Supporting Information

A Novel Pd/C-Catalysed Conversion of Glucose to 1,2-Propanediol by Water Splitting with Zn

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Contents of Supporting Information

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1. General Information:D-(+)-Glucose anhydrous (AR，Sinopharm Chemical Reagent Co., Ltd) was used as reagent.Ethylene glycol (≥ 99.5%, GC),1,2-propanediol(≥ 99.5%, GC) and 1,2-Butanediol (>98.0%, GC) were purchased from TCI for the qualitative analysis of the products in the liquid samples. Pd/C(5 wt. %, wet, water *ca.* 50%, Aldrich Chemistry) was used as reduction catalyst. Fructose(AR，Sinopharm Chemical Reagent Co., Ltd)and Hydroxyacetone (95%,GC, Alfa Aesar) were used as intermediate products.As preliminary tests, various active metals and metal oxide including Zn, Fe, Al,$Ni_2O_3$and CuO (150-200 mesh,AR, Sinopharm Chemical Reagent Co., Ltd) were used in powder form.

2. Product analysis: After reaction the liquid samples' analyses were confirmed by GC-MS (Agilent GC7890A-MS5975C) equipped with anHP-INNOWax polyethylene glycol capillary column with dimensions of 30 m × 250 μm × 0.25 μm.For quantitative determination of 1,2-alkanediol, glucose and fructose,the HPLC was performedon KC-811 columns(SHODEX) with an Agilent Technologies 1260 system, which was equipped with a refractive index(RI) detectors. The solvent was 2mM $HClO_4$ with a flow rate of 0.8 $ml{\cdot}min^{-1}$. Acetol was analyzed by a GC-FID (Agilent7890A GC System) equipped with a HP-INNOWax Polyethylene Glycol column with dimensions of 30 m × 320μm × 0.25 μm. Collected gas was analyzed by a GC-TCD (Agilent 7890A GC System) equipped withTDX-1columm.The solid samples were characterized by X-ray diffraction (XRD) (Shimadzu XRD-6100) to determine the composition and phase purity.TOC (total organic carbon) was analyzed with Shimadzu TOC 5000A.

The yields of productsare defined as the carbon mole ratio of pruduct to the initial reactant as follows below. The yields were obtained from experiments over three times and relative error was less than 5%.

$$Yield,\ mmol\ \% = \frac{C\ in\ products,\ mmol}{C\ in\ the\ initial\ reactants,\ mmol} \times 100\ \%$$

3. General Procedure for reactions: Experiments were conducted in a series of batch SUS316 tubing reactors with an inner volume of 5.7 mL. The typical procedure was as follows. The desired amounts ofreactants and deionized water were loaded into reactor. Then the reactor was sealed and placed into a salt bath that had been preheated to the desired temperature. After the preset reaction time, the reactor was removed from the salt bath and then placed into a cold water bath to quench the reaction. After cooling to room temperature, the reaction mixture was collected

and filtered through a 0.22 μm Syringe for analysis. The water filling was defined as the ratio of the volume of the water put into the reactor to the inner volume of the reactor, and the reaction time was defined as the duration of time which the reactor was kept in the salt bath.

