Supplementary Material

Experimental

All reactants used were of the highest purity and were purchased from Merck, Sigma-Aldrich, BDH Chemicals, Eka Chemicals, M&B or Carlo Erba.

Caesium hydroxide was obtained by precipitation from a solution of caesium sulphate by addition of barium hydroxide.

Lithium borate was synthesized from the corresponding carbonate and boric acid. Caesium borate was synthesized from the corresponding hydroxide and boric acid

^{1}H NMR (300 MHz, D_2O, DOH), and ^{11}B NMR [96.3 MHz, D_2O, $BF_3O(CH_2CH_3)_2$] spectra, were recorded on a Bruker Avance III 300 Ultra Shield spectrometer and ^{13}C NMR spectra were recorded on a Bruker Avance III 400 Ultra Shield spectrometer [100.6 MHz, D_2O, $CO(CH_3)_2$]. All δ values are given in ppm. The assignments of specific proton, carbon and boron signals were achieved by comparison with published data.[1,2]

Study of the cations (lithium and caesium) effect on ribose-borate bound species (BBS) was done as described in the Experimental section of the article.

Nuclear Magnetic Resonance (NMR) Data

^{1}H NMR and ^{11}B NMR

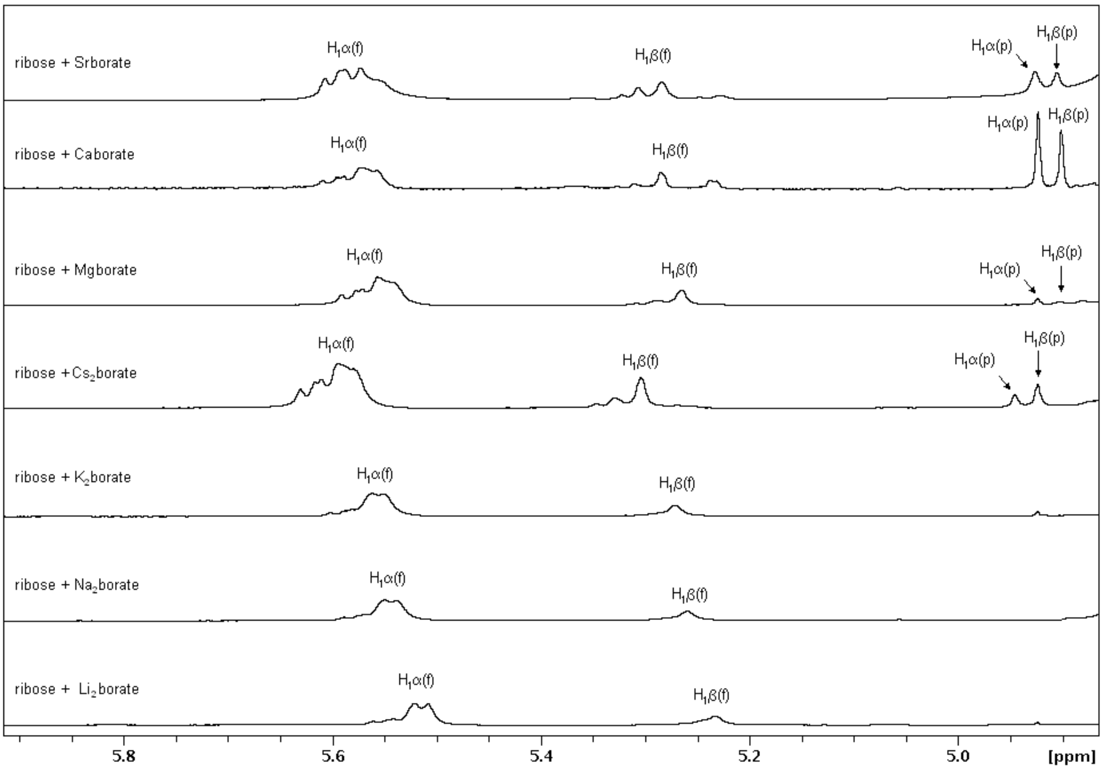

Figure A. Detail of the ^{1}H NMR spectra of ribose-borate bound species synthesized from ribose and lithium borate, sodium borate, potassium borate, caesium borate, magnesium borate, calcium borate or strontium borate. The symbols 'f' and 'p' represent furanose and pyranose, respectively. The spectra were recorded in D_2O.

