

Supporting information for

**Multi-Functional Porous Cobalt Catalyst for the Selective Hydrogenative
Ring-Opening and Rearrangement of Furfural to Cyclopentanol**

Xing-Long Li ^{a,b}, Rui Zhu ^{a*}

^a. *Anhui Province Key Laboratory of Biomass Clean Energy,*

Department of Chemistry, University of Science and Technology of China, Hefei 230026, China. Fax: (+86) -551-63606689;

E-mail: zhr520@mail.ustc.edu.cn

^b. *Institute of Energy, Hefei Comprehensive National Science Center, Hefei 230031, China.*

I. Experimental

General

If not stated otherwise, the reaction was carried out in an autoclave sponsored by Anhui Kemi Machinery Technology Co., Ltd. Usually, the initial temperature is 30 °C.

Catalyst Cycle Experiment

Since the catalyst is magnetic, it can be adsorbed on the magneton. Therefore, the experimental steps of the catalyst circulation are as follows: after the reaction, the reaction solution is taken out, and the magneton is rinsed with methanol and water, and the solutions are combined. The catalyst goes directly to the next cycle without additional treatment under the same reaction conditions. The reaction solution was transferred and diluted into sample vials with methanol, and a quantitative amount of N, N-dimethylformamide (DMF) was added as an internal standard. After centrifugation, the distribution of the product was checked by gas chromatography.

II. Results

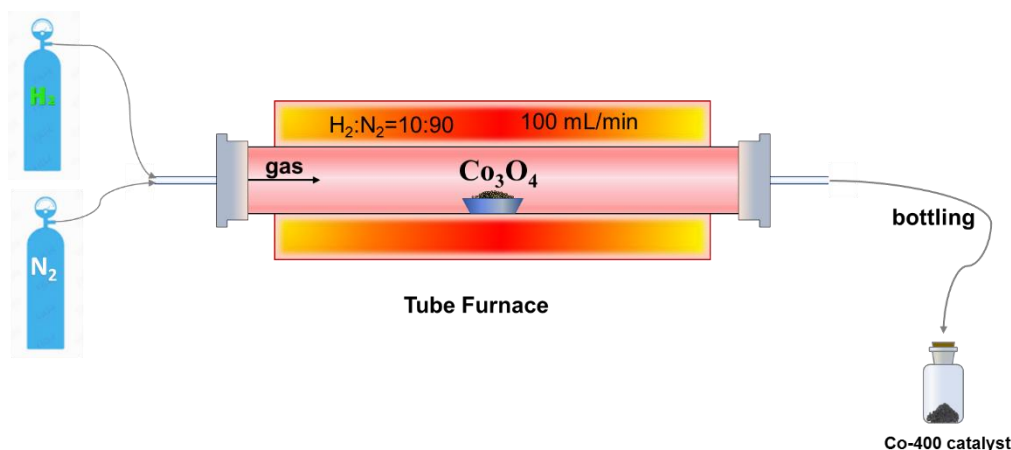


Figure S1. Schematic diagram of catalyst preparation.

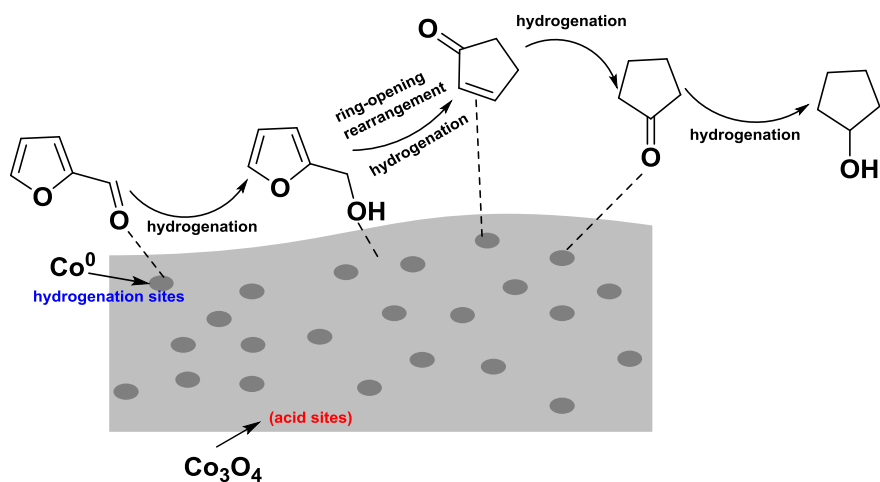


Figure S2. Schematic diagram of reaction mechanism.



