Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

Liquid-liquid extraction of boron from continental brines by 2-butyl-1-octanol diluted in kerosene

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Table S1 Chemical equilibria used for speciation calculations of boron with Phreeqc (databases: Pitzer and Minteq.V4).

Equation	log (K)
$H_3BO_3 \rightleftarrows H_3BO_3$	0
$H_3BO_3 + H_2O \rightleftarrows B(OH)_4^- + H^+$	– 9.2
$H_3BO_3 \rightleftarrows H_2BO_3^- + H^+$	– 9.2
$2H_3BO_3 \rightleftarrows H_5(BO_3)_2^- + H^+$	– 9.3
$3H_3BO_3 \rightleftarrows H_8(BO_3)_3^- + H^+$	– 7.3
$3H_3BO_3 \rightleftarrows B_3O_3(OH)_4^- + 2H_2O + H^+$	– 7.5
$4H_3BO_3 \rightleftarrows B_4O_5(OH)_4^{2-} + 3H_2O + 2H^+$	– 16.1
$Ca^{2+} + H_3BO_3 + H_2O \rightleftarrows CaB(OH)_4^+ + H^+$	– 7.6
$Ca^{2+} + H_3BO_3 \rightleftarrows CaH_2BO_3^+ + H^+$	– 7.5
$Mg^{2+} + H_3BO_3 + H_2O \rightleftarrows MgB(OH)_4^+ + H^+$	– 7.8
$Mg^{2+} + H_3BO_3 \rightleftarrows MgH_2BO_3^+ + H^+$	– 7.7
$Na^+ + H_3BO_3 \rightleftarrows NaH_2BO_3 + H^+$	– 9

Boron speciation calculations with Phreeqc software were validated with data of 0.1 mol kg^{-1} boron speciation in pure water from the literature,[1] and reported in Figure S1 (b). The simulation of the speciation of boron and the other elements, i.e. sodium, calcium, magnesium, potassium and lithium, in the synthetic brine was reported in Figures S2-S6.

Speciation in the aqueous phase plays an important role in solvent extraction. The presence of polyborate species (i.e. diborate, triborate, tetraborate and pentaborate) in aqueous solutions containing 5g L^{-1} boron in pure water was reported in the literature.[2–4] Furthermore, Li et al. reported four species of boron (H_3BO_3, $B(OH)_4^-$, $B_3O_3(OH)_4^-$ and $B_4O_5(OH)_4^{2-}$) in brine. [5] Regarding the composition of the synthetic brine and the databases available in Phreeqc (Pitzer, Core10, Amm and minteq.v4 databases), it was found that 12 boron chemical compounds may exist in the brine. Table S1 gathers the chemical equilibria and the corresponding equilibrium constants used to perform the speciation calculations of boron in pure water and the brine reported in Figures S4 and S5, respectively.