4. GC-MS and HPLC chromatograms of EG, 1,2-PG and 1,2-BD

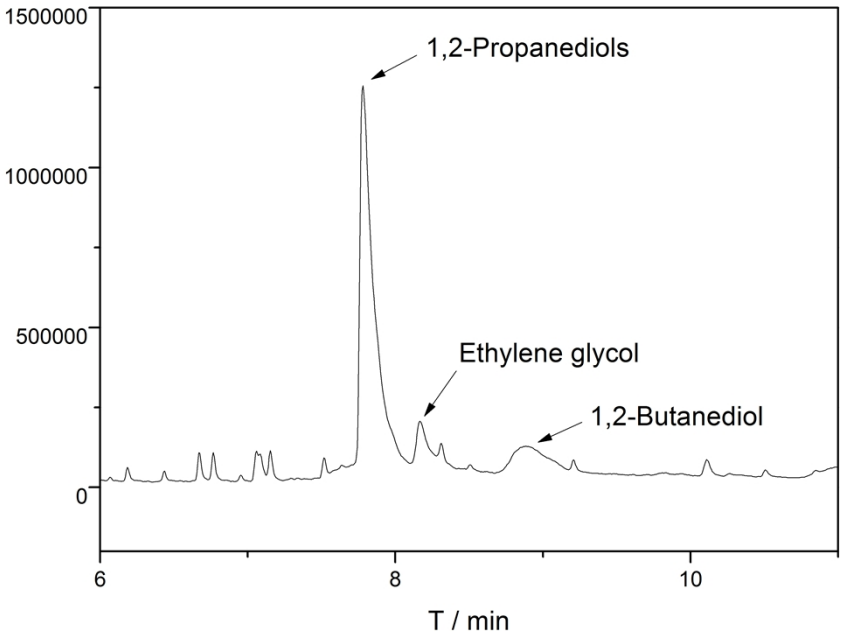


Fig.SI-1(a).GC-MS chromatograms of EG, 1,2-PG and 1,2-BD

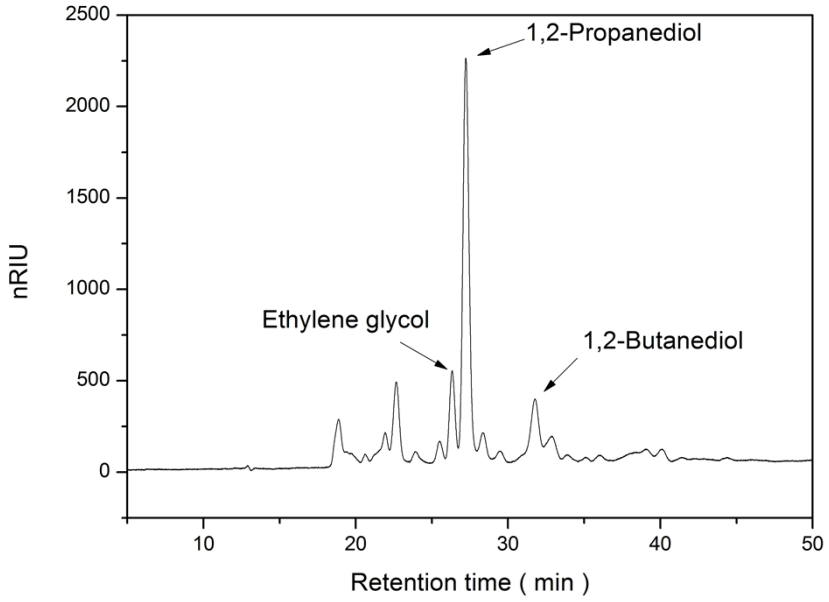


Fig.SI-1(b).HPLCchromatograms of EG, 1,2-PG and 1,2-BD

5. GC-MS chromatograms ofthe products of glucose transformation

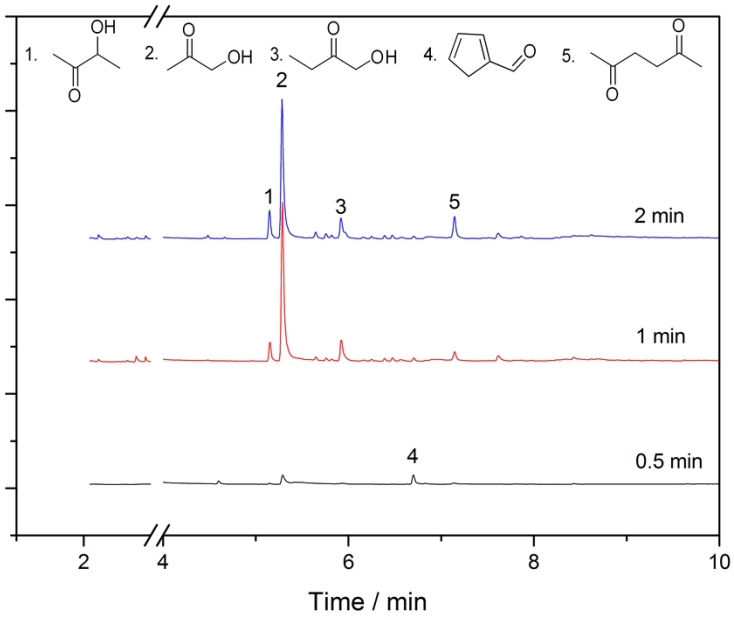


Fig.SI-2 (a).GC-MS chromatograms of the products of glucose transformation over 70mg 5% Pd/C: dependence on reaction time at 250°C and 6.9 mmol Zn.

