Electronic Supplementary Material (ESI) for Green Chemistry

Supporting Information

Highly efficient production of lactic acid from cellulose using lanthanide triflate catalysts

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1. Materials

D-Fructose (99%) and D-glucose (99%) were purchased from Tianjin Chemical Reagents Company. Formic acid (99%), Levulinic acid (99%), Acetic acid (99%), dihydroxyacetone (99%), microcrystalline cellulose (Cat.: 31069-7, CAS No.: 9004346, particles size of 20μm), $La(OTf)_3$ (99.99%), $Ce(OTf)_3$ (99.99%), $Pr(OTf)_3$ (99.99%), $Nd(OTf)_3$ (98%), $Sm(OTf)_3$ (98%), $Dy(OTf)_3$ (99%), $Ho(OTf)_3$ (98%), $Er(OTf)_3$ (99%), $Yb(OTf)_3$ (99.99%), $Lu(OTf)_3$ (99.99%), HMF (98%) were all obtained from Sigma-Aldrich. Lactic acid (98%), pyruvaldehyde (98%), glyceraldehyde (99%) and inulin were purchased from Alfa Aesar. D-(+)-Cellubiose was obtained from Sinopharm Chemical Reagent Co. Ltd. (Shanghai, China). Starch was obtained from Beijing Aoboxing bio-tech Co. Ltd. All the other reagents were analytical reagents and used without further purification.

2. Experimental Section

All the reactions were carried out in a 35 mL stainless steel autoclave equipped with a mechanical stirrer. In a typical experiment, 0.3 g cellulose, 0.05 g catalyst, and 30 mL water were charged into the reactor. The autoclave was purged three times with pure N_2 and then pressurized to 2.0 MPa with N_2 at room temperature. The reaction mixture was heated to 240 ^oC and held at the temperature for 30 min under a stirring rate of 600 rpm. After the reaction, the reactor was cooled quickly down to room temperature, and the post-reaction sample was diluted with mobile phase solution before analysis.

Sample analysis was performed on a Shimadzu HPLC LC-20AT system equipped with a RID-10A detector and a Bio-Rad Aminex HPX-87H ion exclusion column (300 × 7.8 mm). 0.005 M H_2SO_4 was used as the mobile phase that had a flow rate of 0.5 mL/min. The column temperature was 50 ^oC, and the detector temperature was set at 45 ^oC. The amount of products was determined by using calibration curves.

The carbon content in various substrates *i.e.* cellulose, inulin, cellubiose and starch was analyzed by a Vario EL III CHNS analyzer.

3. The cellulose conversion and product yield definitions

The conversion of cellulose and product yields were defined as follows:

Cellulose conversion (wt. %):

$$X = \left(1 - \frac{mass\ of\ unconverted\ cellulose}{mass\ of\ initial\ cell\ ulose}\right) \times 100\%$$

Product yields (C- %):

$$Yi = \frac{mole\ of\ carbon\ contained\ in\ product\ i}{mole\ of\ carbon\ \ contained\ in\ initial\ ce\ llulose} \times 100\%$$

4. Supporting Figures (Figs. S1-S2)

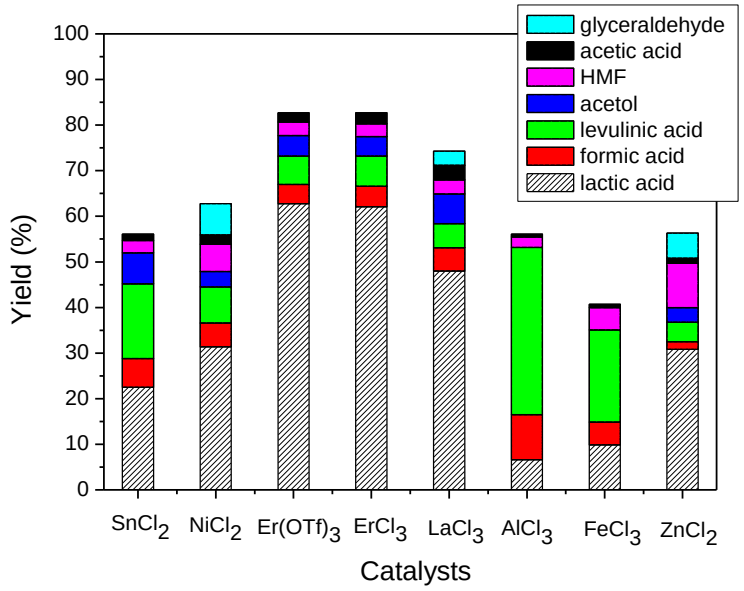

Fig. S1. Comparison of catalytic performance of various catalysts in the hydrolysis of cellulose. (Reaction conditions: cellulose 0.3 g, water 30 mL, catalyst 0.05 g, 240 ºC, 2 MPa N_2, 30 min)

The cellulose was converted completely over all the catalysts.

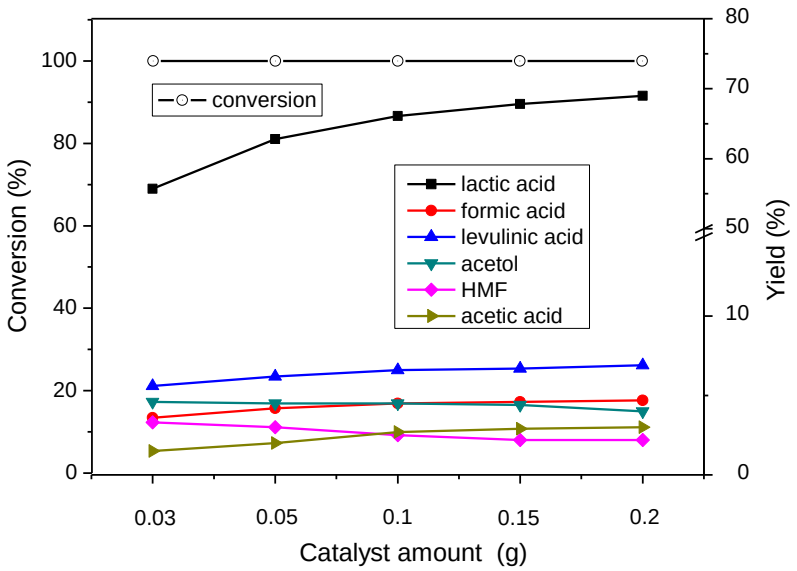

Fig. S2. The influence of catalyst amount on the yield of lactic acid. (Reaction conditions: cellulose 0.3 g, water 30 mL, 240 ºC, 2 MPa N_2, 30 min.)