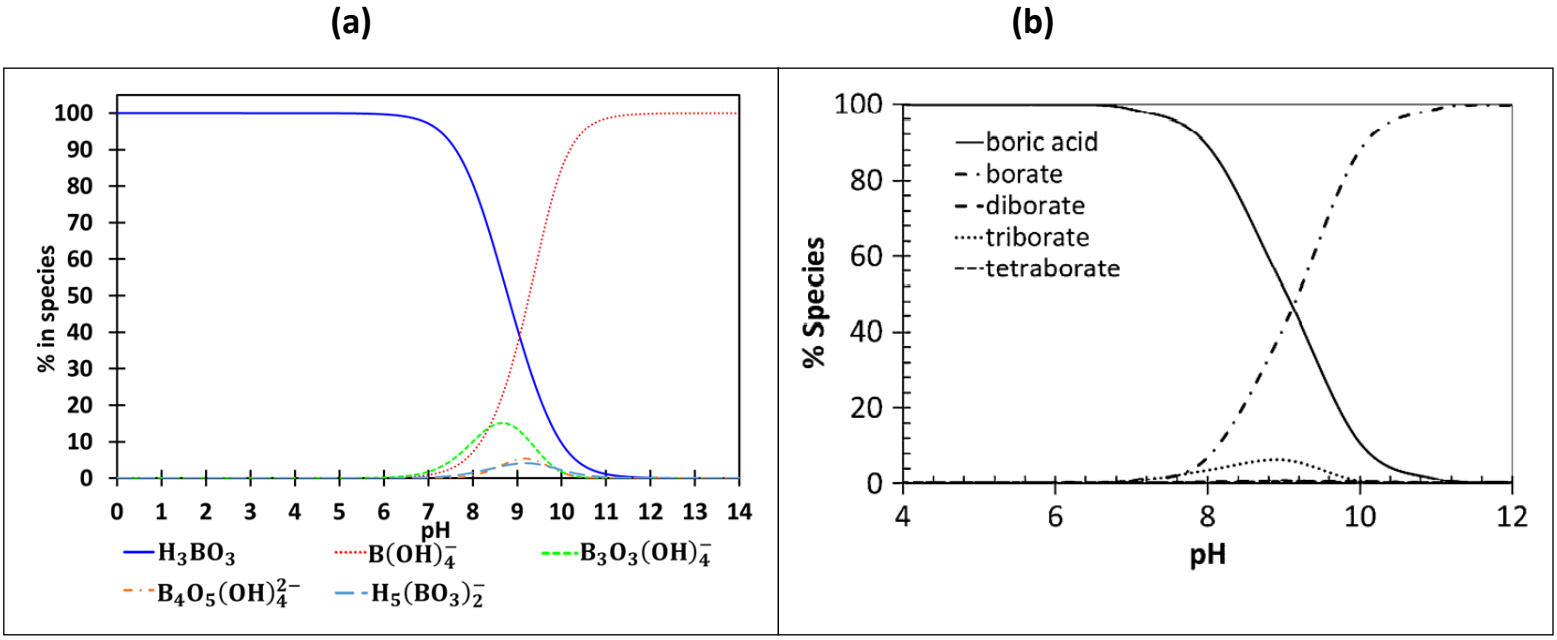


Fig. S1 Comparison of boron speciation in pure water (a) simulated by using the Phreeqc software with the Pitzer and Minteq.V4 databases and (b) reported in literature,[1] [Boron] = 0.1 mol kg^{-1}) .

