Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information for

Mullite-derivative $Bi_2Mn_xAl_{7-x}O_{14}$ ($x \sim 1$): Structure determination by powder X-ray diffraction from a multi-phase sample

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Table S1. Atomic ratio of Bi:Mn:Al in sample **A** from EDS.

Spot Number	Bi	Mn	Al
1	1.77	1.07	5.93
2	1.52	0.81	6.19
3	1.73	0.89	6.11
4	1.76	1.16	5.84
5	1.60	0.95	6.05
6	1.74	1.58	5.42
7	1.64	1.03	5.97
8	1.47	1.02	5.98
9	1.67	0.86	6.14
10	1.79	1.05	5.95
11	1.73	0.80	6.20
12	1.88	1.02	5.98
13	1.89	1.03	5.97
14	1.71	0.86	6.14
15	1.69	0.90	6.10
16	1.68	0.98	6.02
17	1.73	1.06	5.94
18	1.62	1.00	6.00
Average	1.70	1.00	6.00

Table S2. Cell parameters of mullite phases and $Bi_2Mn_xAl_{7-x}O_{14}$.

	Space Group	*a* / Å	*b* / Å	*c* / Å
$Bi_2Al_4O_9$	*Pbam*	7.71	8.11	5.69
$Bi_2Mn_4O_{10}$	*Pbam*	7.54	8.53	5.77
$Bi_2Mn_xAl_{7-x}O_{14-\delta}$	*Pbam*	7.60	8.21	8.54

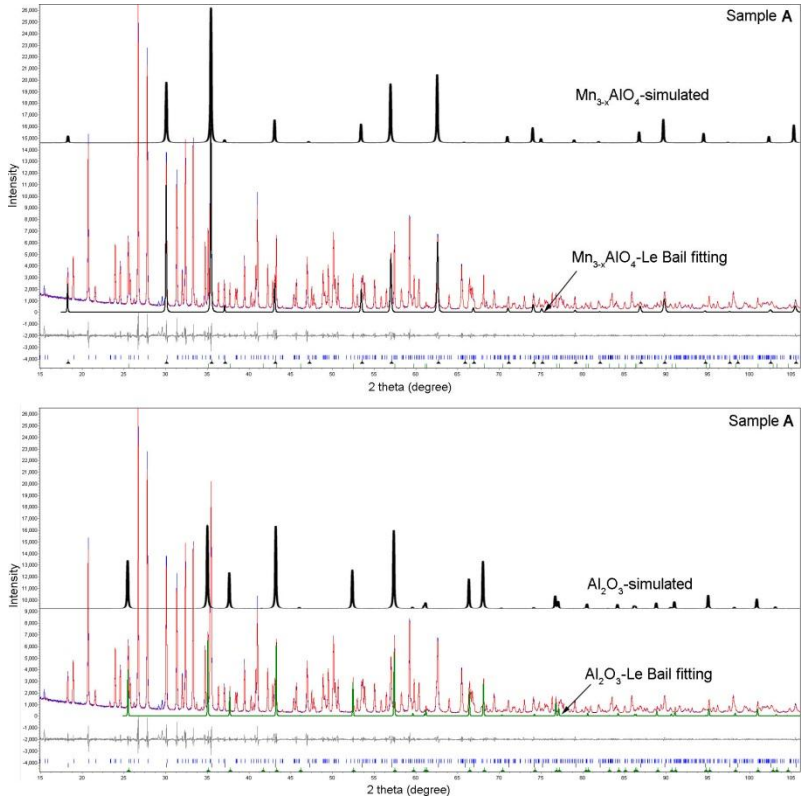

Fig. S1 The comparison of the simulated intensities (according to reported structure information) and extracted intensities by usual Le Bail fitting on sample **A**.