Figure S3. Schematic diagram of Co-400 catalyst dispersed in aqueous solution (left); Schematic diagram of Co-400 catalyst dispersed in aqueous solution after adsorption with magnet (right)

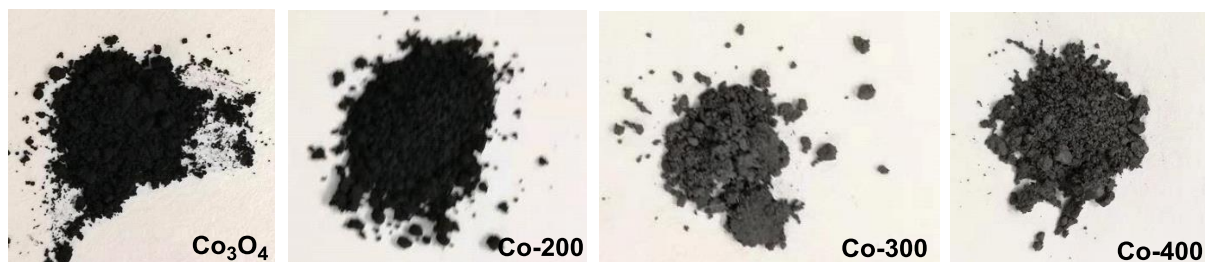


Figure S4. Appearance comparison of the reduced Co catalyst and Co_3O_4 .

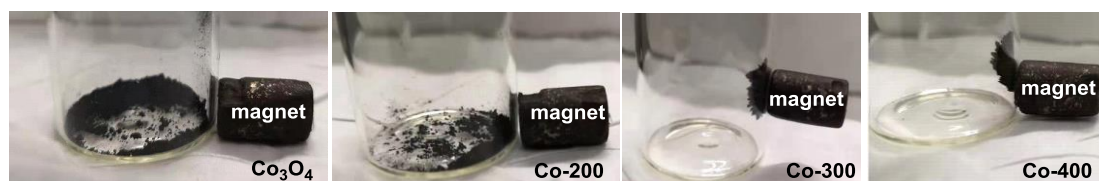


Figure S5. The magnetic effects of the reduced Co catalyst and Co_3O_4 .

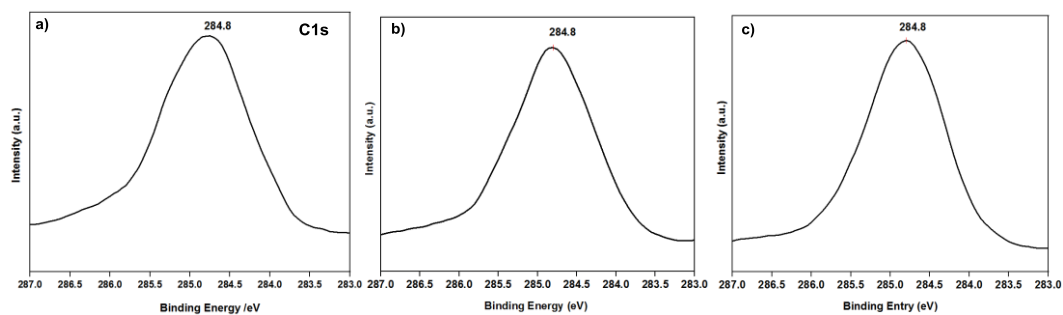


Figure S6. The C1s XPS spectra of Co catalysts with different reduction temperature. a) Co-200 catalyst, b) Co-300 catalyst, c) Co-400 catalyst.

