Supporting Information

Combined Experimental and Computational Approach toward the Structural Design of Borosilicate-Based Bioactive Glasses

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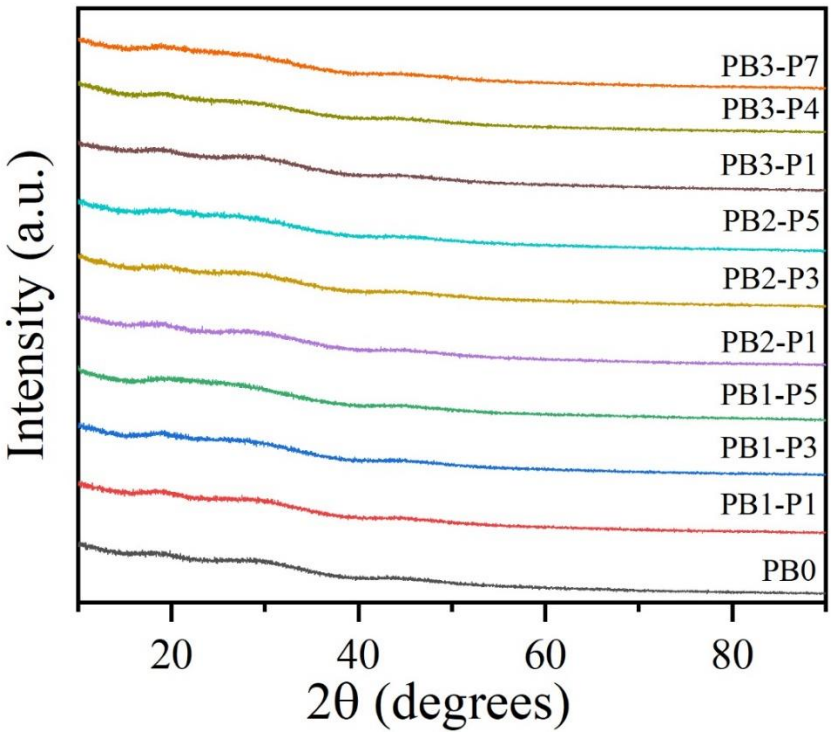
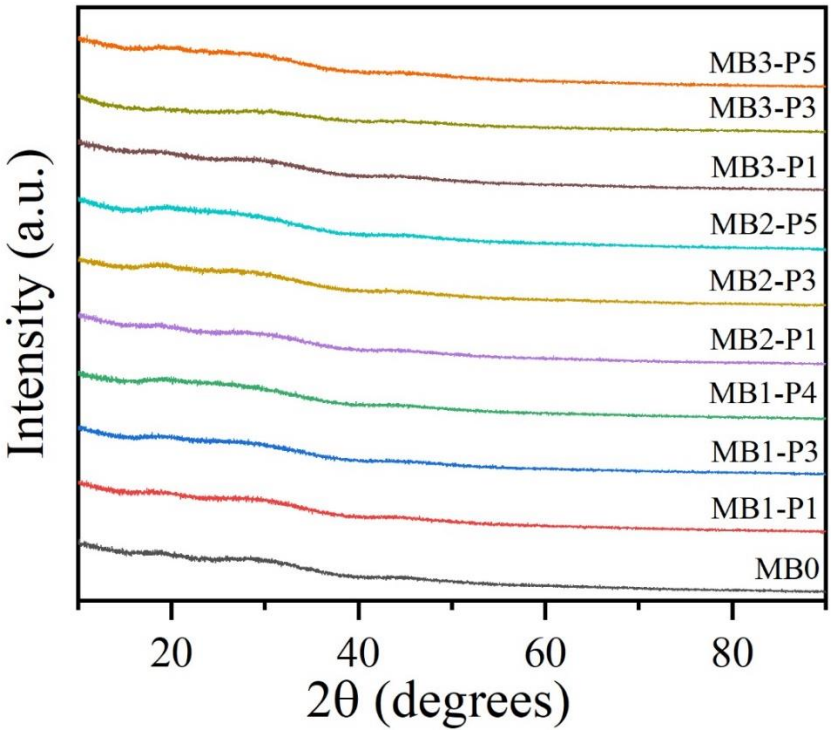
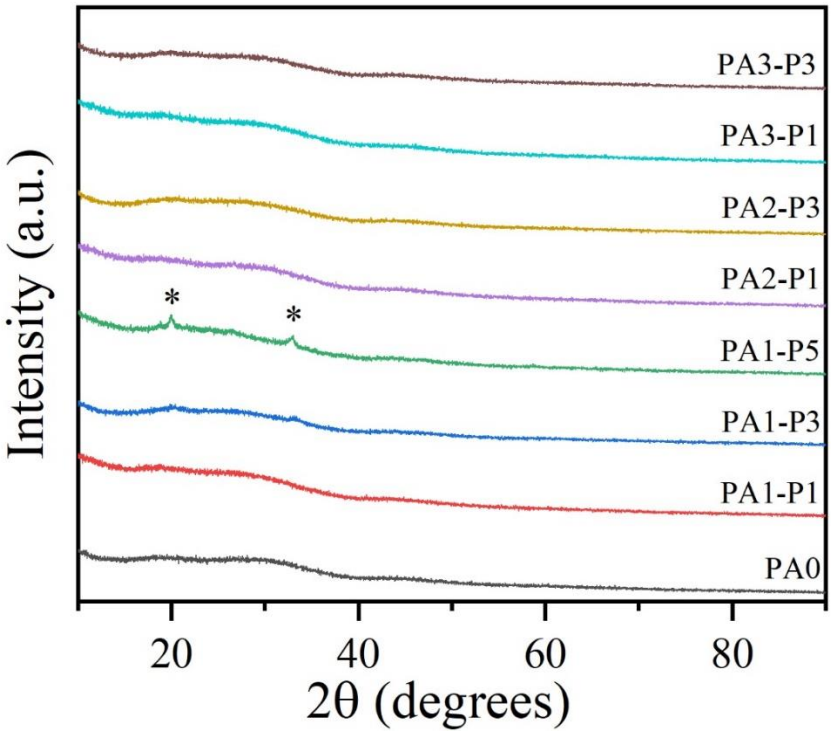
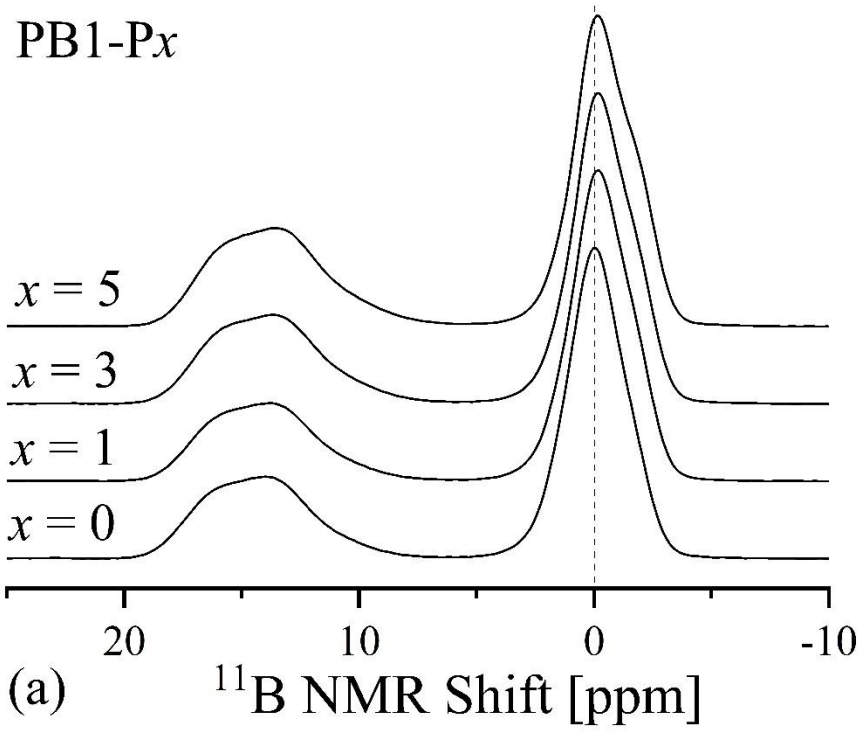