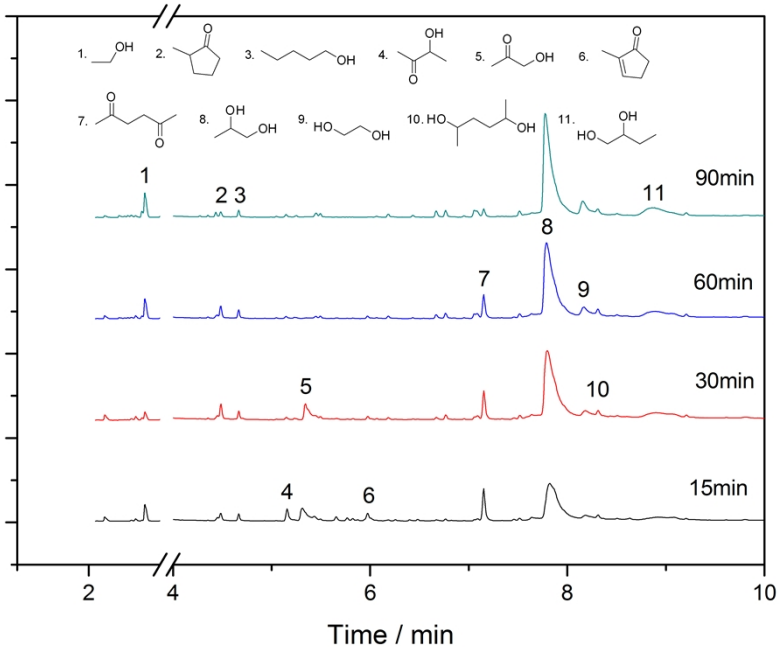


Fig.SI-2 (b).GC-MS chromatograms of the products of glucose transformation over 70mg 5% Pd/C: dependence on reaction time at 250°C and 6.9 mmol Zn.

