

Electronic Supporting Information

Condition Screening and Process Investigation of Aldose Transformation in Borate-containing Acidic Phosphate Buffer System under Microwave Irradiation

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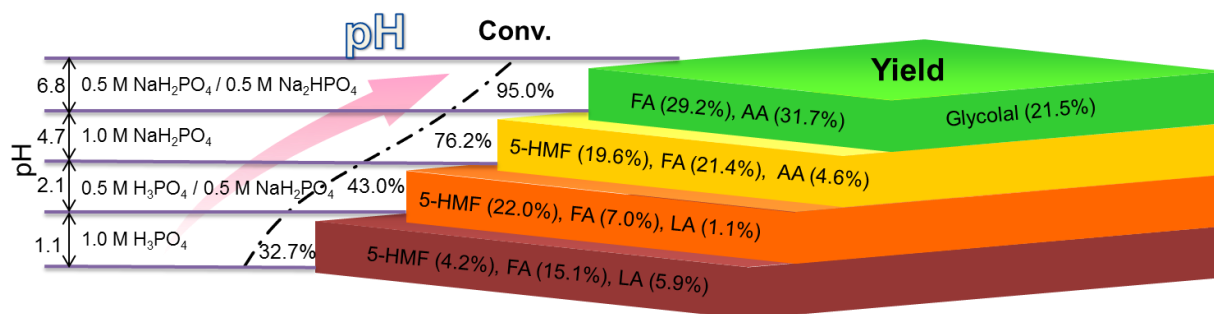


Figure S1. The conversion of glucose (10 wt.%) and the corresponding product distributions in PBS system without borate at different pH values under microwave irradiation. Conditions: reaction time = 90 min, and reaction temperature = 160 °C. 5-HMF: 5-hydromethylfurfural; LA: levulinic acid; FA: formic acid; AA: acetic acid; Conv.: Conversion.

Table S1. Influence of B/F ratio on the conversion of fructose into 5-HMF under microwave irradiation.^[a]

B/F	Conv. (%)	Y. 5-HMF (%)	S. 5-HMF (%)	Y. Glucose (%)
0	96.6	51.8	53.6	2.6
0.5	93.6	49.2	52.6	4.7
1	91.2	44.7	49.0	5.5
1.5	96.7	22.0	22.8	4.5

^[a] Reaction conditions: 10 wt.% fructose in 0.5 M H₃PO₄ / 0.5 M NaH₂PO₄ PBS system, B/F = 0-1.5, reaction time = 30 min and reaction temperature = 160 °C

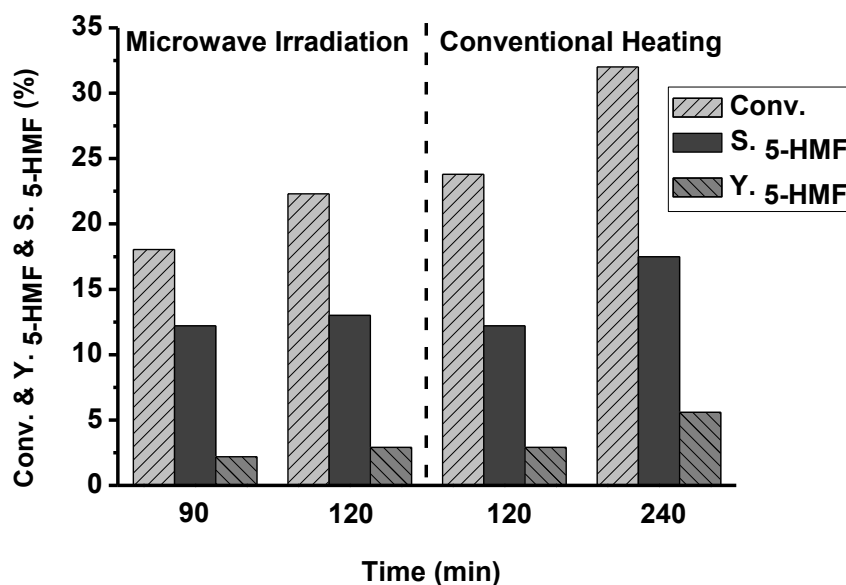


Figure S2. The conversions of 10 wt.% glucose in the pure water under microwave irradiation and conventional heating at 160 °C. 5-HMF: 5-hydroxymethylfurfural; Conv.: Conversion; Y.: Yield; S.: Selectivity.