PB3-P7
PB3-P4
PB3-P1
PB2-P5
PB2-P3
PB2-P1
PB1-P5
PB1-P3
PB1-P1
PB0
Intensity (a.u.)
20
40
60
80
2θ (degrees)

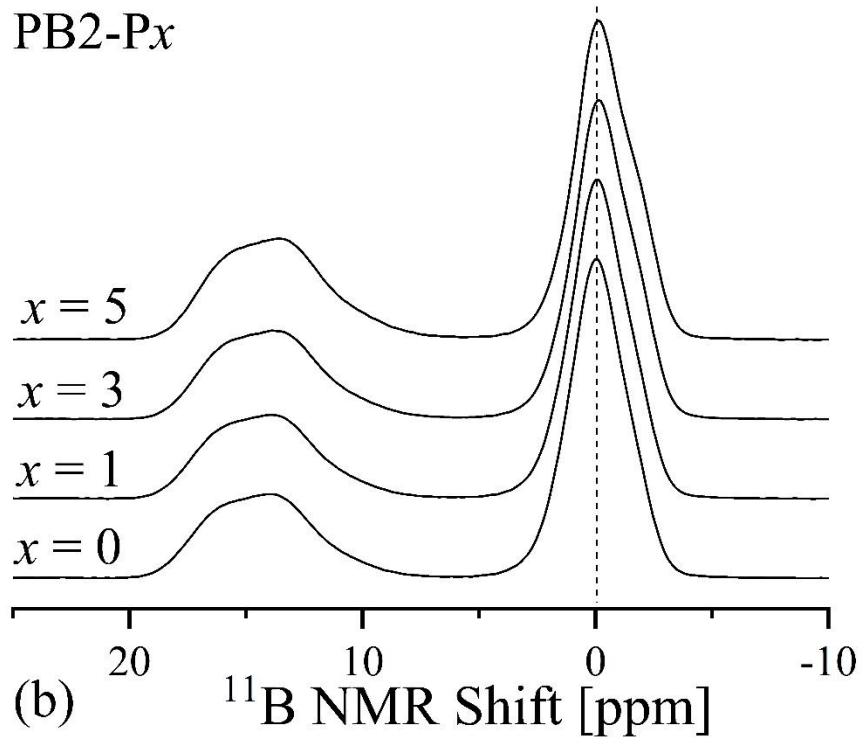

MB3-P5
MB3-P3
MB3-P1
MB2-P5
MB2-P3
MB2-P1
MB1-P4
MB1-P3
MB1-P1
MB0
Intensity (a.u.)
20
40
60
80
2θ (degrees)



* XRD peaks associated with tetrasodium diphosphate crystals

Figure S1. X-ray diffraction patterns of PB, MB, and PA glass compositions, respectively. All samples shown, with the exception of PA1-P5, were used in this study due to their amorphous / visibly transparent nature. PA1-P5 displays an example of a glass which developed crystalline phases upon quenching, as was seen in all $x = 5$ PA glasses.


PB1-Px
$x = 5$
$x = 3$
$x = 1$
$x = 0$
20
10
0
-10
(a)
^{11}B NMR Shift [ppm]


PB2-Px
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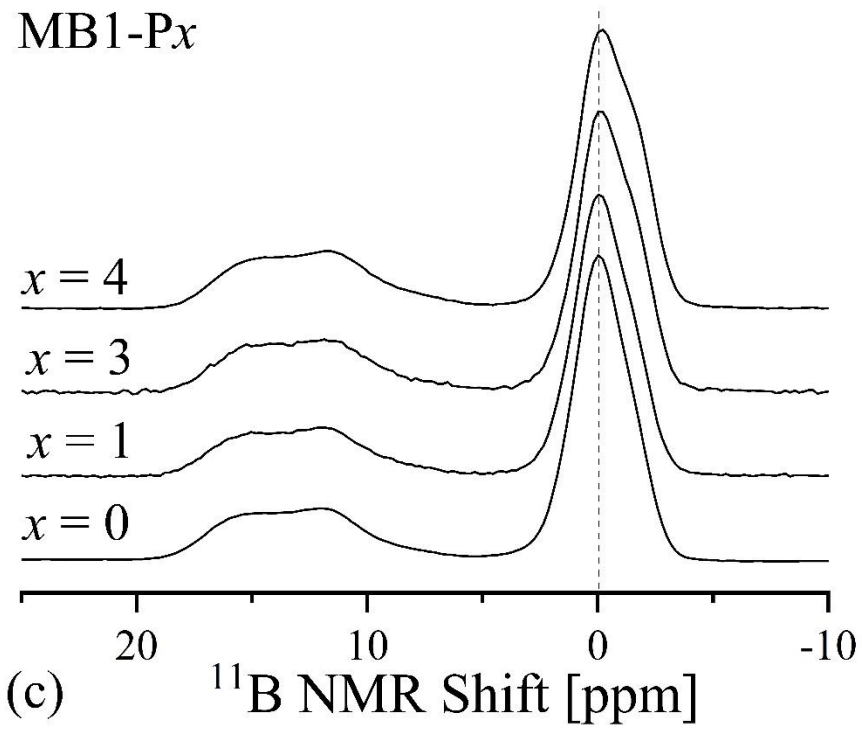
$x = 3$
$x = 1$
$x = 0$
20
10
0
-10
(b)
^{11}B NMR Shift [ppm]


MB1-Px
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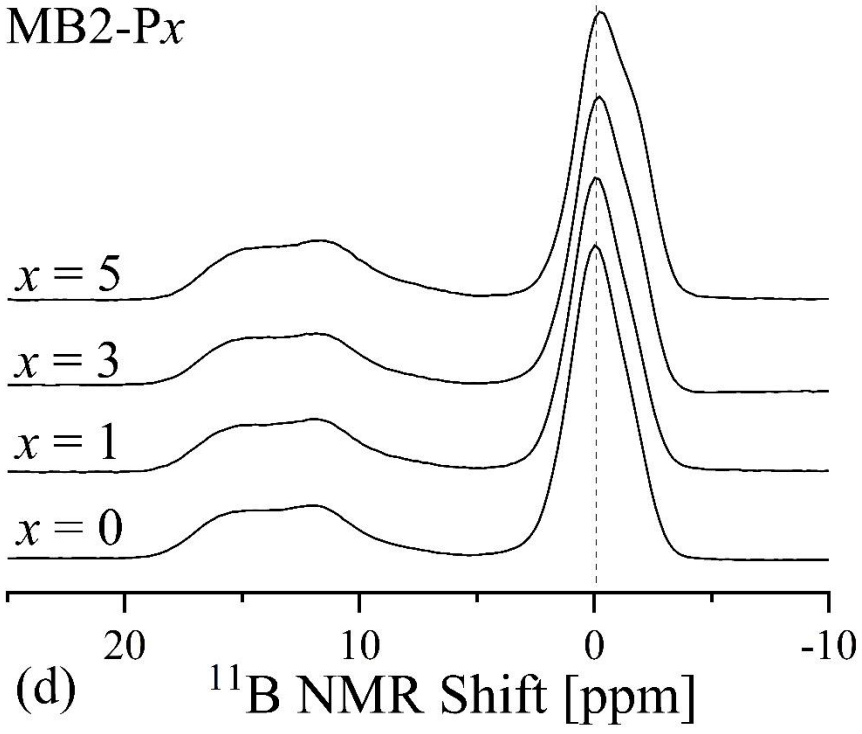
x = 3
x = 1
x = 0
20
10
0
-10
(c)
^{11}B NMR Shift [ppm]


MB2-Px
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x = 3
x = 1
x = 0
20
10
0
-10
(d)
^{11}B NMR Shift [ppm]

