Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information (ESI)

We performed energy minimisation, geometry optimisation and cell optimisation calculations in the final glass structure at 300 K in order to calculate the residual pressure in our glass models and determine its effect on the final cell volume. The results shown in Table S1 indicate that relaxation of the cell has an effect on the density of the MCNB glass but the difference is comparable to the DFT error. The results shown in Table S2 indicate almost no difference in the final glass volume after relaxation for the MLNB composition.

Table S1 Calculation of the pressure and the volume of the cell for the MCNB glass structure before and after relaxation.

Type of calculation	Residual pressure (kbar)	Cell volume ($Å^3$)
Energy minimisation	-17.75	2715.87
Geometry optimisation	-8.68	2715.87
Cell & geometry optimisation	0.05	2671.59

Table S2 Calculation of the pressure and the volume of the cell for the MLNB glass structure before and after relaxation.

Type of calculation	Residual pressure (kbar)	Cell volume ($Å^3$)
Energy minimisation	-4.57	2687.36
Geometry optimisation	-2.98	2687.36
Cell & geometry optimisation	0.04	2678.48