

Electronic Supplementary Information

An investigation of Al₂O₃ induced variations in the structural parameters in strontium borosilicate glasses using solid state NMR

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Table – S1: Radius of oxide ions and modifier atom ¹⁻³

Oxide ions	Radius (Å)
SrO	1.4
AlO ₆	1.4
AlO ₅	1.334
AlO ₄	1.437
BO ₄	1.204
BO ₃	1.187
SiO ₄	1.306
Sr ⁺² ion in SrO	1.18
Al ⁺³ ion in AlO ₆	0.535

Table – S2: Molar volume and oxygen number density of the glass samples

Glass Code	Molar Volume (cc/mol)	Oxygen number Density (Angstrom ⁻³)
SBS	24.97	0.0523
SABS 5	25.44	0.051

SABS 10	25.76	0.0499
SABS 15	25.94	0.0492
SABS 20	26.69	0.0474
SABS 25	27.31	0.046
SABS 30	27.79	0.0448

Calculation of Oxygen packing fraction

The oxygen packing fraction is calculated using Equation 2. The details of the calculation of the oxygen packing fraction of one of the glass materials are explained below. In the case of SBS, the V_o in Equation 2 is calculated as,

$$V_o = \frac{4}{3}\pi \frac{F_{BO_3} C_{BO_3} r_{BO_3}^3 + F_{BO_4} C_{BO_4} r_{BO_4}^3 + F_{SiO_4} C_{SiO_4} r_{SiO_4}^3}{F_{BO_3} C_{BO_3} + F_{BO_4} C_{BO_4} + F_{SiO_4} C_{SiO_4}}$$

Where F_{BO_3} , F_{BO_4} , and F_{SiO_4} are the fraction of BO_3 , BO_4 and SiO_4 respectively and C_{BO_3} , C_{BO_4} and C_{SiO_4} are the coordination number and r_{BO_3} , r_{BO_4} , r_{SiO_4} are the radii of the BO_3 , BO_4 and SiO_4 units respectively. The ρ_o is calculated by using Equation No. 1. The $V_M \rho_M$ of the modifier atom (in these case Sr) is further calculated by Equation 5.

$$V_M \rho_M = \frac{4}{3}\pi r_{Sr^{2+}}^3 + \rho_{Sr}$$

Where $r_{Sr^{2+}}$ is the radii of the Sr^{2+} in the SrO and ρ_{Sr} is the number density of the Sr atoms. In the case of Al incorporated samples, AlO_5 and AlO_6 were also included in the calculation of $V_M \rho_M$. The ρ_{Sr} can be calculated using the following equation.

$$\rho_{Sr} = \frac{N_{Sr} N_{avo}}{V_m}$$

N_{Sr} is the number of Sr atoms in the composition, calculated from the molecular formula. N_{avo} is the Avogadro number, and V_m is the molar volume

¹¹B deconvolution procedure

The quadrupolar coupling constant (Cq) and asymmetric constant (η) value of the different borate species are deduced from the fitting of the ^{11}B MQMAS spectra (shown in Fig S1). These parameters are used for deconvoluting the ^{11}B MAS spectra. The consistency in the

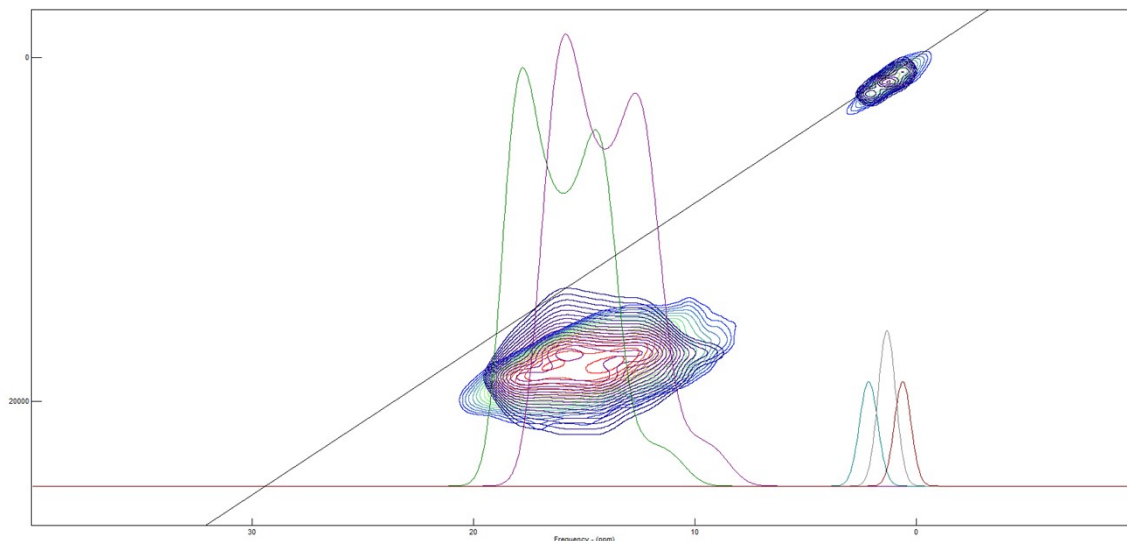


Fig. S1. ^{11}B MQMAS NMR spectra of SABS 30 fitted with two components for the BO_3 species and three for the BO_4 species.

