Metal-Free Dehydration of Glucose to 5-(Hydroxymethyl)furfural in Ionic Liquids with Boric Acid as a Promoter

The dehydration of glucose and other hexose carbohydrates to 5-(hydroxymethyl)furfural (HMF) was investigated in imidazolium-based ionic liquids with boric acid as a promoter. A yield of up to 42% from glucose and as much as 66% from sucrose was obtained. The yield of HMF decreased as the concentration of boric acid exceeded one equivalent, most likely as a consequence of stronger fructose–borate chelate complexes being formed. Computational modeling with DFT calculations confirmed that the formation of 1:1 glucose–borate complexes facilitated the conversion pathway from glucose to fructose. Deuterium-labeling studies elucidated that the isomerization proceeded via an ene–diol mechanism, which is different to that of the enzyme-catalyzed isomerization of glucose to fructose. The introduced non-metal system containing boric acid provides a new direction in the search for catalyst systems allowing efficient HMF formation from biorenewable sources.