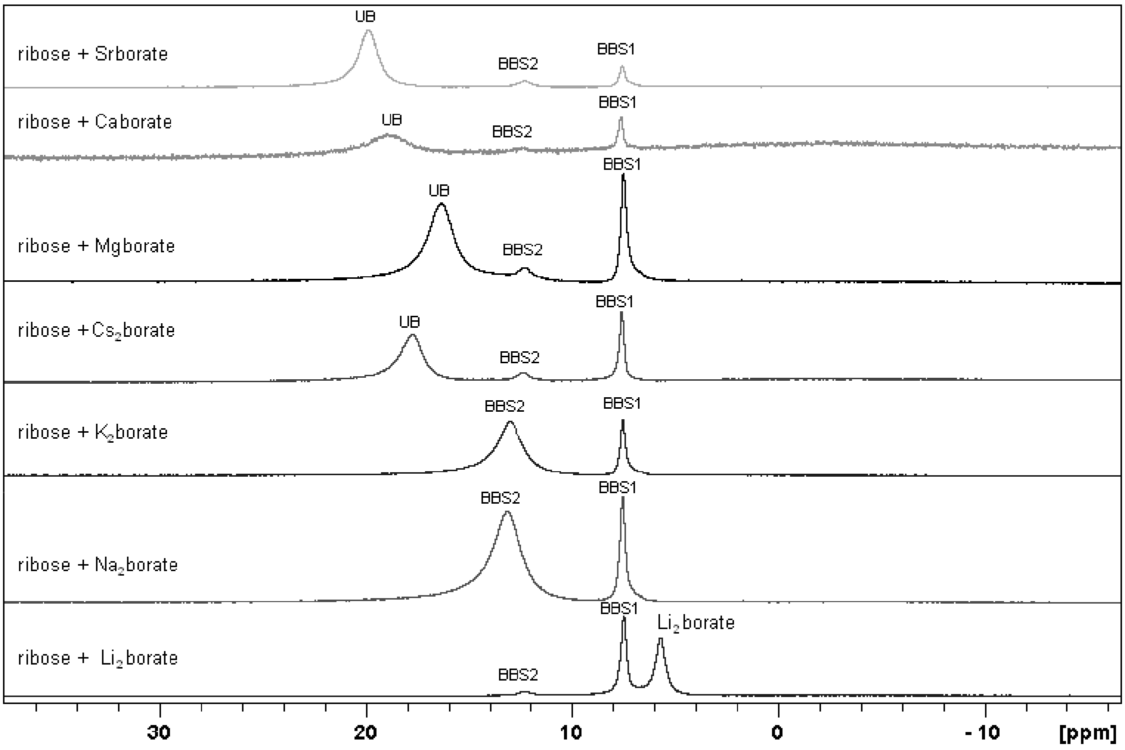

Figure B. ^{11}B NMR spectra of ribose-borate bound species synthesized from ribose and lithium borate, sodium borate, potassium borate, caesium borate, magnesium borate, calcium borate or strontium borate. The symbol 'UB' represents unbound borate. The spectra were recorded in D_2O.

Table A. Ribofuranose percentages after incubation with lithium, sodium, potassium, caesium, magnesium, calcium and strontium borates and charge densities of the cations

Cation	% D-ribofuranose borate bound species (BBS)	ξ[a] (e/Å^3)	M-O[b] (Å)	Ionic Radius[5] (Å)	Nuclear effective charge[c] (Z_{eff})
Li^+	100	0.088	2.25	0.78	1.28
Na^+	100	0.017	2.41	0.98	2.51
K^+	100	0.012	2.70	1.33	3.50
Cs^+	88	0.039	2.95	1.65	6.36
Mg^{2+}	96	0.054	2.07	0.78	3.31
Ca^{2+}	89	0.038	2.33	1.06	4.40
Sr^{2+}	77	0.027	2.60	1.27	6.07

[a] Charge densities of metal cations.[3]

[b] Length of metal (M) oxygen bond. Fully hydrated ions are larger due to contributions from hydrogen atoms and additional water layers.[4]

[c] The effective nuclear charge (Z_{eff}) used was the one according to Clementi.[5]