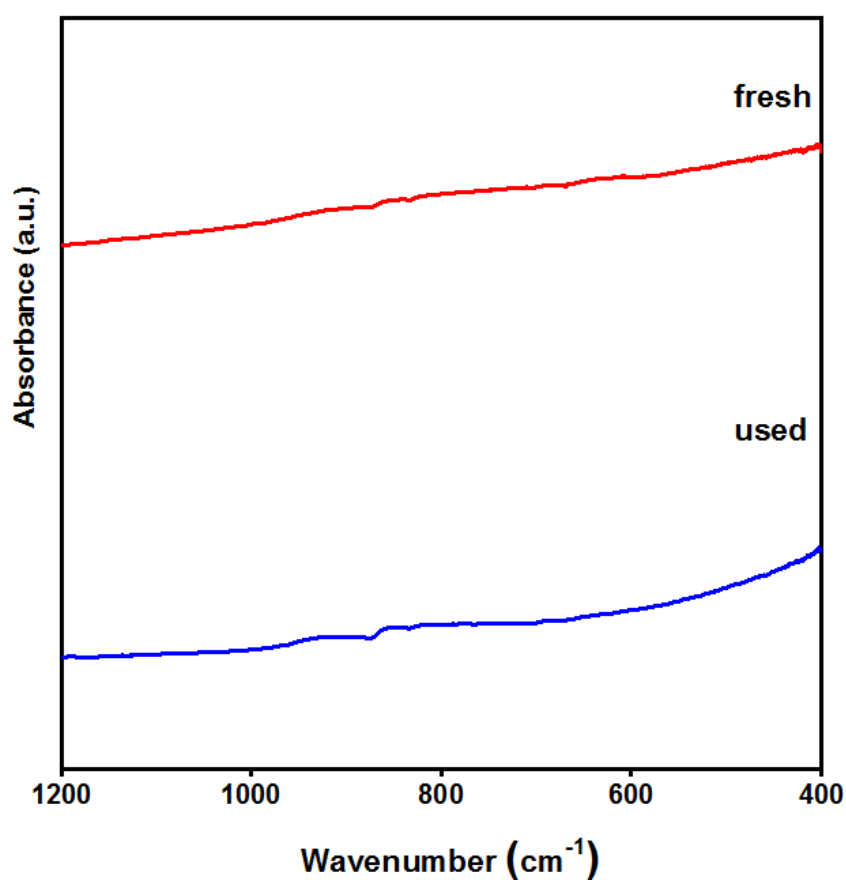


Figure S7. The FT-IR spectra of fresh Co-400 catalyst and Co-400 catalyst after reused 4 times.

It can be seen from the FT-IR spectra that the structure and composition of the Co-400 catalyst did not change significantly after the cycle. No apparent crystalline Co_3O_4 was observed.

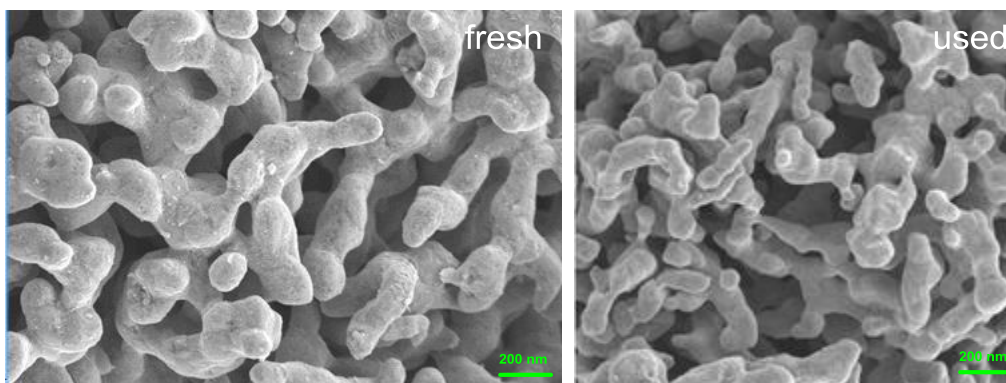


Figure S8. The SEM image of fresh Co-400 catalyst and Co-400 catalyst after reused 4 times.

It can be seen from the SEM image that the catalyst after recycling is still porous and rough, and the overall structure has not changed significantly.