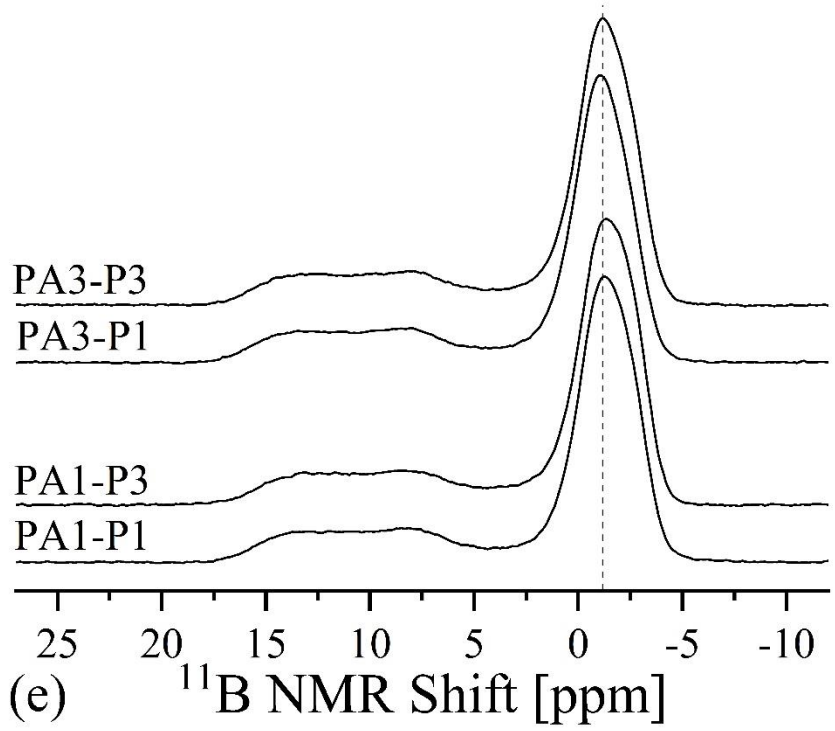
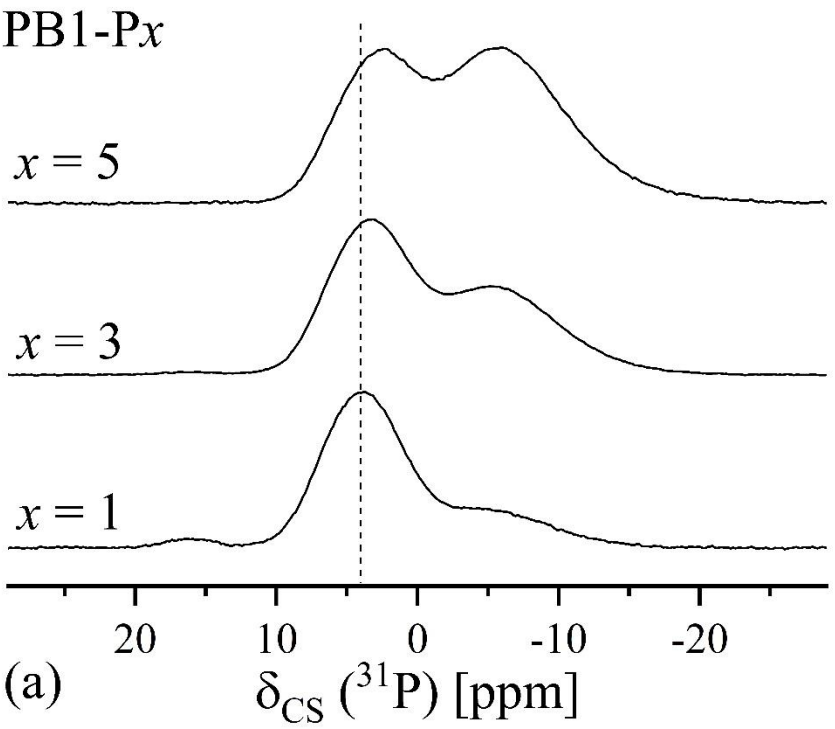
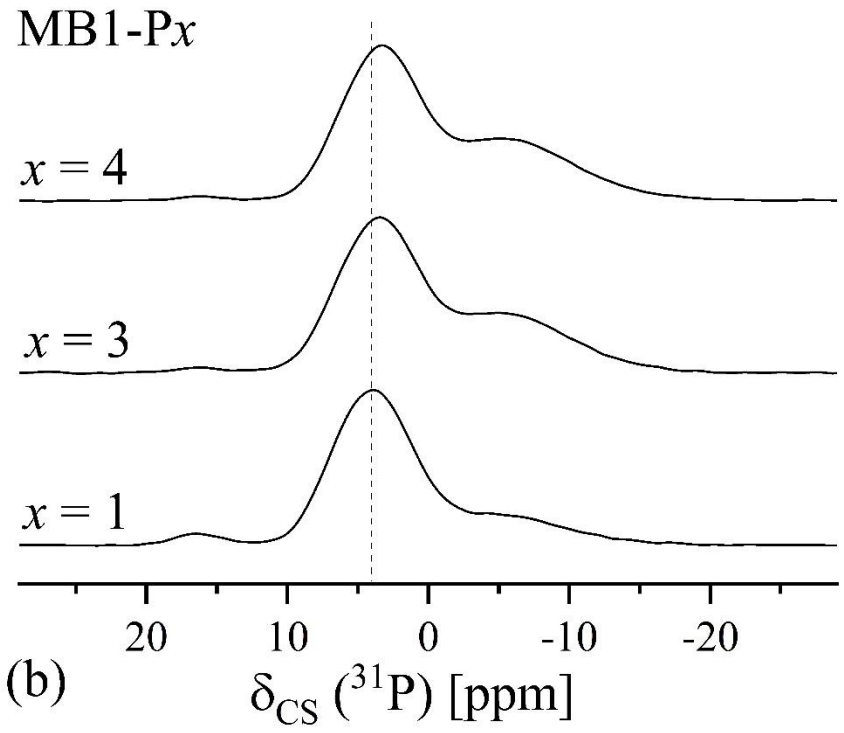
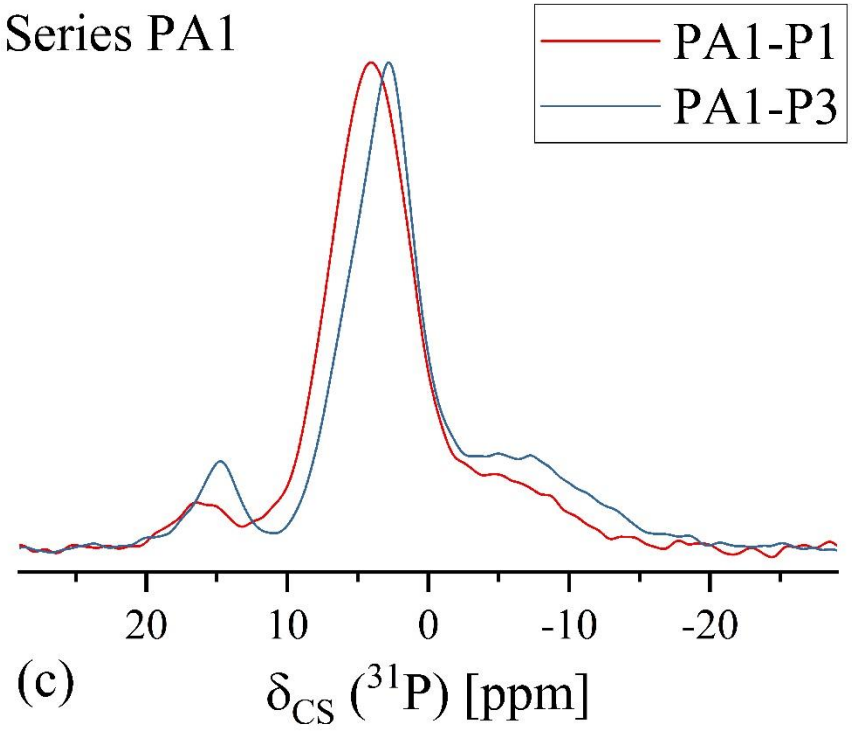


Figure S2. ^{11}B MAS NMR spectra of all Series "1" and "2" glasses in the perboric and metaboric regimes, in addition to Series "1" and "3" in the peralkaline regime. Spectra on the perboric, metaboric, and peralkaline glasses were collected at 16.4 T, 14.1 T, and 11.7 T, respectively.




