

Fig. 1. 5-HMF yield in the cellobiose decomposition in DMSO/water mixture solvent.

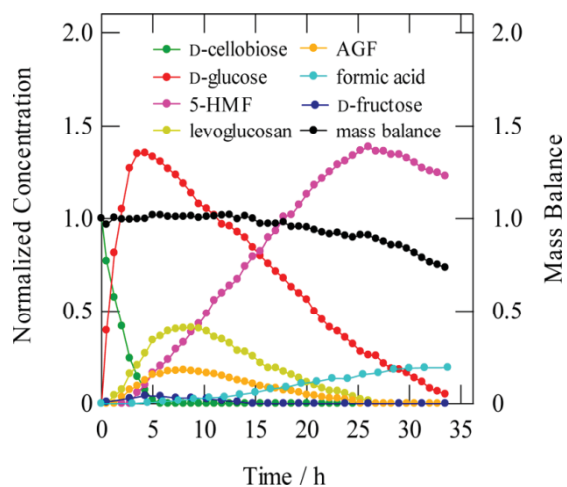


Fig. 2. Time course of the reactant and product of the decomposition of cellobiose determined by using  $^{13}\text{C}$  in situ NMR monitoring.

## Content:

Biomass-derived poly-saccharides have attracted attentions as the novel renewable sources. Recently we succeeded in the production of 5-hydroxymethyl-2-furaldehyde (5-HMF) from cellobiose, the model disaccharide for cellulose (H. Kimura et al., *J. Phys. Chem. A*, 117, 10987 (2013); Fig. 1). 5-HMF is a center of focus today as a biomass-derived valuable that can be converted into biofuels, fine chemicals, and polymers.

In the decomposition reaction steps of saccharides, a variety of isomers, tautomers, and precursors are generated as intermediate products. Solution NMR spectroscopy is a powerful method to monitor all of those species involved in the reactions. By using  $^{13}\text{C}$  NMR, each of the individual species can be distinguished from each other. The positions of the glucose units in the oligomers can be specified. The in situ NMR method allows us to determine the time course of the product and reactant species. As shown in Fig. 2, reliable data are obtained with a single setup of the in-situ experiment. The best conditions for the target species can be determined on the basis of the reaction kinetics.

Keywords: saccharides, in situ NMR, 5-HMF

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