

Supporting Information

Direct synthesis of jet fuel range dicycloalkane by the aqueous phase hydrodeoxygenation of polycarbonate

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Properties of pure PC pellets and chopped DVD disk

In this work, the average molecular weights, the melt points and the decomposition temperatures of the pure PC pellets and chopped DVD disk were measured by a waters 1525 & Agilent PL-GPC220 gel permeation chromatography (GPC), a X-5 micro melting point apparatus (Beijing Tech Instrument Co. LTD) and a SDTQ600 thermogravimetric (TG), respectively. The chemical composition of the chopped DVD disk was measured by an elemental vario el III elemental analyzer. According to our analysis, the weight percentages of C (75.8 wt%), H (5.4 wt%), O (18.8 wt%) in the chopped DVD disk are very close to their theoretical values (C (75.6 wt%), H (5.5 wt%), O (18.9 wt%)), indicating the chopped DVD disk has high purity and can be considered as pure PC in the calculation of conversion and the yield of different products.

CO-chemisorption

The metal dispersions in M/C (M = Rh, Ru, Pd) catalysts (see Table S1) were measured with a Micromeritics AutoChem II 2920 Automated Catalyst Characterization System based on the molar ratios of CO chemisorption and noble metals in the catalysts. These values correspond to the ratios of surface metal atoms to total metal atoms assuming that the stoichiometry of adsorbed CO to surface metal atom is one. Before the tests, the samples (100 mg) were flushed with H₂ for 0.5 h at room temperature, dried in He flow at 473 K for 0.5 h and cooled down in He flow to 323 K. After the stabilization of baseline, the CO adsorption was carried out at 323 K by the pulse adsorption of 5% CO in He.

NH₃-TPD

The acidity of the Rh/C catalyst was characterized by NH₃-temperature programmed desorption (NH₃-TPD). Before each test, 0.1 g sample was placed in a quartz reactor,

pretreated in He flow at 773 K for 0.5 h and cooled down in He flow to 373 K. After the stabilization of base line, pulses of NH₃ (1 mL) were dosed in the reactor until saturation. Subsequently, the desorption of NH₃ was conducted in He flow from 373 K to 1073 K at a heating rate of 10 K min⁻¹. The desorbed NH₃ molecules were detected by a mass spectrometry (MS) OminiStar equipped with the software quadstar.

Table S1. Metal dispersion of the investigated M/C (M = Rh, Ru, Pd) catalysts.

Catalyst	Metal dispersion (%) ^a
Rh/C	2.1
Ru/C	4.0
Pd/C	11.5

^a Measured by CO-chemisorption.