MB1-Px
x = 4
x = 3
x = 1
20
10
0
-10
-20
(b)
δCS (31P) [ppm]


Series PA1
PA1-P1
PA1-P3
20
10
0
-10
-20
(c)
δCS (31P) [ppm]

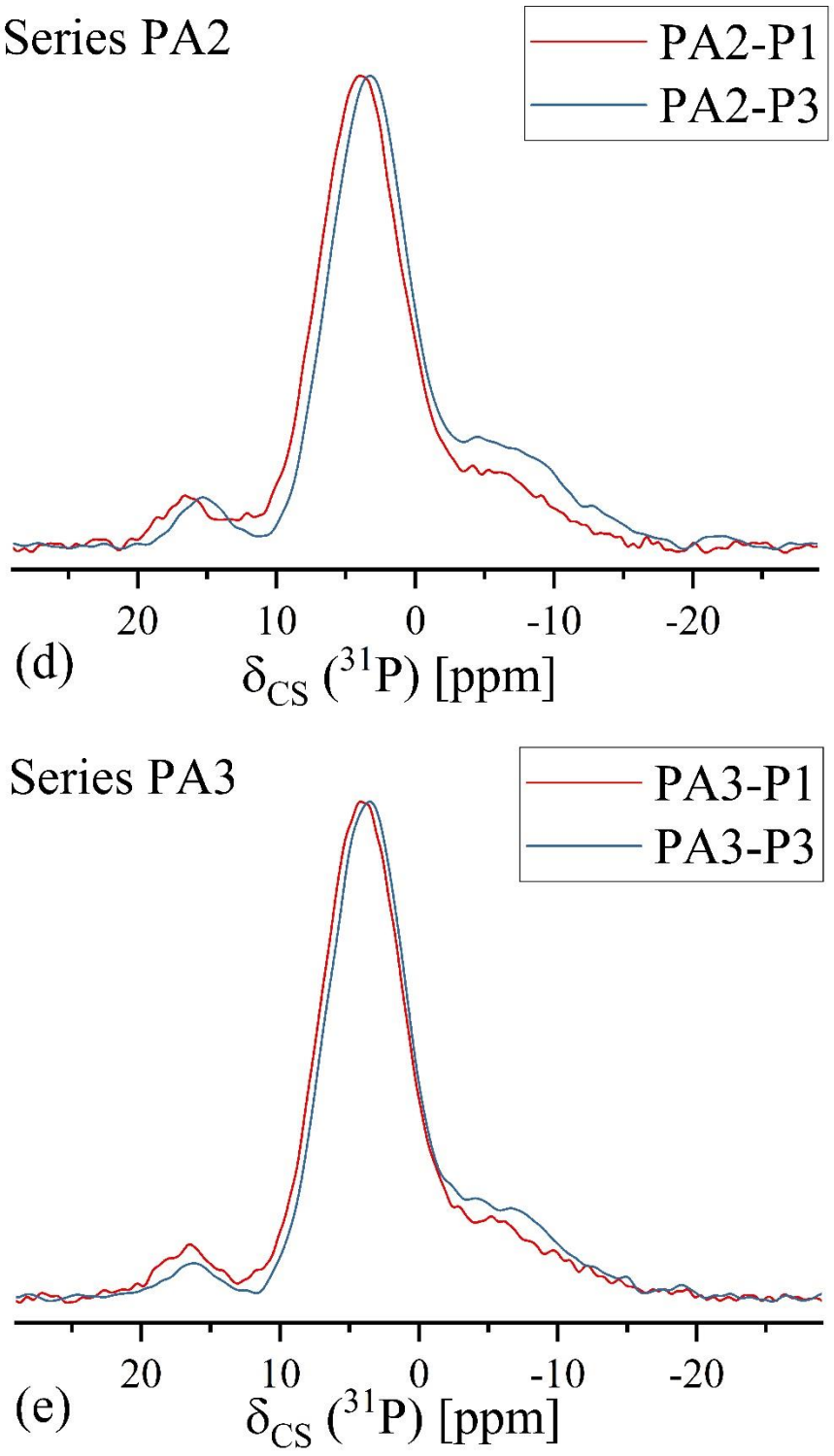


Figure S3. ^{31}P MAS NMR spectra of Series "1" PB and MB samples and all PA samples.

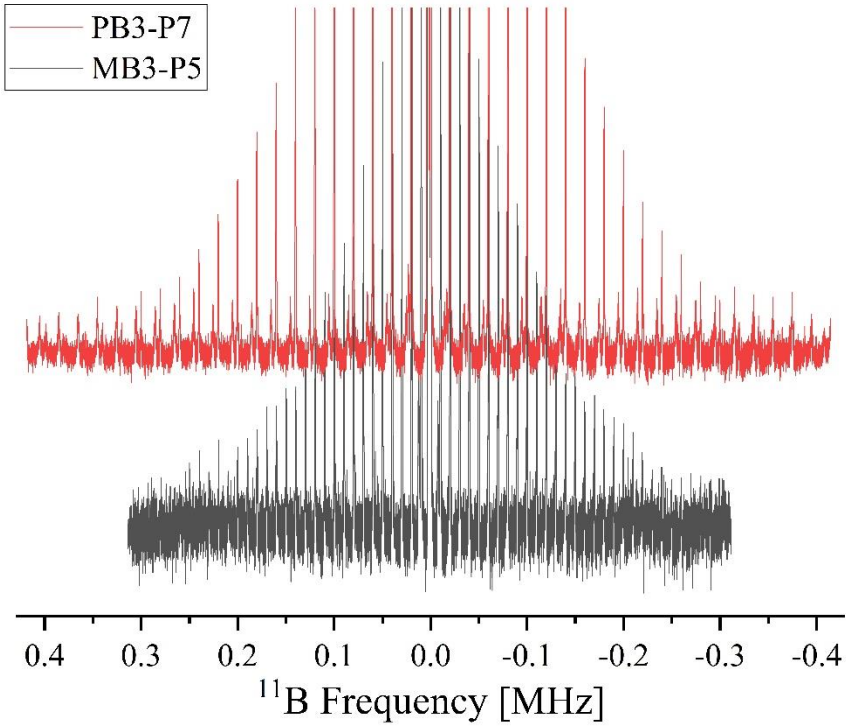
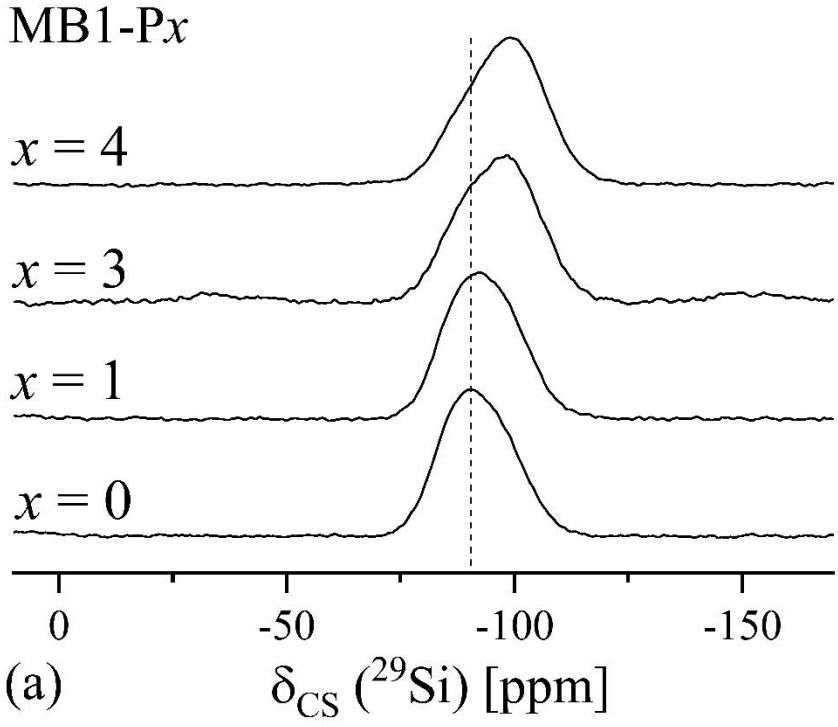
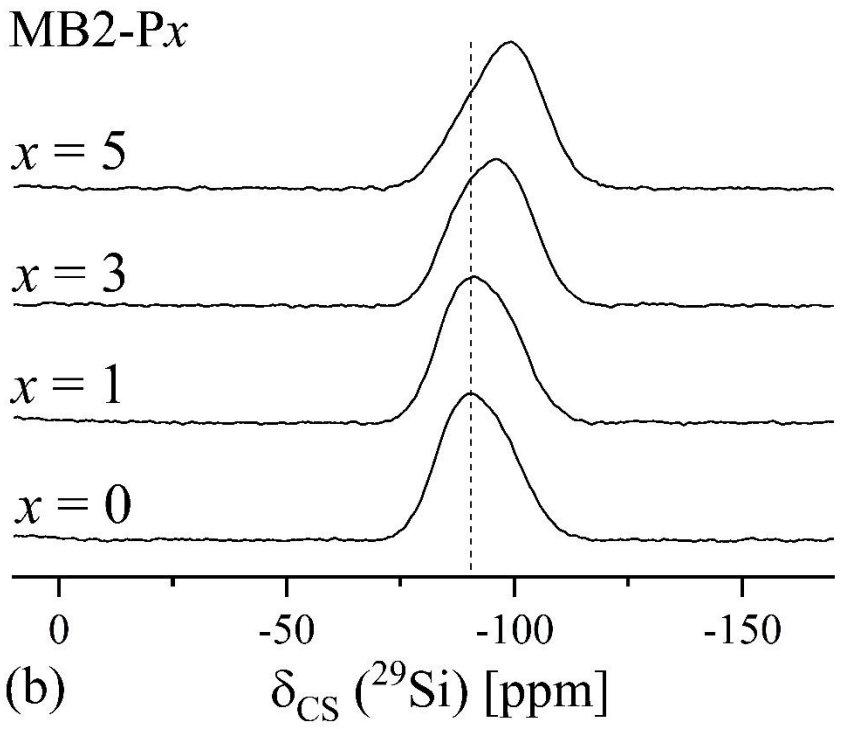
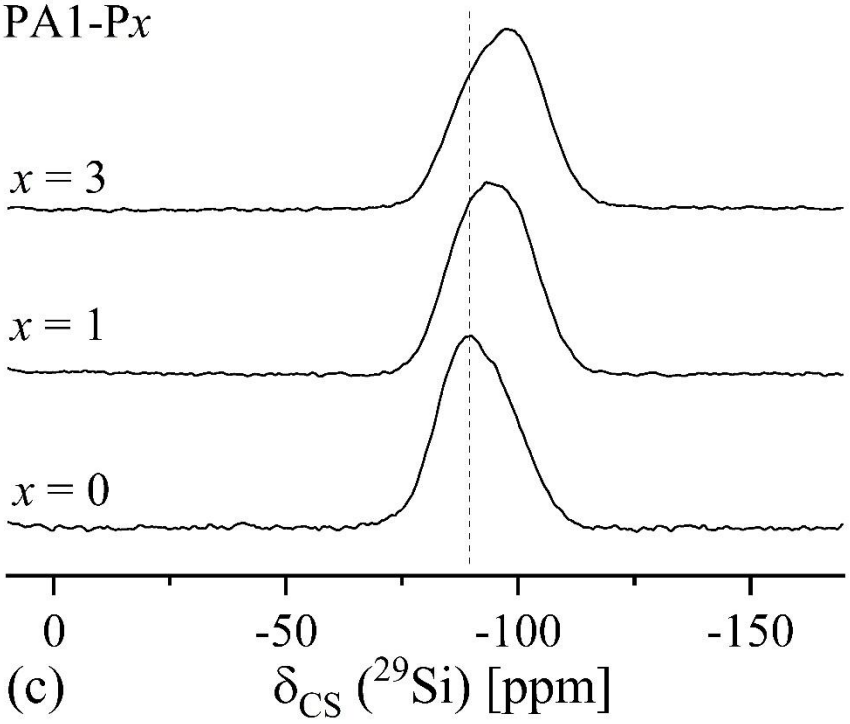