6. GC-FID chromatograms of Acetol

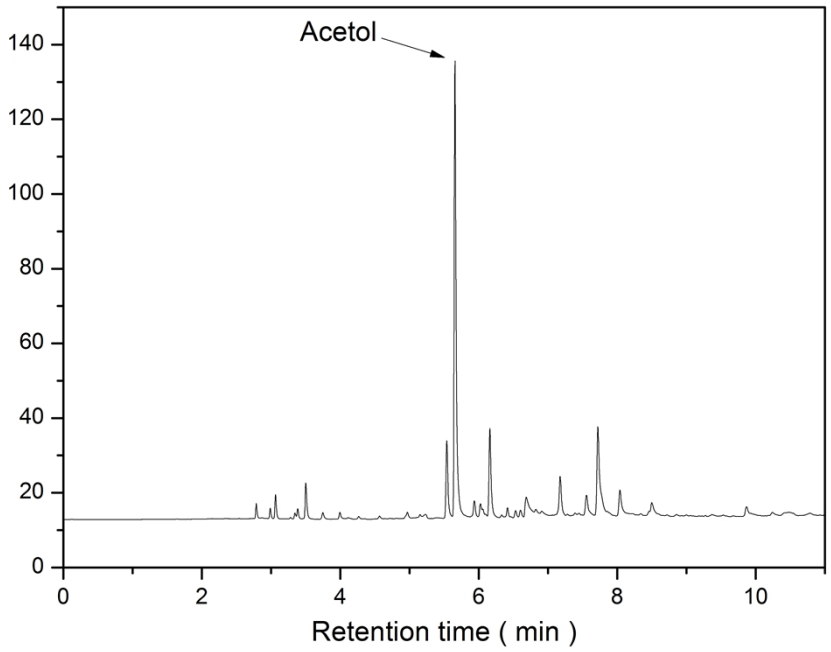


Fig. SI-3 GC-FID chromatograms of Acetol

7. HPLC chromatograms of Glucose and Fructose

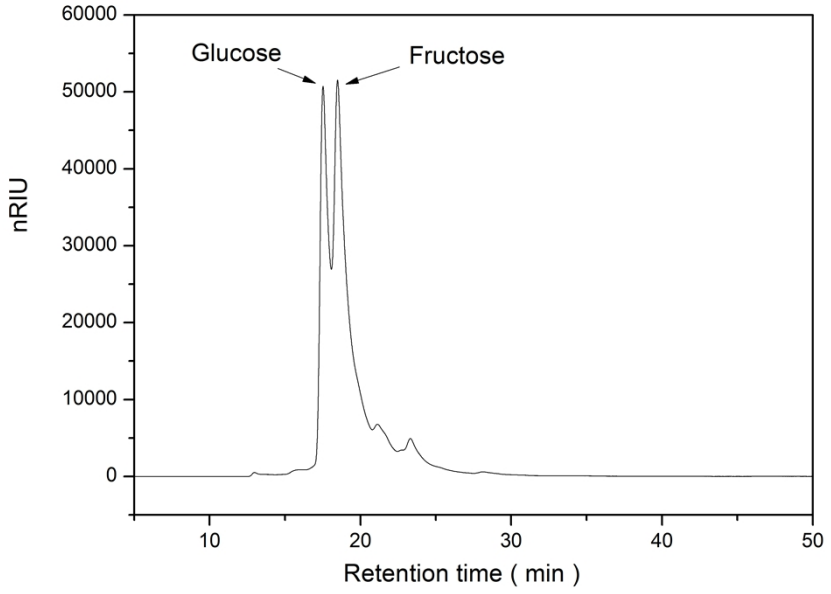


Fig. SI-4 HPLC chromatograms of Glucose and Fructose

8. XRD analysis

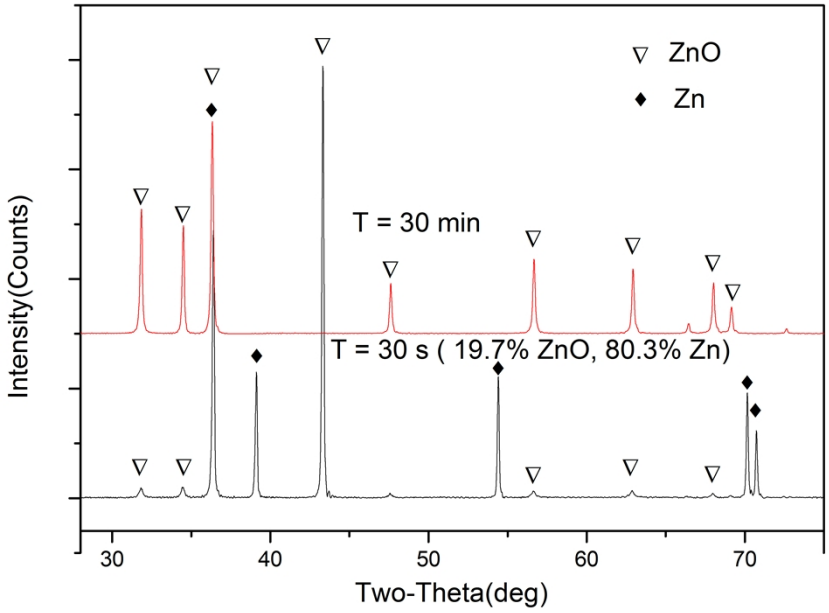


Fig.SI-5. XRD patterns of solid samples after reaction (glucose: 1.11mmol; Zn: 6.9mmol;Pd/C: 35 mg; water filling: 50%; 30 min; 250 °C). The conversion of Zn is defined as the percentage of amount of ZnO, which was quantified by MDI jade software based on XRD patterns.