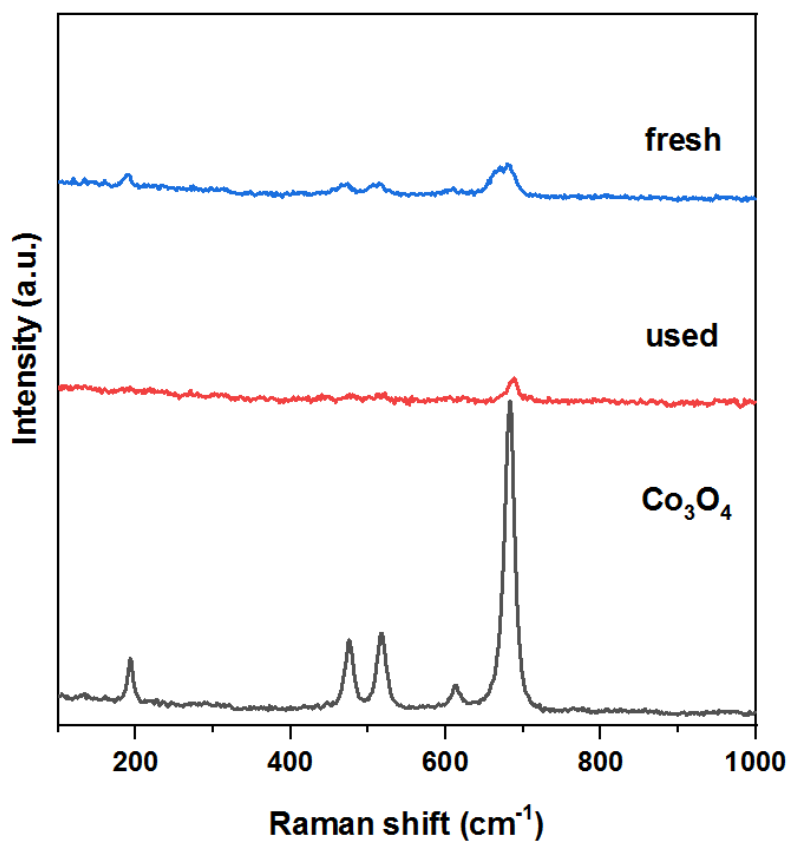


Figure S9. The Raman spectra of Co₃O₄, fresh Co-400 catalyst and Co-400 catalyst after reused 4 times.

It can be seen from the Raman spectra that the crystallinity of the recovered Co-400 catalyst has further decreased, which may be related to the reduction atmosphere in the reaction.

Surface composition of Co catalysts with different reduction temperature obtained according to the XPS analysis.

Table S1. Surface composition of Co catalysts obtained from XPS analysis

| Entry | Catalysts | Content (%) | | |
|-------|-----------|-----------------|------------------|------------------|
| | | Co ⁰ | Co ²⁺ | Co ³⁺ |
| 1 | Co-200 | 34.0 | 31.2 | 34.8 |
| 2 | Co-300 | 32.1 | 31.6 | 36.3 |
| 3 | Co-400 | 29.3 | 32.0 | 38.7 |

The leaching of metal Co in reaction solution were detected by ICP-AES analysis

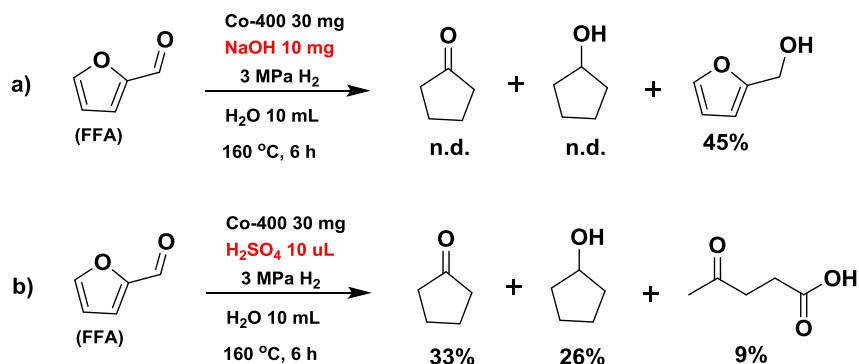
Table S2. The leaching of metal Co

| Entry | Catalyst recirculation | The leaching of Co /% |
|-------|------------------------|-----------------------|
| 1 | fresh | 0.4 |
| 2 | 1 | 0.3 |
| 3 | 2 | 0.2 |
| 4 | 3 | 0.2 |

Reaction conditions: FFA 0.1 g, Co-400 catalyst 30 mg, H₂O 10 mL, 160 °C, 5 h, 3 MPa H₂, mole Yield.

The leaching of Co in the reaction solutions was measured by Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES, Thermo-Jarrell ASH-Atom Scan Advantage). ICP-AES tests: after the reaction, magnets separate out the catalyst. The reaction solution was centrifuged and evaporated to dryness under reduced pressure. The residue were dissolved with concentrated nitric acid and diluted with pure water.

The effect of additional addition of acid and alkali on the production distribution.



Scheme S1. The effect of additional addition of acid and alkali on the production distribution.