Figure S4. Overall spectral range of ^{11}B MAS NMR spectra of PB3-P7 and MB3-P5 samples, which was used to estimate ^{11}B quadrupolar coupling constants, based on the spinning sideband pattern of the satellite transition.




MB2-Px
x = 5
x = 3
x = 1
x = 0
0
-50
-100
-150
(b)
δCS (29Si) [ppm]


PA1-Px
x = 3
x = 1
x = 0
0
-50
-100
-150
(c)
δCS (29Si) [ppm]

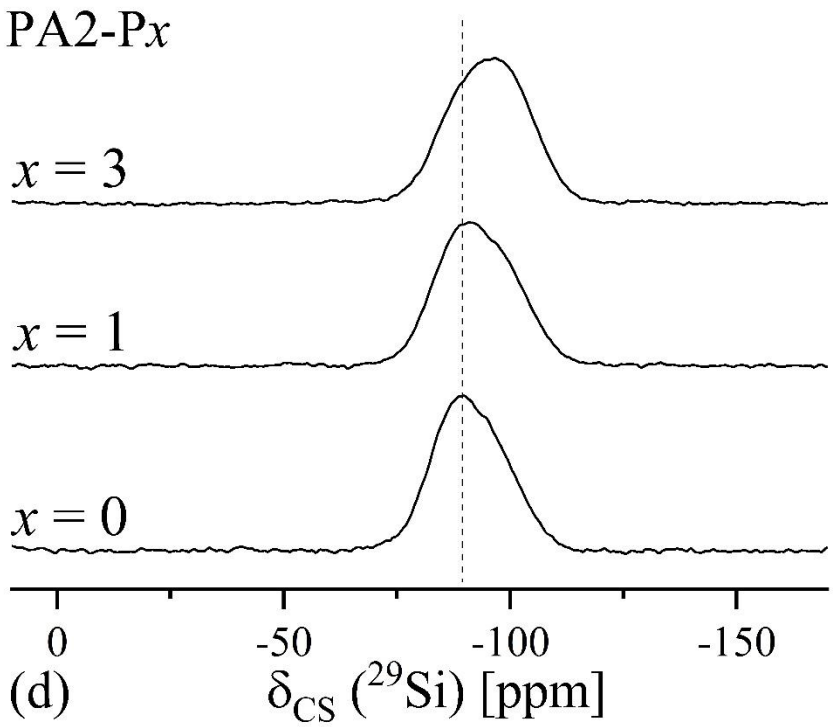


Figure S5. ^{29}Si MAS NMR spectra of Series "1" and "2" samples.

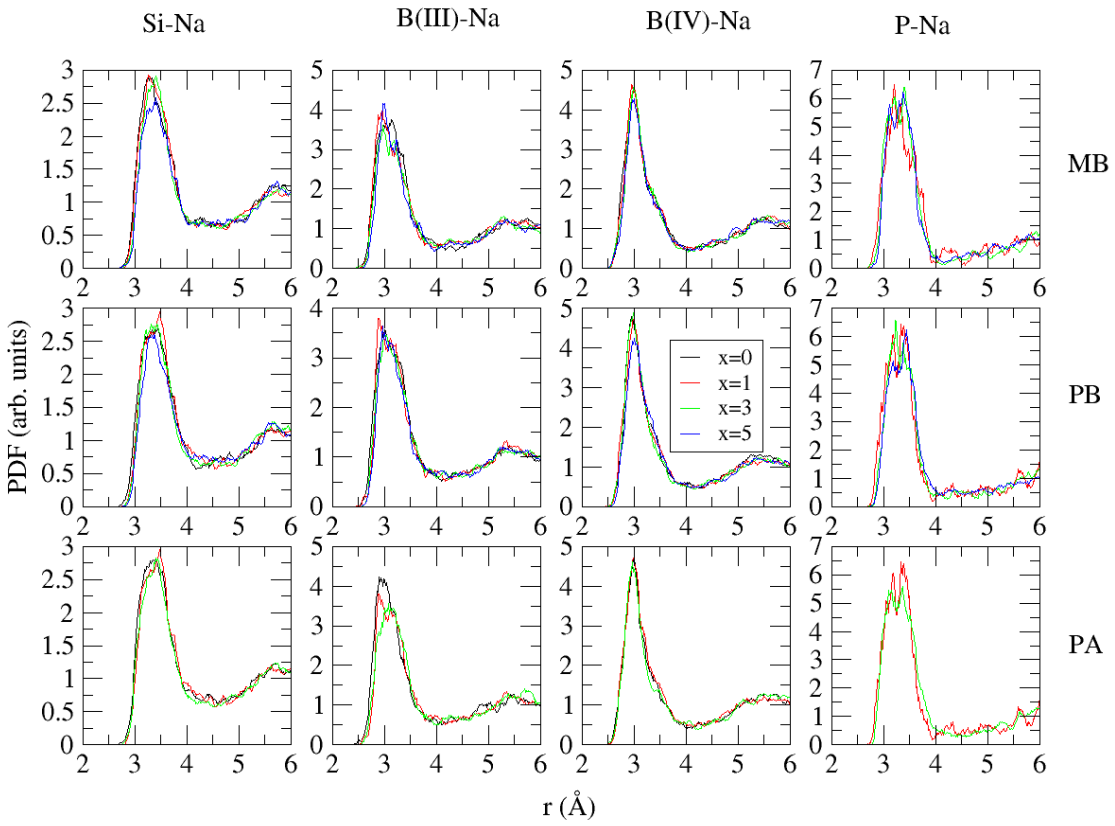


Figure S6. T-Na (T=Si, B(III), B(IV), P) pair distribution functions of the glasses investigated. *x* is the content of P_2O_5 in the glass.