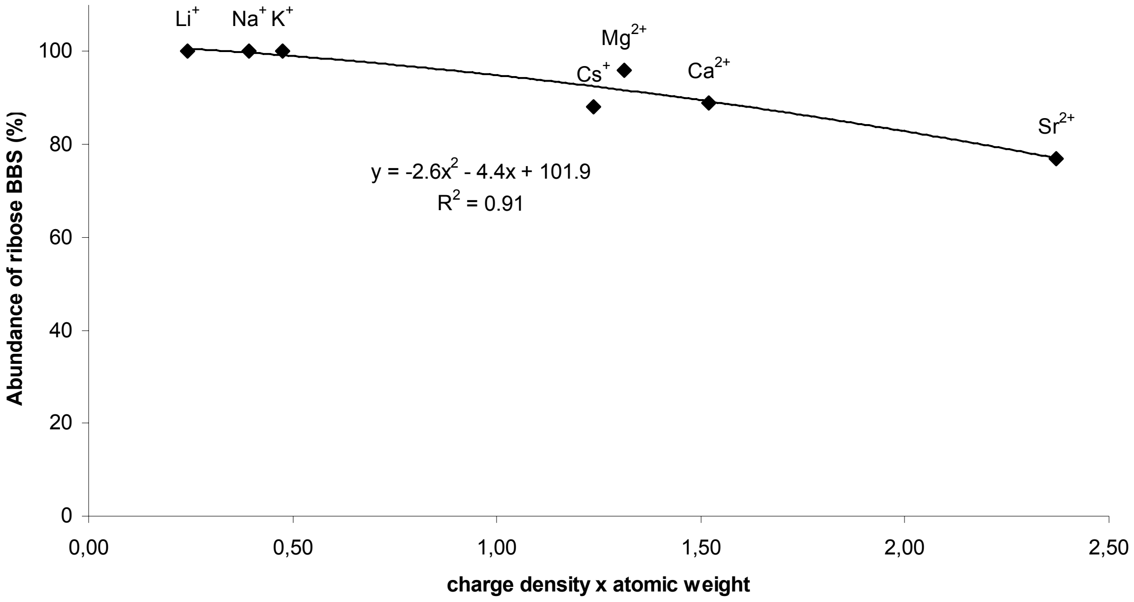

Figure C. Correlation of the (cation charge density × atomic weight) with the percentage of ribofuranose in solutions of lithium, sodium, potassium, caesium, magnesium, calcium and strontium borates*.

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* It should be noticed that the regression coefficient R^2 is also quite high (0.85) when representing the abundance of ribose BBS *vs.* (charge density x atomic number).

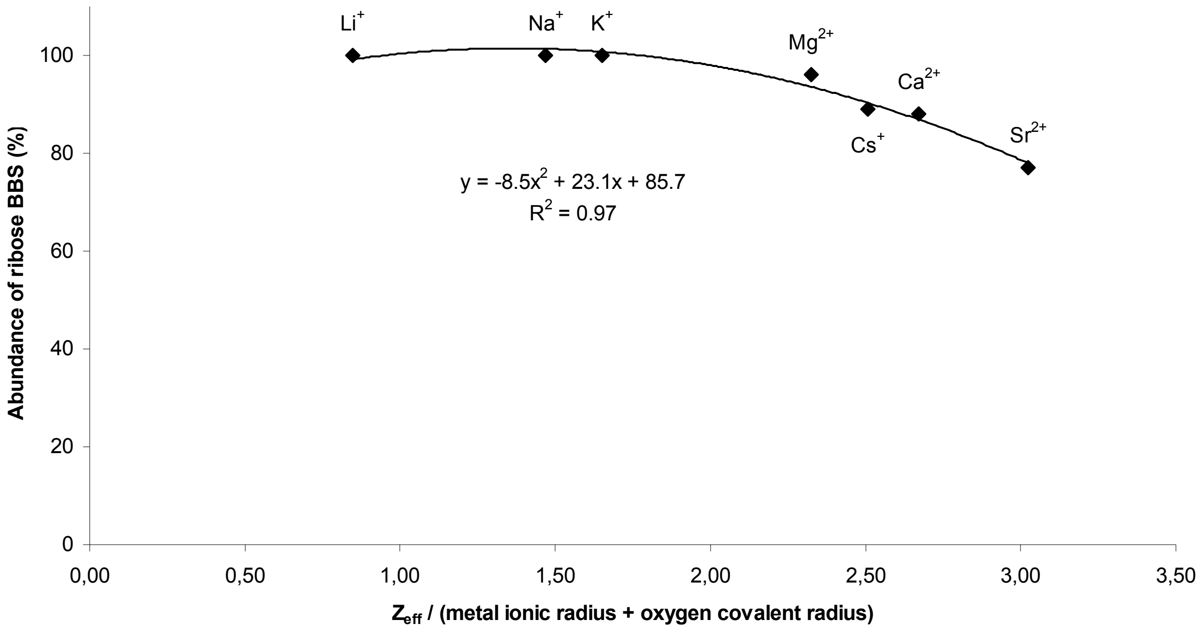

Figure D. Correlation of the (cation effective nuclear charge/metal ionic radius + oxygen covalent radius) with the percentage of ribofuranose in solutions of lithium, sodium, potassium, caesium, magnesium, calcium and strontium borates.