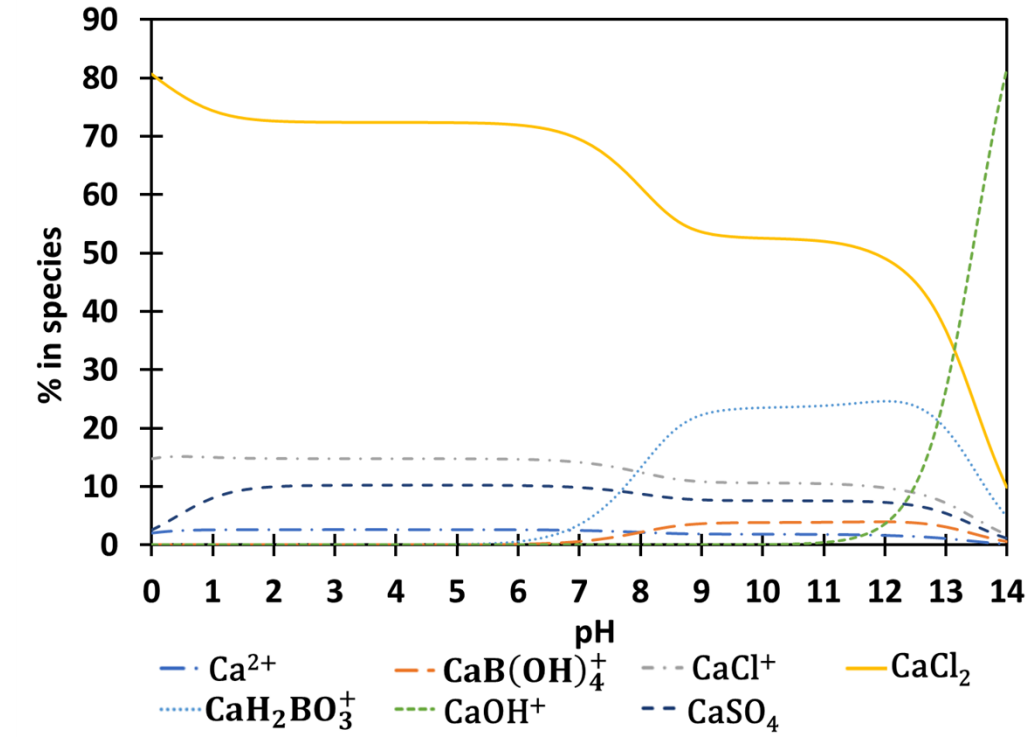


Fig. S2 Calcium speciation in the synthetic brine vs. pH.

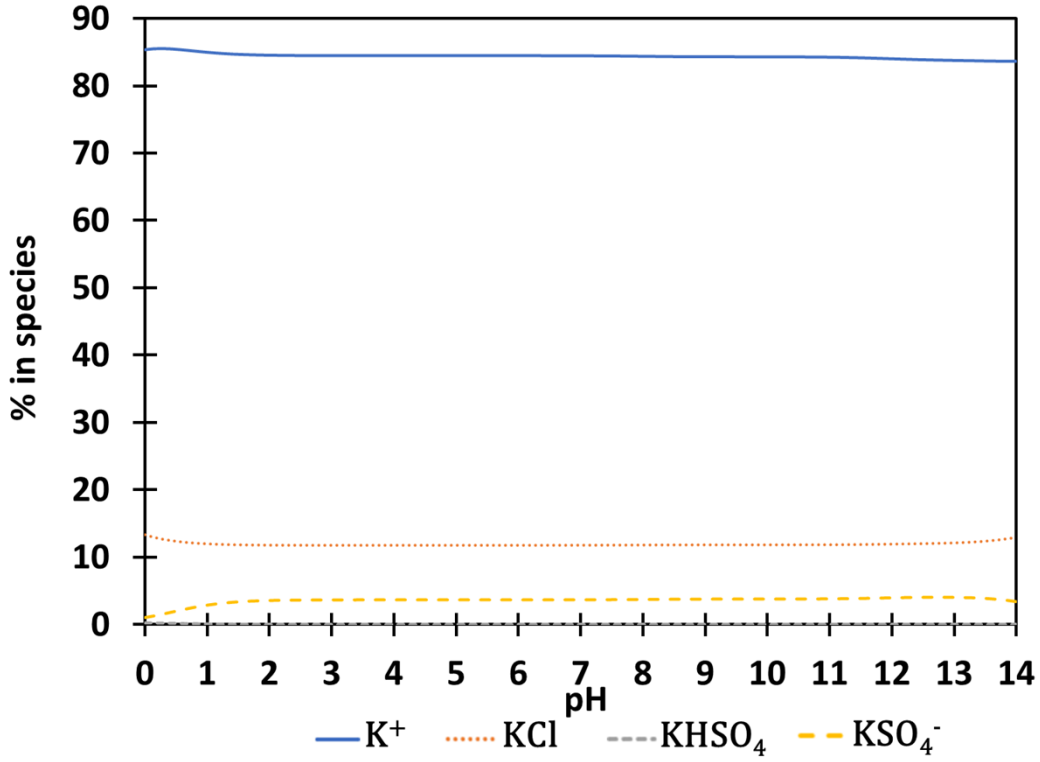


Fig. S3 Potassium speciation in the synthetic brine vs. pH.