9. Yields of 1,2-propandiol over ZnO + Pd/C + H_2 or Zn with acetol as feedstock

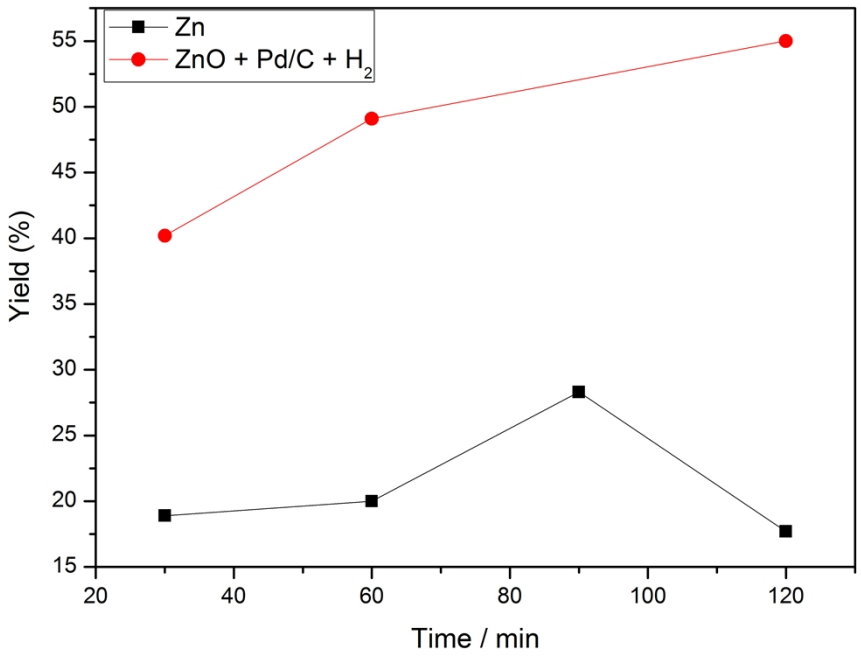


Fig.SI-6. Yields of 1,2-propanediols over ZnO + Pd/C + H_2 or Zn with acetol as feedstock: dependence on the time at 250°C, 1.1mmolacetol, 35mg Pd/C, 6MPa H_2, and water filling: 50%.

10. Products distribution of glucose isomerization

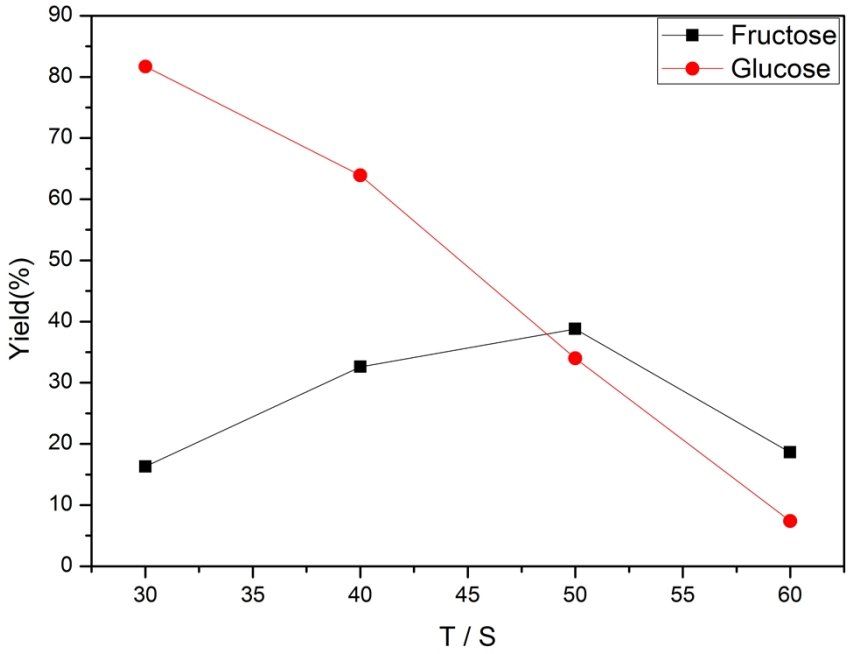


Fig.SI-7. Products distribution of glucose isomerization over 112 mg ZnO at 250°C