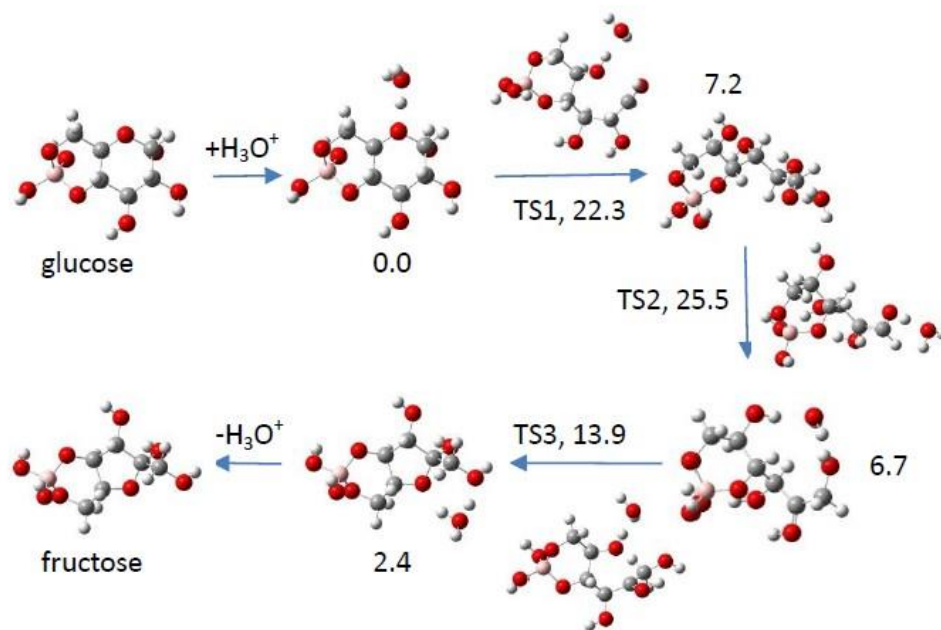


Figure S3. Gibbs free-energy profiles at 298.15 K and structures of the intermediates and transition states of the isomerization of glucose to fructose via 4,6-boroglucofuranose with the help of proton. The numbers are relative free energies (in kcal/mol) to the complex between D-glucose and H_3O^+ .

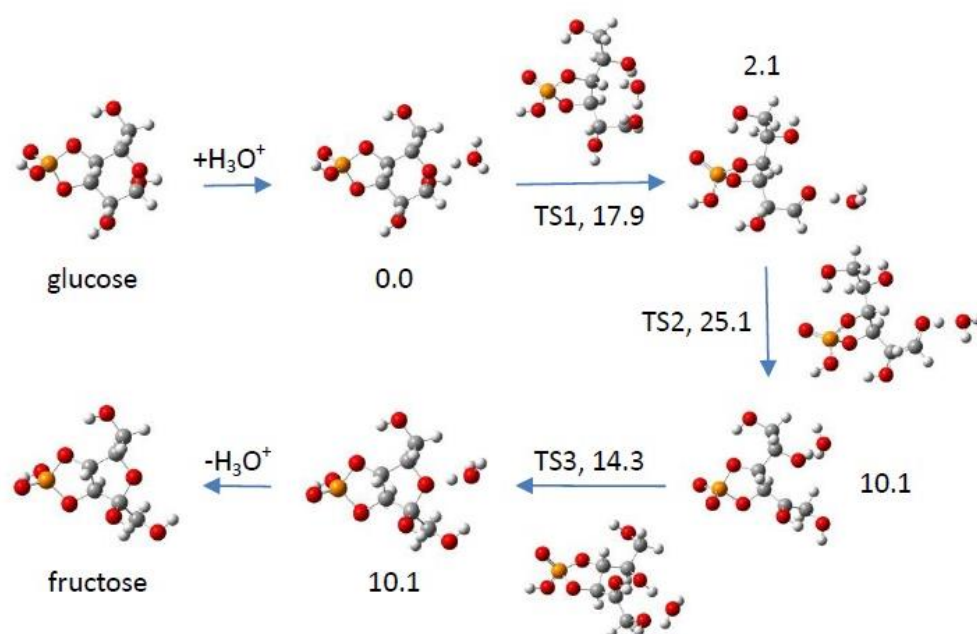


Figure S4. Gibbs free-energy profiles at 298.15 K and structures of the intermediates and transition states of the isomerization of glucose to fructose with the help of proton and H_3PO_4 . The numbers are relative free energies (in kcal/mol) to the complex between D-glucose and H_3O^+ .