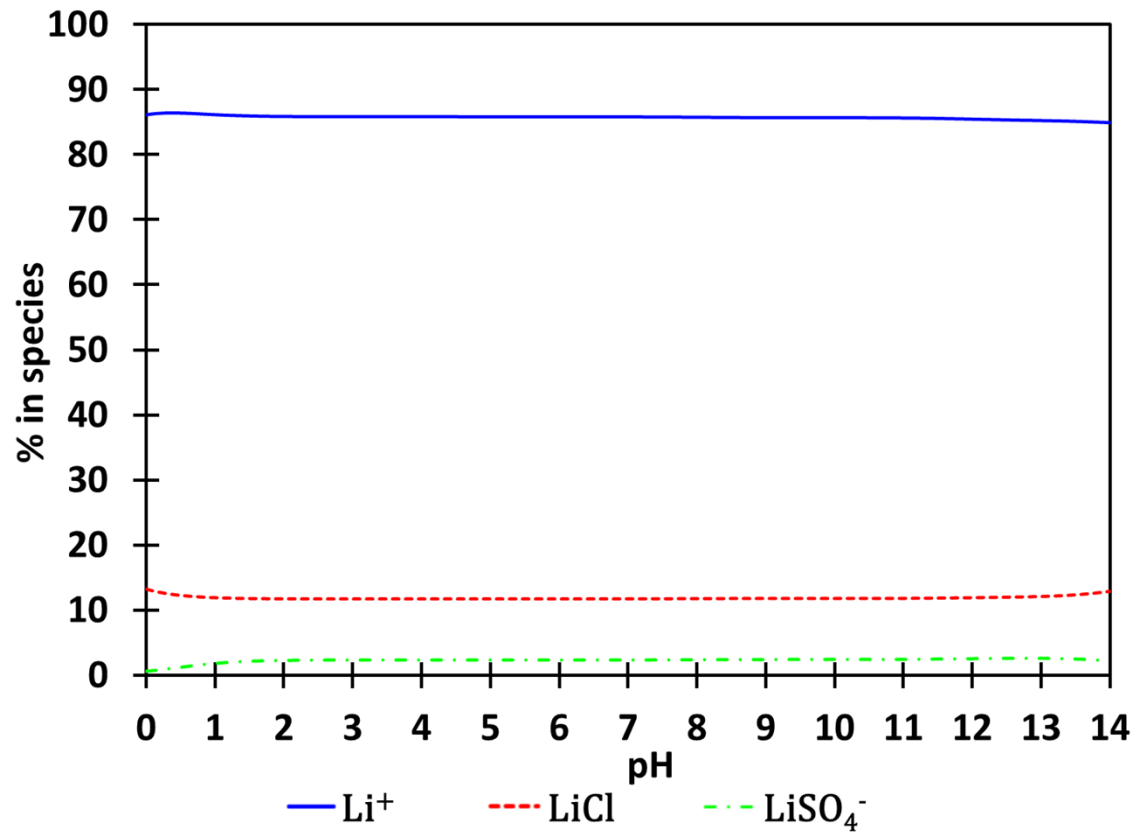


Fig. S4 Lithium speciation in the synthetic brine vs. pH.