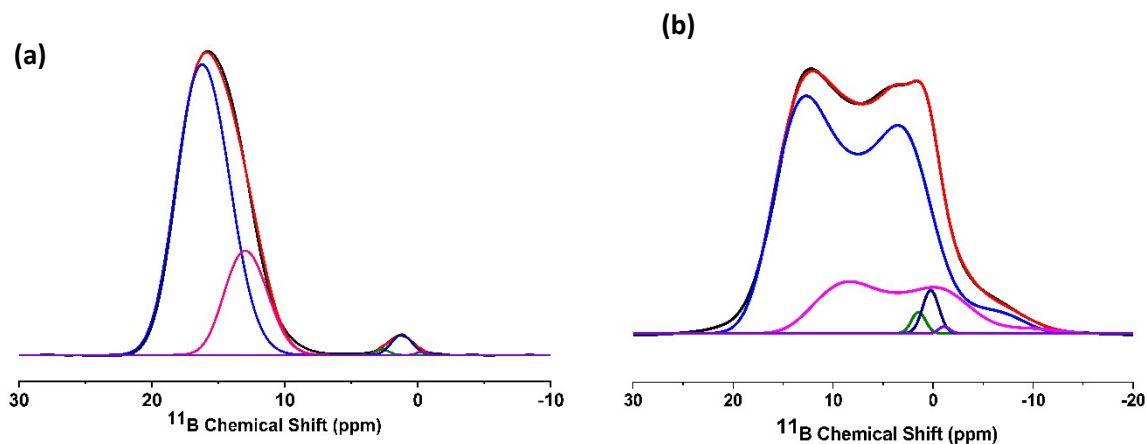


Fig. S2. ^{11}B MAS NMR spectra of SABS 30 (Black, Experimental; Red, Fitted) recorded at (a) 16.5T and (b) 9.4T accompanied by its components (Blue, ^{3}B (non-ring); Magenta, ^{3}B (ring); Green, ^{4}B (0B, 4Si); Indigo, ^{4}B (1B,3Si); Violet; ^{4}B (2B,2Si)) derived from deconvolution.

fitting parameters were further checked by deconvoluting the spectra recorded at different field strengths. The deconvoluted spectra of SABS 30 recorded at two field strengths (16.5T and 9.4T

are given in Fig S2. The deconvolution of the spectra from both field strengths gives the same values for the parameters Cq and η for B (III) and B (IV) units. However, the percentage of occupancy of these species is different in both cases. It is observed that the 2.5mm triple resonance probe of the Bruker 700MHz (16.5T) spectrometer gives a background signal which leads to the wrong estimation of the percentage of occupancy of the B (III) and the B (IV) units. Thus the ^{11}B NMR data from Jeol 400 MHz (9.4T) has been used for the deconvolution and the quantitative estimation of different sites.

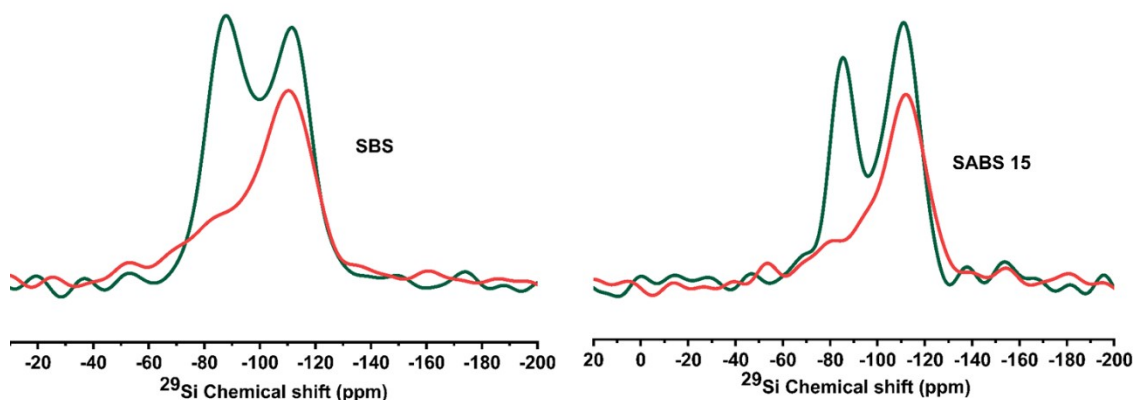


Fig. S2 ^{29}Si static (Red) and MAS NMR (Green) of SBS and SABS 15 glasses

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