCu_{0.4}Mn_{6.6}O_{12}$ (space group *Immm*, *I*2/*m* and *Im*-3) from synchrotron X-ray diffraction data on heating

T (K)	a_M (Å)	b_M (Å)	c_M (Å)	β_M (deg)	V_M (Å^3)	a_C or a_O (Å)	c_O (Å)	Fraction of O or C	V_O or V_C (Å^3)
100						7.43583	7.44327	1	411.962
110						7.43600	7.44344	1	411.990
120						7.43614	7.44361	1	412.017
130						7.43626	7.44377	1	412.041
135						7.43632	7.44391	1	412.060
140						7.43643	7.44406	1	412.083
145						7.43653	7.44420	1	412.104
150						7.43659	7.44434	1	412.122
155						7.43660	7.44445	1	412.135

160						7.43669	7.44456	1	412.152
165						7.43676	7.44465	1	412.166
170						7.43698	7.44471	1	412.185
175						7.43717	7.44477	1	412.202
180						7.43730	7.44485	1	412.218
185						7.43740	7.44505	1	412.246
190	fixed at 195 K					7.43812	7.44490	0.88	412.269
195	7.42569	7.45151	7.44862	90.3705	412.143	7.43870	7.44482	0.77	412.293
200	7.42605	7.45128	7.44894	90.3644	412.168	7.43914	7.44502	0.62	412.339
205	7.42643	7.45092	7.44922	90.3657	412.185	7.43909	7.44538	0.48	412.376
210	7.42683	7.45073	7.44949	90.3692	412.211	7.43871	7.44596	0.35	412.419
215	7.42730	7.45055	7.44982	90.3735	412.245	7.43807	7.44704	0.24	412.503
220	7.42747	7.45056	7.45026	90.3782	412.280	fixed at 215 K		0.14	
225	7.42784	7.45054	7.45048	90.3819	412.311	fixed at 215 K		0.09	
230	7.42821	7.45051	7.45065	90.3854	412.339	fixed at 215 K		0.06	
240	7.42906	7.45048	7.45095	90.3902	412.401			0	
250	7.42984	7.45047	7.45132	90.3962	412.464			0	
260	7.43066	7.45042	7.45159	90.4009	412.521			0	
270	7.43155	7.45045	7.45192	90.4040	412.591			0	
280	7.43242	7.45049	7.45227	90.4062	412.660			0	
290	7.43330	7.45058	7.45252	90.4075	412.728			0	
300	7.43413	7.45069	7.45278	90.4075	412.795			0	
310	7.43497	7.45088	7.45302	90.4060	412.865			0	
320	7.43584	7.45116	7.45326	90.4031	412.942			0	
330	7.43670	7.45145	7.45343	90.3987	413.016			0	
340	7.43755	7.45183	7.45352	90.3918	413.089			0	
350	7.43832	7.45195	7.45341	90.3806	413.133			0	
360	fixed at 350 K					7.44848		0.84	413.241
370						7.44888		1	413.307
380						7.44927		1	413.372
400						7.45017		1	413.522
420						7.45105		1	413.668
440						7.45199		1	413.825
460						7.45304		1	414.000

$BiCu_{0.5}Mn_{6.5}O_{12}$ (space group *I*2/*m* and *Im*-3) from laboratory X-ray diffraction

T (K)	a_M (Å)	b_M (Å)	c_M (Å)	β_M (deg)	V_M (Å^3)
10	7.4230	7.4439	7.4404	90.276	411.124
20	7.4232	7.4442	7.4405	90.274	411.158
30	7.4235	7.4444	7.4408	90.274	411.201
40	7.4232	7.4443	7.4407	90.274	411.169
50	7.4233	7.4445	7.4409	90.275	411.201
60	7.4233	7.4447	7.4408	90.275	411.206
70	7.4237	7.4450	7.4413	90.276	411.272
80	7.4234	7.4447	7.4411	90.275	411.228
90	7.4236	7.4449	7.4410	90.273	411.244
100	7.4244	7.4455	7.4411	90.261	411.325
110	7.4245	7.4452	7.4405	90.249	411.279
120	7.4245	7.4450	7.4410	90.268	411.298
130	7.4232	7.4441	7.4434	90.344	411.308