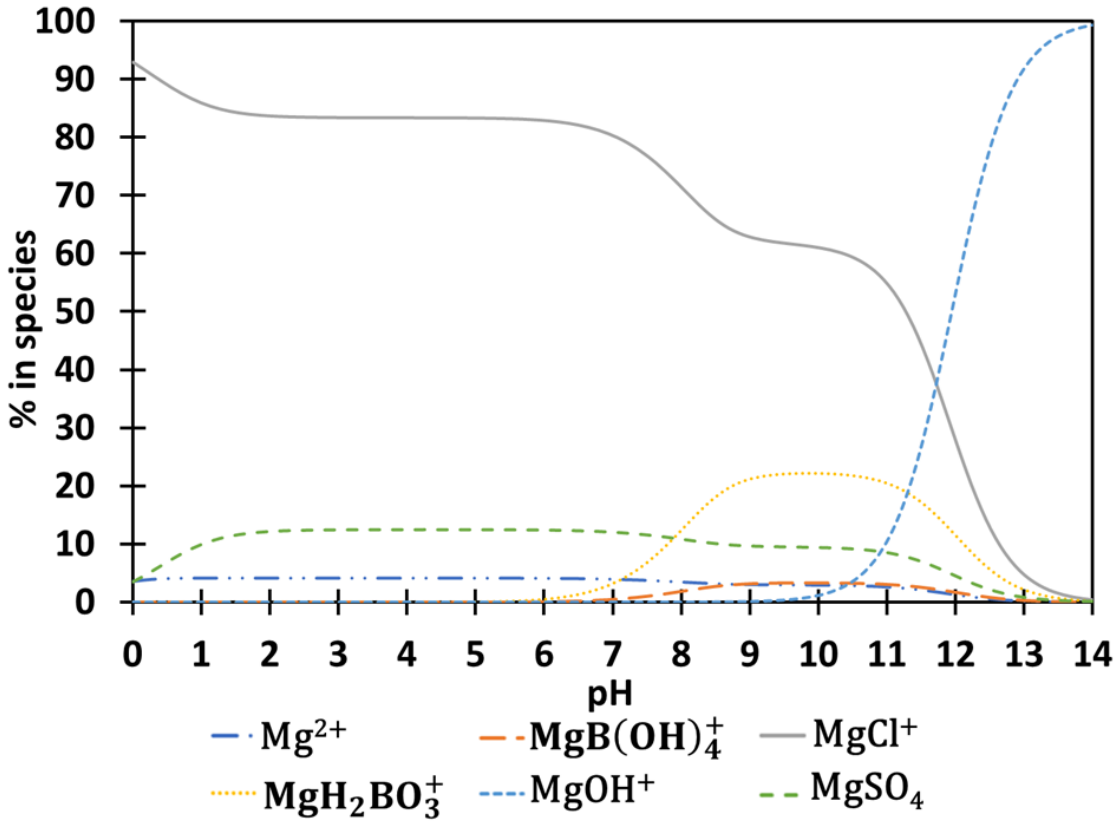


Fig. S5 Magnesium speciation in the synthetic brine vs. pH.