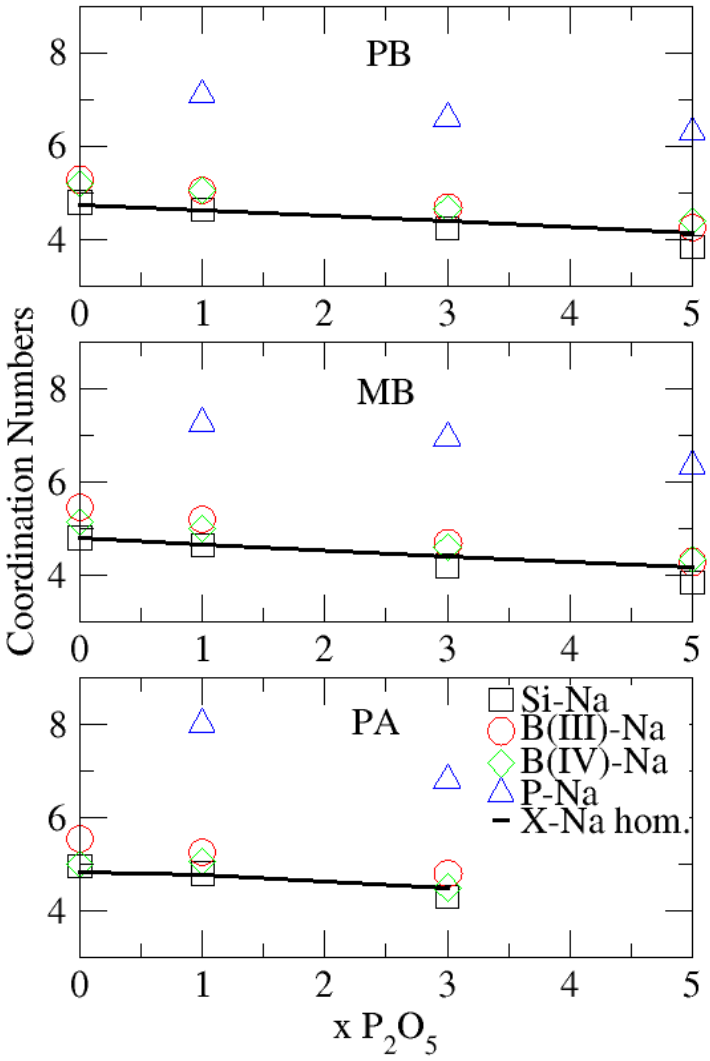


Figure S7. T-Na coordination numbers (computed using a cutoff = 4.5 Å) as a function of P_2O_5 content. The black line represents the coordination numbers for models in which sodium is homogeneously distributed.

Table S1. Summary of measurement conditions for all samples and nuclei studied by MAS NMR.

Single Resonance Parameters		Perboric	Metaboric	Peralkaline
^{23}Na	Magnetic field (T) / Resonance frequency (MHz)	16.4 / 185.1	5.7 / 64.1	5.7 / 64.1
	Spinning frequency (kHz)	22.0	15.0	15.0
	Pulse length (μs) / Tip angle	0.6 / (π/12)	0.8-1.2 / (π/6)	0.8-1.2 / (π/6)
	Recycle delay (s)	2	0.25-0.5	0.25-0.5
	Number of acquisitions	200	≥2000	≥2000
	Reference standard	NaCl (aq.) (0.0 ppm)	NaCl (7.2 ppm)	NaCl (7.2 ppm)
^{11}B	Magnetic field (T) / Resonance frequency (MHz)	16.4 / 224.6	14.1 / 192.6	11.7 / 160.5 or 14.1 / 192.6
	Spinning frequency (kHz)	20.0	15.0	14.0 or 15.0
	Pulse length (μs) / (Tip Angle)	0.6 / (π/12)	0.5-1.0 / (π/6)	0.4-1.0 / (π/6)
	Recycle delay (s)	2	1-5	1-15
	Number of acquisitions	200	≥400	≥400
	Reference standard	H_3BO_3 (aq.) (19.6 ppm)	BPO_4 (-3.5 ppm)	BPO_4 (-3.5 ppm)
^{31}P	Magnetic field (T) / Resonance frequency (MHz)	16.4 / 283.3	5.7 / 98.1	5.7 / 98.1
	Spinning frequency (kHz)	20.0	12.0	12.0
	Pulse length (μs) / (Tip angle)	1.0 / (π/6)	4.0-5.2 / (π/2)	4.0-5.2 / (π/2)
	Recycle delay (s)	45	90-150	90-150
	Number of acquisitions	160-800	80	80
	Reference standard	85 % H_3PO_4 (0.0 ppm)	BPO_4 (-29.3 ppm)	BPO_4 (-29.3 ppm)
^{29}Si	Magnetic Field (T) / Resonance frequency (MHz)	11.7 / 99.3	5.7 / 48.2	5.7 / 48.2
	Spinning frequency (kHz)	6.0	5.0	5.0
	Pulse length (μs) / (Tip angle)	1.6 / (π/6)	5.0 / (π/2)	5.0 / (π/2)
	Recycle delay (s)	300	150	150
	Number of acquisitions	300-800	150	150
	Reference standard	Tetramethylsilane (0.0 ppm)	$CaSi_2O_5$ (-71.3 ppm)	$CaSi_2O_5$ (-71.3 ppm)

Experimental Parameters of Double Resonance Experiments		
$^{11}B\{^{31}P\}$	$\nu_{nut.}$, observed (kHz)	71.0
	$\nu_{nut.}$, non-observed (kHz)	161.0
	Spinning frequency (kHz)	15.0
	π-Pulse length, observed (μs)	5.6-6.0
	π-Pulse length, non-observed (μs)	3.1
	Recycle delay (s)	1
	Number of acquisitions (per point)	≥112
$^{23}Na\{^{31}P\}$	$\nu_{nut.}$, observed (kHz)	31.3
	$\nu_{nut.}$, non-observed (kHz)	62.5
	Spinning frequency (kHz)	11.0
	π-Pulse length, observed (μs)	6.0
	π-Pulse length, non-observed (μs)	6.4
	Recycle delay (s)	0.5
	Number of acquisitions (per point)	512
$^{31}P\{^{23}Na\}$	$\nu_{nut.}$, observed (kHz)	62.5
	$\nu_{nut.}$, non-observed (kHz)	31.3
	Spinning frequency (kHz)	11.0
	π-Pulse length, observed (μs)	6.4
	π-Pulse length, non-observed (μs)	6.0
	Recycle delay (s)	40-100
	Number of acquisitions (per point)	256
$^{31}P\{^{11}B\}$	$\nu_{nut.}$, observed (kHz)	161.0
	$\nu_{nut.}$, non-observed (kHz)	71.0
	Spinning frequency (kHz)	15.0
	π-Pulse length, observed (μs)	3.1
	π-Pulse length, non-observed (μs)	22.0
	Recycle delay (s)	90
	Number of acquisitions (per point)	192

*7.75 μs used for B(III) and 11.25 μs for B(IV)

Table S2. Number of atoms in the simulation cells of the investigated glasses.