140	7.4231	7.4436	7.4445	90.379	411.333
150	7.4237	7.4437	7.4455	90.397	411.432
160	7.4238	7.4432	7.4457	90.406	411.413
170	7.4243	7.4433	7.4460	90.413	411.465
180	7.4247	7.4433	7.4462	90.419	411.498
190	7.4252	7.4433	7.4463	90.424	411.527
200	7.4257	7.4434	7.4466	90.429	411.583
210	7.4265	7.4435	7.4469	90.429	411.647
220	7.4271	7.4434	7.4469	90.433	411.678
230	7.4279	7.4438	7.4472	90.433	411.759
240	7.4284	7.4437	7.4470	90.435	411.772
250	7.4295	7.4442	7.4478	90.434	411.902
260	7.4301	7.4445	7.4479	90.433	411.949
270	7.4306	7.4445	7.4479	90.432	411.983
280	7.4312	7.4448	7.4480	90.432	412.041
290	7.4322	7.4452	7.4488	90.428	412.164
300	7.4330	7.4455	7.4487	90.429	412.214
313	7.4340	7.4454	7.4486	90.420	412.262
323	7.4347	7.4458	7.4490	90.417	412.343
333	7.4354	7.4461	7.4494	90.411	412.427
343	7.4362	7.4465	7.4499	90.405	412.516
353	7.4368	7.4472	7.4500	90.397	412.596
363	7.4374	7.4475	7.4499	90.378	412.643
	a_C (Å)				V_C (Å^3)
373	7.4455				412.738
383	7.4459				412.808
393	7.4463				412.876
403	7.4468				412.959
413	7.4472				413.021
423	7.4476				413.101
433	7.4483				413.204
453	7.4492				413.354
463	7.4497				413.440
473	7.4502				413.524
483	7.4507				413.602
493	7.4511				413.683
503	7.4516				413.767
513	7.4523				413.872
523	7.4527				413.942

$BiCu_{0.6}Mn_{6.4}O_{12}$ (space group *Im*-3 and *I*2/*m*) from laboratory X-ray diffraction

T (K)	a_C (Å)	V_C (Å^3)	a_M (Å)	b_M (Å)	c_M (Å)	β_M (deg)	V_M (Å^3)	Fraction of M
10	7.4283	409.884						0
20	7.4284	409.912						0
30	7.4280	409.841						0
40	7.4281	409.851						0
50	7.4284	409.912						0
60	7.4288	409.967						0
70	7.4288	409.967						0
80	7.4290	409.999						0

90	7.4289	409.990						0
100	7.4287	409.962						0
110	7.4288	409.977						0
120	7.4290	410.012						0
130	7.4291	410.020						0
140	7.4294	410.070						0
150	7.4295	410.085						0
160	7.4296	410.105						0
170	7.4301	410.189						0
180	7.4302	410.202						0.23
190	7.4292	410.033	7.4189	7.4352	7.4349	90.394	410.109	0.77
200			7.4197	7.4353	7.4350	90.388	410.163	1
210			7.4205	7.4361	7.4355	90.395	410.274	1
220			7.4205	7.4361	7.4359	90.397	410.297	1
230			7.4206	7.4356	7.4354	90.402	410.245	1
240			7.4210	7.4360	7.4362	90.403	410.338	1
250			7.4218	7.4368	7.4367	90.403	410.455	1
260			7.4227	7.4370	7.4371	90.408	410.534	1
270			7.4234	7.4371	7.4370	90.398	410.578	1
280			7.4238	7.4372	7.4371	90.401	410.605	1
290			7.4246	7.4381	7.4376	90.398	410.730	1
300			7.4252	7.4382	7.4377	90.394	410.774	1