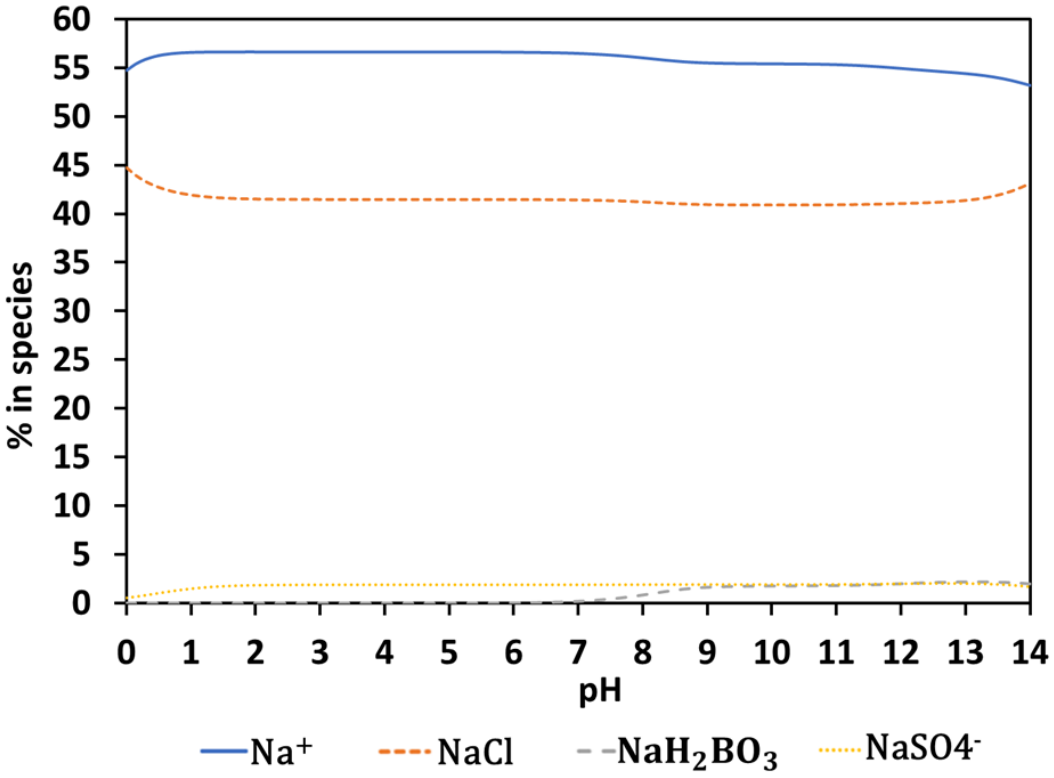
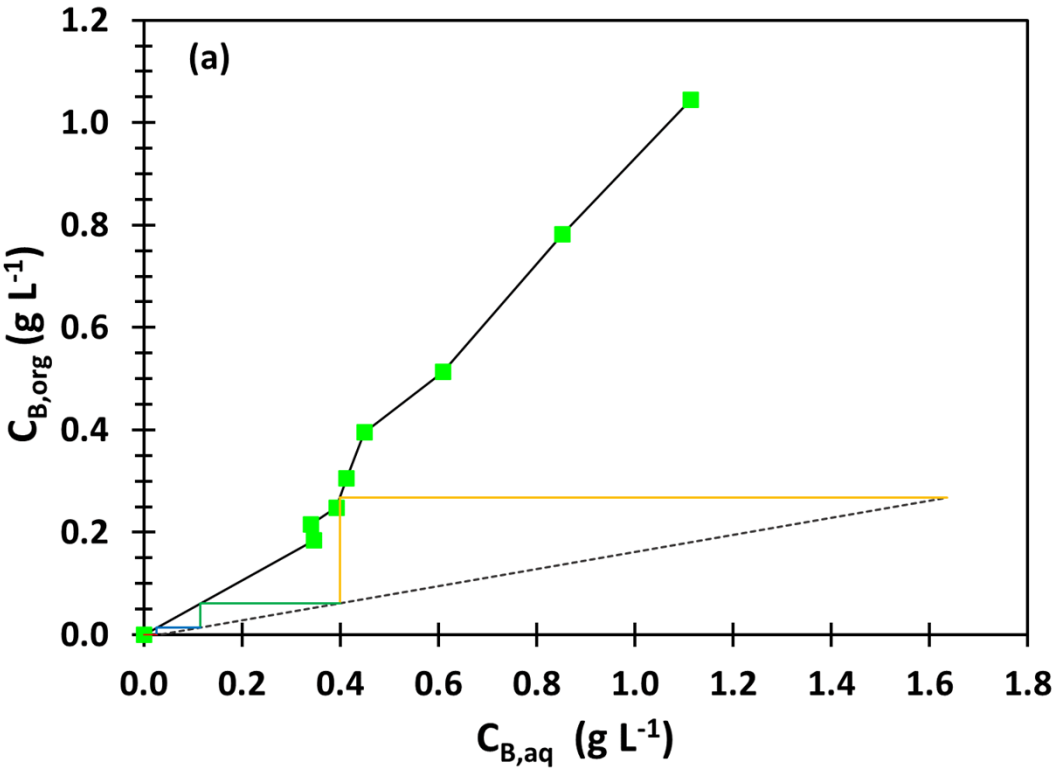


Fig. S6 Sodium speciation in the synthetic brine vs. pH.