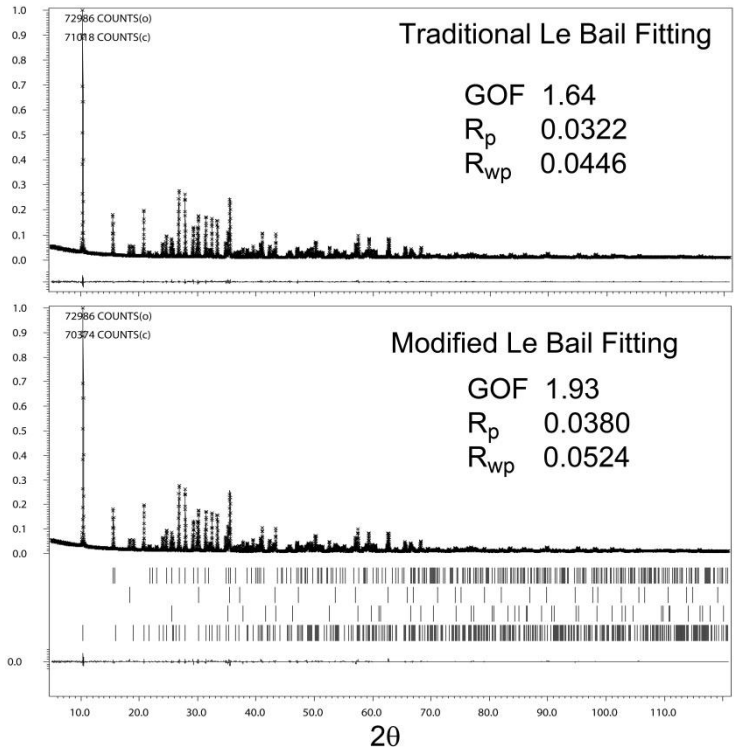

Fig. S2. A comparison of the traditional and modified Le Bail fitting on sample **B**. The marks below the diffraction patterns from up to bottom are the expected reflection positions for Mullite, $Mn_{3-x}AlO_4$, Al_2O_3 and $Bi_2Mn_xAl_{7-x}O_{14}$, respectively.