$BiCu_{0.7}Mn_{6.3}O_{12}$ (space group *Im*-3 and *I*2/*m*) from laboratory X-ray diffraction

T (K)	a_C (Å)	V_C (Å^3)	a_M (Å)	b_M (Å)	c_M (Å)	β_M (deg)	V_M (Å^3)	Fraction of M
10	7.4228	408.975						0
20	7.4230	409.021						0
30	7.4232	409.039						0
40	7.4226	408.950						0
50	7.4232	409.054						0
60	7.4232	409.047						0
70	7.4230	409.014						0
80	7.4235	409.095						0
90	7.4233	409.067						0
100	7.4237	409.130						0
110	7.4240	409.180						0
120	7.4239	409.156						0
130	7.4237	409.135						0
140	7.4238	409.151						0
150	7.4242	409.208						0
160	7.4239	409.163						0
170	7.4246	409.272						0
180	7.4246	409.275						0
190	7.4251	409.355	fixed at 200 K					0.21
200			7.4148	7.4309	7.4285	90.377	409.294	1
210			7.4150	7.4315	7.4289	90.389	409.357	1
220			7.4150	7.4316	7.4293	90.393	409.387	1
230			7.4158	7.4320	7.4297	90.393	409.470	1
240			7.4160	7.4320	7.4297	90.394	409.481	1
250			7.4170	7.4327	7.4306	90.393	409.624	1

260			7.4173	7.4326	7.4301	90.390	409.614	1
270			7.4184	7.4334	7.4308	90.382	409.752	1
280			7.4185	7.4330	7.4302	90.372	409.707	1
290	7.4287	409.960	7.4220	7.4340	7.4312	90.380	410.007	0.45
300	7.4284	409.899	fixed at 290 K					0.14

$BiCu_{0.8}Mn_{6.2}O_{12}$ (space group *Im*-3) from laboratory X-ray diffraction

T (K)	a_C (Å)	V_C (Å^3)
10	7.4156	407.792
20	7.4158	407.822
30	7.4161	407.868
40	7.4156	407.794
50	7.4160	407.860
60	7.4161	407.866
70	7.4157	407.809
80	7.4159	407.848
90	7.4163	407.899
100	7.4165	407.942
110	7.4164	407.919
120	7.4166	407.960
130	7.4167	407.969
140	7.4169	408.003
150	7.4172	408.050
160	7.4170	408.015

$BiCu_{0.8}Mn_{6.2}O_{12}$ (space group *Im*-3, *I*2/*m*, *R*-3 and *Im*-3) from synchrotron X-ray diffraction

T (K)	a_C (Å)	V_C (Å^3)	a_M (Å)	b_M (Å)	c_M (Å)	β_M (deg)	V_M (Å^3)	a_R (Å)	c_R (Å)	V_R (Å^3)	fraction of R
121	7.41654	407.947									0
138	7.41673	407.979									0
155	7.41691	408.008									0
172	7.41716	408.050									0
189	7.41757	408.117									0
206			7.40629	7.42404	7.42057	90.3943	408.0074				0
223			7.40662	7.42495	7.42160	90.4027	408.1318				traces
241			7.40794	7.42633	7.42316	90.4027	408.3662	10.52358	6.38191	612.0802	0.51
258			7.40997	7.42763	7.42490	90.3904	408.6460	10.52499	6.38317	612.3651	0.78
275			fixed at	258 K				10.52604	6.38461	612.6255	0.87
292	7.42260	408.948						10.52614	6.38629	612.7983	0.65
300	7.42367	409.125									0
300	7.42367	409.125									0
320	7.42460	409.279									0
330	7.42506	409.355									0
340	7.42551	409.429									0
360	7.42643	409.581									0
380	7.42735	409.734									0
400	7.42830	409.891									0
420	7.42932	410.060									0
440	7.43040	410.239									0