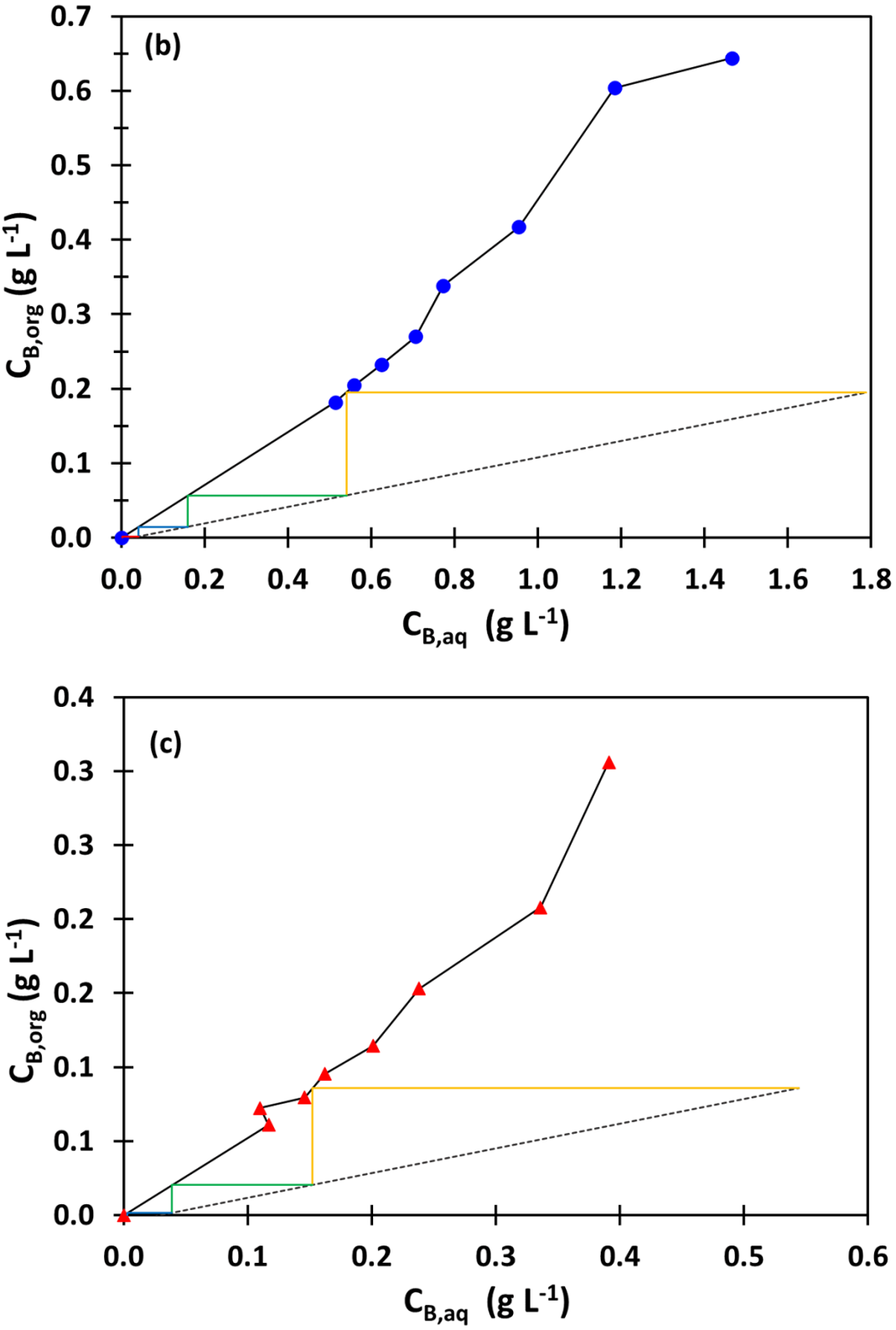


Fig. S7 McCabe-Thiele diagrams for boron removal from (a) the synthetic brine (SB) at O/A=6, (b) the native brine 1 (NB1) at O/A=9 and (c) the native brine 2 (NB2) at O/A=6 .

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