Glass	B	Si	P	O	Na	# atoms
PB0	600	450	-	2050	500	3600
PB2-P1	590	440	20	2060	490	3600
PB2-P3	580	430	60	2120	480	3670
PB2-P5	570	420	100	2180	470	3740
MB0	500	500	-	2000	500	3500
MB2-P1	490	500	20	2030	490	3530
MB2-P3	480	490	60	2090	480	3600
MB2-P5	470	480	100	2150	470	3670
PA0	400	550	-	1950	500	3400
PA2-P1	390	540	20	1910	490	3350
PA2-P3	380	530	60	2020	480	3470
55 Na_2O – 45 P_2O_5	-	-	72	224	88	384
40 Na_2O – 18 B2O3 – 42 P_2O_5	27	-	63	228	60	378

Table S3. Shell model interatomic potential parameters used in this work.

	Buckingham			***Ref.***
Pairs	**A (eV)**	**ρ (Å)**	**C (eV Å^6)**	
O_s-O_s	22764.30	0.1490	27.88	[1]
Si-O_s	1283.91	0.32052	10.661580	[1]
Na-O_s	56465.345	0.193931	0.000000	[2]
B-O_s	511.0	0.3310	0.0	this work
P-O_s	1120.09	0.33477	0.0	[3]
	Three-body potential			
	k_b (eV rad^{-2})	**θ_0 (deg)**	**ρ (Å)**	***Ref.***
O-Si-O	100.0	109.47	1.0	[3]
O-P-O	50.0	109.47	1.0	[3]
	Core-shell potential			
	k_s (eV Å^{-2})	**Y(e)**	**m_{shell} (uma)**	
O_c-O_s	74.92	-2.8482	3.0	

(1) Sanders, M. J.; Leslie, M.; Catlow, C. R. A. Interatomic Potentials for SiO_2. *J. Chem. Soc. Chem. Commun.* **1984**, No. 19, 1271–1273.

(2) Tilocca, A.; De Leeuw, N. H.; Cormack, A. N. Shell-Model Molecular Dynamics Calculations of Modified Silicate Glasses. *Phys. Rev. B Condens. Matter* **2006**, *73* (10), 1–14.

(3) Tilocca, A.; Cormack, A. N.; De Leeuw, N. H. The Structure of Bioactive Silicate Glasses: New Insight from Molecular Dynamics Simulations. *Chem. Mater.* **2007**, *19* (1), 95–103.

Table S4. Fitting parameters of ^{11}B MAS NMR in the studied glasses, including fraction of each species f (± 1.0 %), isotropic chemical shift, δ_{CS}^{iso} (± 0.5 ppm), quadrupolar coupling constant, C_Q (± 0.2 MHz), η_Q (± 0.05), and overall N_4 fractions (± 1 %) where N_4 as simulated from MD models are displayed in brackets.

Sample ID	B(III) Ring				B(III) Non-Ring				B(IV)-I		B(IV)-II		N_4
	f (%)	δ_{CS}^{iso} (ppm)	C_Q (MHz)	η_Q	f (%)	δ_{CS}^{iso} (ppm)	C_Q (MHz)	η_Q	f (%)	δ_{CS}^{iso} (ppm)	f (%)	δ_{CS}^{iso} (ppm)	
PB0	27.8	18.5	2.7	0.3	9.3	16.2	2.6	0.3	59.3	-0.1	3.6	-2.1	62.9 [59.5]
PB1-P1	25.7	18.2	2.7	0.3	9.5	16.1	2.6	0.3	60.2	-0.2	4.6	-2.2	64.8
PB1-P3	28.2	18.1	2.7	0.3	10.1	15.8	2.6	0.3	55.3	-0.2	6.4	-2.2	61.7
PB1-P5	29.9	18.0	2.7	0.3	11.3	15.7	2.6	0.3	47.4	-0.1	11.4	-2.1	58.8
PB2-P1	26.2	18.4	2.7	0.3	10.3	16.4	2.7	0.3	60.1	-0.1	3.4	-2.1	63.5 [60.5]
PB2-P3	28.6	18.1	2.7	0.3	9.3	16.1	2.6	0.3	54.7	-0.1	7.4	-2.1	62.1 [58.6]
PB2-P5	28.7	18.1	2.7	0.3	12.2	16.1	2.6	0.3	49.9	-0.1	9.2	-2.1	59.1 [54.6]
PB3-P1	27.0	18.3	2.7	0.3	9.6	16.3	2.6	0.3	58.5	-0.1	4.9	-2.1	63.4
PB3-P4	29.4	18.2	2.7	0.3	10.6	16.1	2.6	0.3	53.8	-0.1	6.2	-2.2	60.0
PB3-P7	31.2	18.0	2.7	0.3	12.4	16.0	2.6	0.3	48.4	-0.1	8.0	-2.2	56.4 [53.8]
MB0	25.1	17.7	2.6	0.3	5.9	14.6	2.5	0.5	62.4	-0.5	6.6	-2.4	67.2 [61.7]
MB1-P1	23.6	17.7	2.6	0.3	6.5	14.6	2.5	0.5	61.9	-0.5	8.0	-2.4	69.9
MB1-P3	26.3	17.5	2.6	0.4	5.6	14.1	2.6	0.4	56.9	-0.6	11.2	-2.4	68.1
MB1-P4	26.8	17.4	2.6	0.3	7.7	14.0	2.5	0.5	50.6	-0.6	14.9	-2.4	65.5
MB2-P1	25.8	17.6	2.6	0.3	6.7	14.6	2.6	0.5	62.4	-0.6	5.1	-2.5	67.5 [63.4]
MB2-P3	25.5	17.4	2.6	0.3	7.3	14.8	2.6	0.5	59.6	-0.7	7.6	-2.6	67.2 [60.9]
MB2-P5	26.1	17.3	2.6	0.3	8.4	14.1	2.5	0.5	54.6	-0.7	10.9	-2.6	65.5 [60.3]
MB3-P1	23.1	17.5	2.6	0.3	9.3	15.2	2.6	0.5	62.6	-0.9	5.0	-2.8	67.6
MB3-P3	23.0	17.4	2.6	0.3	10.0	15.3	2.6	0.5	59.6	-0.9	7.4	-2.8	67.0
MB3-P5	26.6	17.2	2.6	0.3	9.4	14.2	2.4	0.5	56.0	-0.9	8.0	-2.9	64.0
PA0	21.7	18.2	2.6	0.4	6.4	15.2	2.6	0.4	60.8	-0.1	11.1	-1.9	71.0 [67.2]
PA1-P1	22.5	18.0	2.5	0.4	8.9	11.4	2.5	0.5	62.1	-0.2	6.4	-1.8	68.5
PA1-P3	22.0	18.0	2.5	0.4	10.1	11.4	2.5	0.5	59.3	-0.2	8.6	-1.8	67.9
PA2-P1	21.2	18.1	2.5	0.4	6.5	14.4	2.6	0.4	58.0	-0.1	14.3	-1.8	71.4 [58.9]
PA2-P3	21.9	18.0	2.6	0.4	5.5	14.4	2.6	0.4	57.7	-0.3	14.9	-2.1	71.9 [66.6]
PA3-P1	24.6	18.4	2.5	0.4	8.2	10.0	2.4	0.5	62.6	0.0	4.6	-1.7	67.2
PA3-P3	23.5	18.2	2.5	0.4	9.1	10.3	2.4	0.5	61.7	-0.2	5.8	-1.8	67.4

Table S5. Fitting parameters of ^{31}P MAS NMR in all studied glasses, including species designations, fraction of each species f (±1.0 %), isotropic chemical shift, δ_{CS}^{iso} (±0.2 ppm) and FWHM (±0.1 ppm). Average number of B next nearest neighbors around P and total average P coordination are also displayed.