Effect of pH on ribose borate bound species (BBS)

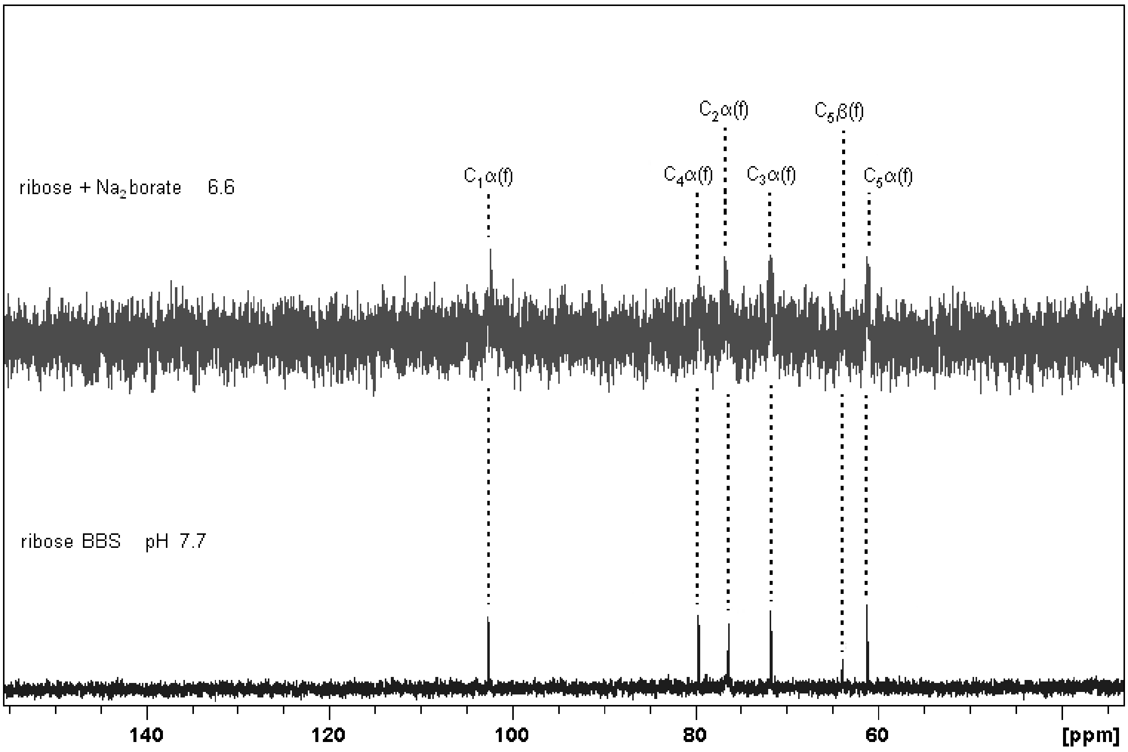

Figure E. ^{13}C NMR spectra of ribose borate bound species (BBS) synthesized from ribose and sodium borate: at pH 6.6 and at pH 9.3 with subsequent acidification to pH 7.7. The symbols ‘f’ and ‘p’ represent furanose and pyranose, respectively. The spectra were recorded in D_2O.

References

[1] P. Ortiz, J. Fernández-Bertrán and E. Reguera, *Spect. Chim. Acta Part A*, 2005, **61**, 1977.

[2] S. Chapelle and J.-F. Verchere, *Tetrahedron*, 1988, **44**, 4469.

[3] E. Koculi, C. Hyeon, D. Thirumalai and S. A. Woodson, *J. Am. Chem. Soc.*, 2007, **129**, 2676.

[4] H. Ohtaki and T. Radnai, *Chem. Rev.*, 1993, **93**, 1157.

[5] J. Emsley, *The Elements*, Clarendon Press, Oxford, 2nd edn., 1991.