11. GC-TCD chromatograms of collected gas

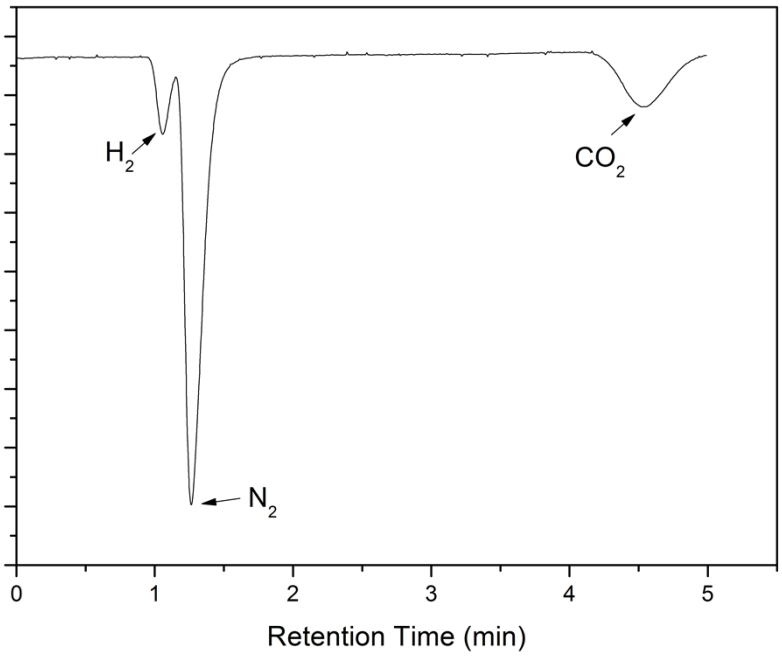
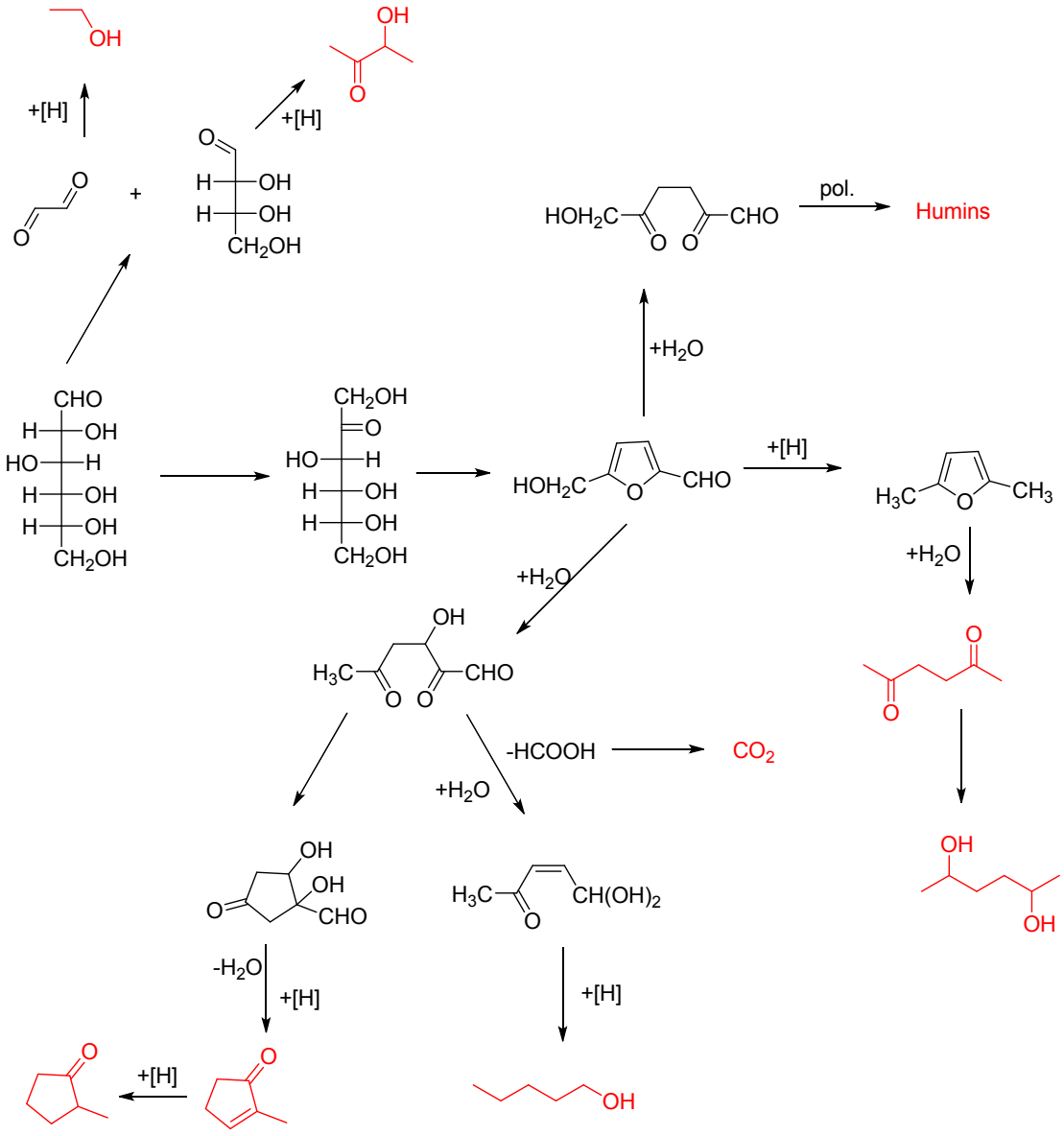


Fig. SI-8GC-TCD chromatograms of gas sample under the optimized condition

12. The possible side reactions.



Scheme. SI-1 The possible side reactions under the optimized conditions. The side products are highlighted in red.