Sample ID		^{31}P MAS NMR								
		PB1-P1	**PB1-P3**	**PB1-P5**	**PB2-P1**	**PB2-P3**	**PB2-P5**	**PB3-P1**	**PB3-P4**	**PB3-P7***
P^0	***f* (%)**	2.0	0.6	0.0	3.3	0.9	0.0	2.7	0.5	0.0/0.0
	δ_{CS}^{iso} **(ppm)**	16.0	16.0	--	16.3	15.9	--	16.0	16.0	--
	FWHM (ppm)	3.9	4.6	--	3.9	4.6	--	3.9	3.9	--
P^1_{1B}	***f* (%)**	11.3	6.2	4.3	12.0	7.8	4.7	12.0	10.2	3.2/4.2
	δ_{CS}^{iso} **(ppm)**	6.6	6.6	6.1	6.9	6.6	6.1	6.6	6.2	6.2/4.6
	FWHM (ppm)	4.0	4.0	4.0	4.0	4.0	4.0	4.0	4.0	3.9/3.8
P^1_{1P}	***f* (%)**	59.9	45.5	32.3	60.5	50.8	33.2	60.8	45.0	25.7/21.6
	δ_{CS}^{iso} **(ppm)**	3.4	3.1	2.6	3.6	3.2	2.6	3.5	2.8	2.3/1.6
	FWHM (ppm)	5.8	5.8	5.8	5.8	5.8	5.8	5.7	5.7	5.8/5.7
P^2_{2B}	***f* (%)**	8.7	11.7	12.4	9.1	12.0	12.1	9.7	12.4	16.6/32.7
	δ_{CS}^{iso} **(ppm)**	-2.1	-2.1	-2.1	-2.1	-2.1	-2.1	-2.1	-2.7	-2.7/-4.6
	FWHM (ppm)	5.1	5.1	5.1	5.1	5.1	5.1	5.1	5.1	5.1/8.0
$P^2_{1B,1P}$	***f* (%)**	15.1	26.5	36.5	12.8	23.4	36.1	12.7	25.6	40.4/26.8
	δ_{CS}^{iso} **(ppm)**	-6.4	-6.2	-6.3	-6.6	-6.5	-6.3	-6.6	-6.6	-6.8/7.4
	FWHM (ppm)	6.3	6.3	6.4	6.3	6.4	6.4	6.3	6.3	6.4/7.1
$P^3_{2B,1P}$	***f* (%)**	3.1	8.6	12.9	2.2	5.1	12.4	2.1	6.3	12.5/12.0
	δ_{CS}^{iso} **(ppm)**	-12.4	-11.5	-11.7	-12.4	-12.4	-11.7	-12.4	-12.4	-12.4/-12.1
	FWHM (ppm)	6.4	6.3	6.4	6.4	6.4	6.4	6.4	6.4	6.4/6.4
P^2_{2P}	***f* (%)**	0.0	0.8	1.7	0.0	0.0	1.4	0.0	0.0	1.5/2.8
	δ_{CS}^{iso} **(ppm)**	--	-18.7	-18.7	--	--	-18.7	--	--	-18.7/-17.5
	FWHM (ppm)	--	5.9	5.9	--	--	5.9	--	--	5.9/6.2
$\langle m_B(P) \rangle$ **Av. # of B neighbors per P**		0.50	0.73	0.91	0.47	0.65	0.90	0.48	0.73	1.02/1.20
$\langle n \rangle$		1.28	1.56	1.77	1.23	1.45	1.74	1.24	1.50	1.83/1.86

*two separate sets of measurements with fits constrained by refocused INADEQUATE experiments

Sample ID		^{31}P MAS NMR								
		MB1-P1	**MB1-P3**	**MB1-P4**	**MB2-P1**	**MB2-P3**	**MB2-P5**	**MB3-P1**	**MB3-P3**	**MB3-P5**
P^0	***f* (%)**	3.2	1.3	1.0	3.7	1.4	1.2	3.7	1.7	1.1
	δ_{CS}^{iso} (ppm)	16.4	16.3	16.3	16.4	16.3	15.6	16.4	16.3	15.8
	FWHM (ppm)	4.1	4.2	4.2	4.1	4.2	4.9	4.1	4.2	4.2
P^1_{1B}	***f* (%)**	29.6	20.4	18.1	31.6	22.5	14.5	32.5	23.4	15.2
	δ_{CS}^{iso} (ppm)	6.0	6.0	5.9	6.0	6.0	6.2	6.0	6.0	6.2
	FWHM (ppm)	4.5	4.5	4.5	4.5	4.5	3.9	4.5	4.5	3.9
P^1_{1P}	***f* (%)**	39.7	35.6	34.5	40.1	37.1	36.6	39.5	37.6	37.4
	δ_{CS}^{iso} (ppm)	2.9	2.9	2.9	2.9	2.9	2.9	2.9	2.9	2.9
	FWHM (ppm)	4.6	4.6	4.6	4.6	4.6	4.6	4.6	4.6	4.6
P^2_{2B}	***f* (%)**	10.3	13.1	13.4	9.0	12.4	14.1	9.5	12.5	13.5
	δ_{CS}^{iso} (ppm)	-0.9	-0.9	-0.5	-1.1	-0.9	-0.9	-0.8	-0.9	-1.0
	FWHM (ppm)	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0	5.0
$P^2_{1B,1P}$	***f* (%)**	12.8	21.4	22.9	12.0	19.5	23.8	11.8	18.4	23.7
	δ_{CS}^{iso} (ppm)	-5.8	-5.8	-5.6	-5.6	-5.8	-5.8	-5.8	-5.8	-5.8
	FWHM (ppm)	6.5	6.5	6.5	6.5	6.5	6.4	6.5	6.5	6.5
$P^3_{2B,1P}$	***f* (%)**	4.4	8.2	10.1	3.6	7.1	9.8	3.0	6.4	9.2
	δ_{CS}^{iso} (ppm)	-10.9	-10.9	-10.9	-10.9	-10.9	-10.9	-10.9	-10.9	-10.9
	FWHM (ppm)	6.5	6.5	6.5	6.5	6.5	6.5	6.5	6.5	6.5
P^2_{2P}	***f* (%)**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	δ_{CS}^{iso} (ppm)	--	--	--	--	--	--	--	--	--
	FWHM (ppm)	--	--	--	--	--	--	--	--	--
$\langle m_B(P) \rangle$		0.72	0.84	0.88	0.69	0.81	0.86	0.69	0.80	0.84
$\langle n \rangle$		1.29	1.50	1.56	1.25	1.45	1.56	1.24	1.42	1.55

Sample ID		^{31}P MAS NMR					
		PA1-P1	**PA1-P3**	**PA2-P1**	**PA2-P3**	**PA3-P1**	**PA3-P3**
P^0	***f* (%)**	4.7	7.4	4.8	4.7	5.5	3.2
	δ_{CS}^{iso} (ppm)	16.0	14.8	16.4	15.3	16.5	16.3
	FWHM (ppm)	4.1	3.8	4.5	4.5	4.6	4.5
P^1_{1B}	***f* (%)**	27.6	16.5	26.8	21.1	29.0	23.1
	δ_{CS}^{iso} (ppm)	6.4	6.2	6.3	5.8	6.4	6.2
	FWHM (ppm)	4.6	4.3	4.6	4.6	4.6	4.6
P^1_{1P}	***f* (%)**	45.5	46.7	42.7	40.6	42.2	43.1
	δ_{CS}^{iso} (ppm)	3.1	2.8	3.1	2.9	3.1	3.1
	FWHM (ppm)	4.6	4.2	4.6	4.6	4.6	4.6
P^2_{2B}	***f* (%)**	8.0	7.9	11.1	12.2	9.9	11.7
	δ_{CS}^{iso} (ppm)	-1.0	-1.2	-0.5	-0.3	-0.7	-0.5
	FWHM (ppm)	5.0	5.0	5.0	5.0	5.0	5.0
$P^2_{1B,1P}$	***f* (%)**	10.8	13.6	10.9	14.4	9.6	13.2
	δ_{CS}^{iso} (ppm)	-5.8	-5.8	-5.8	-5.8	-5.8	-5.8
	FWHM (ppm)	6.5	6.5	6.5	6.5	6.5	6.5
$P^3_{2B,1P}$	***f* (%)**	3.4	7.9	3.6	7.1	3.8	5.7
	δ_{CS}^{iso} (ppm)	-10.9	-10.9	-10.9	-10.9	-10.9	-10.9
	FWHM (ppm)	6.5	6.5	6.5	6.5	6.5	6.5
P^2_{2P}	***f* (%)**	0.0	0.0	0.0	0.0	0.0	0.0
	δ_{CS}^{iso} (ppm)	--	--	--	--	--	--
	FWHM (ppm)	--	--	--	--	--	--
$\langle m_B(P) \rangle$		0.61	0.62	0.67	0.74	0.66	0.71
$\langle n \rangle$		1.21	1.30	1.24	1.39	1.21	1.33