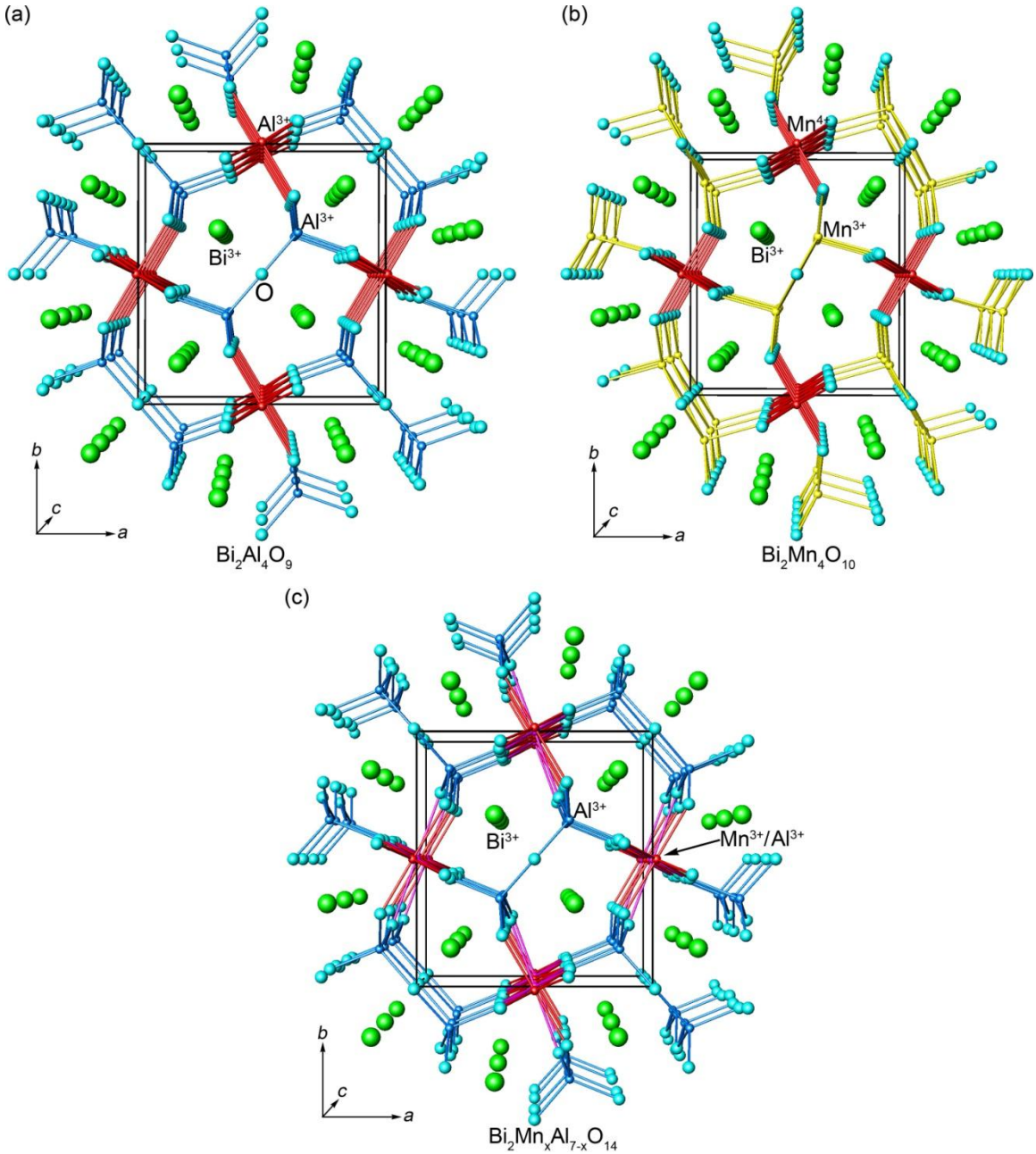

Fig. S3. Projected structure views along the *c*-direction of mullite phase and $Bi_2Mn_xAl_{7-x}O_{14}$.

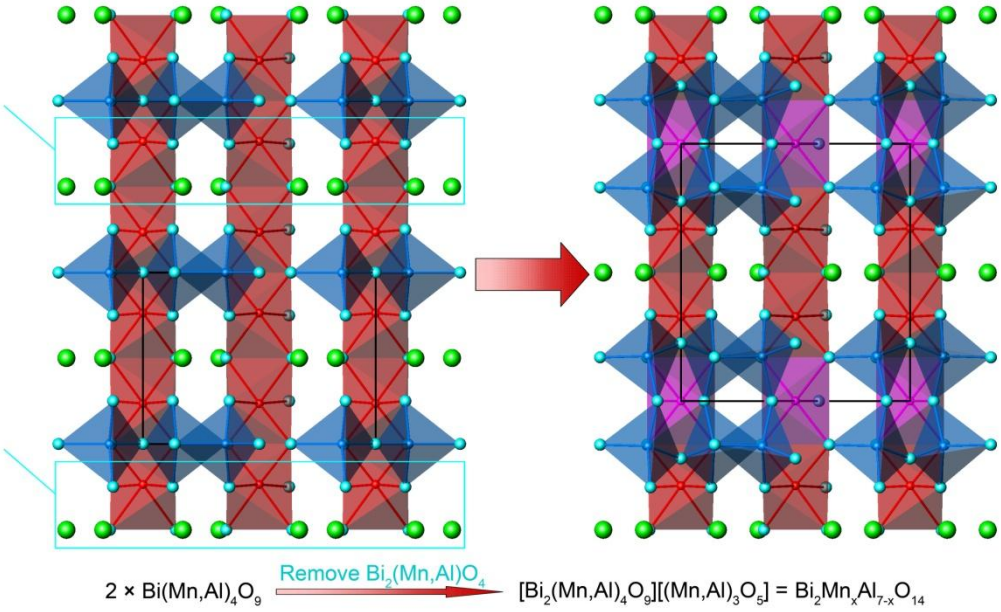

Fig. S4. Scheme of the formation of $Bi_2Mn_xAl_{7-x}O_{14}$ from the decomposition of mullite-$Bi_2(Mn,Al)_4O_9$.