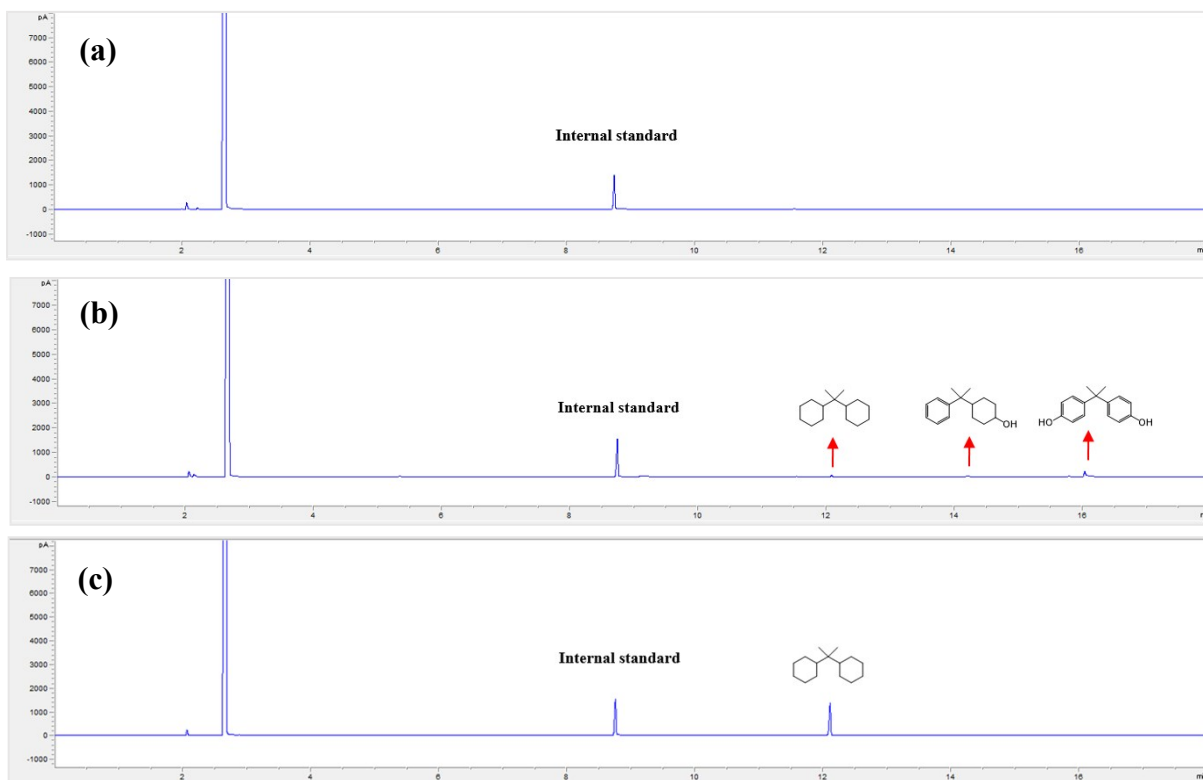


Figure S1. GC chromatograms of the products obtained the reaction of pure PC pellets over the H-USY (a), Rh/C (b) and Rh/C + H-USY (c) catalysts. Reaction conditions: 473 K, 3.5 MPa H₂, 12 h; 1 g pure PC pellets, 0.1 g Rh/C and/or 0.1 g H-USY catalyst and 40 mL H₂O were used in the tests.

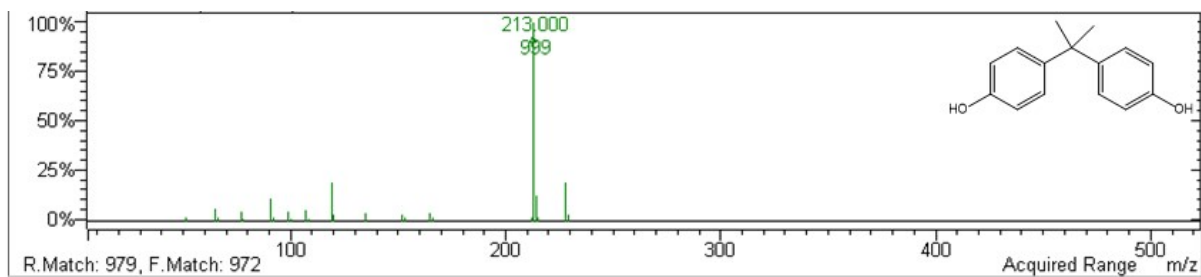


Figure S2. Mass spectrogram of the bisphenol A (BPA) from the aqueous phase hydrodeoxygenation (APHDO) of pure PC pellets over the Rh/C catalyst. Reaction conditions: 473 K, 3.5 MPa H₂, 12 h; 1 g pure PC pellets, 0.1 g Rh/C catalyst and 40 mL H₂O were used in the test.

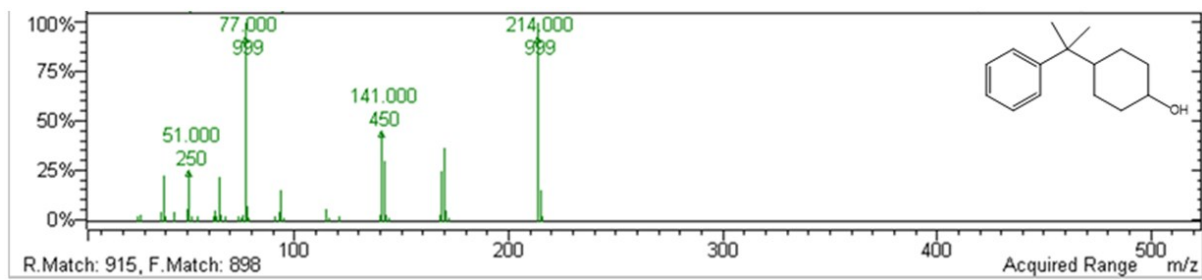


Figure S3. Mass spectrogram of the 4-(2-phenylpropan-2-yl)cyclohexanol from the APHDO of pure PC pellets over the Rh/C catalyst. Reaction conditions: 473 K, 3.5 MPa H₂, 12 h; 1 g pure PC pellets, 0.1 g Rh/C catalyst and 40 mL H₂O were used in the test.

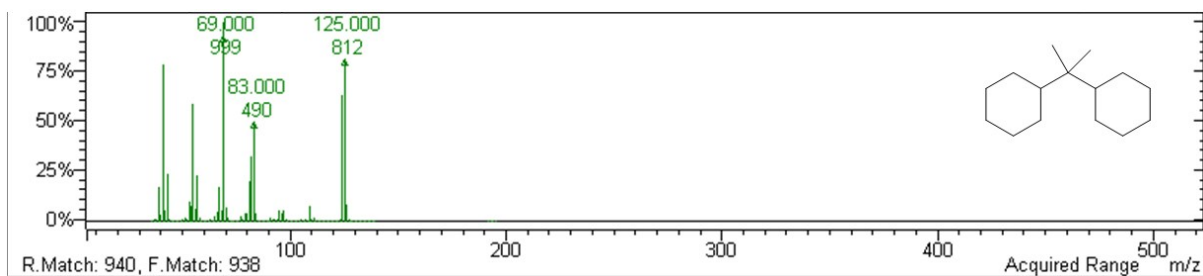


Figure S4. Mass spectrogram of the propane-2,2-diylidicyclohexane from the APHDO of pure PC pellets over the Rh/C catalyst. Reaction conditions: 473 K, 3.5 MPa H₂, 12 h; 1 g pure PC pellets, 0.1 g Rh/C and 40 mL H₂O were used in the test.

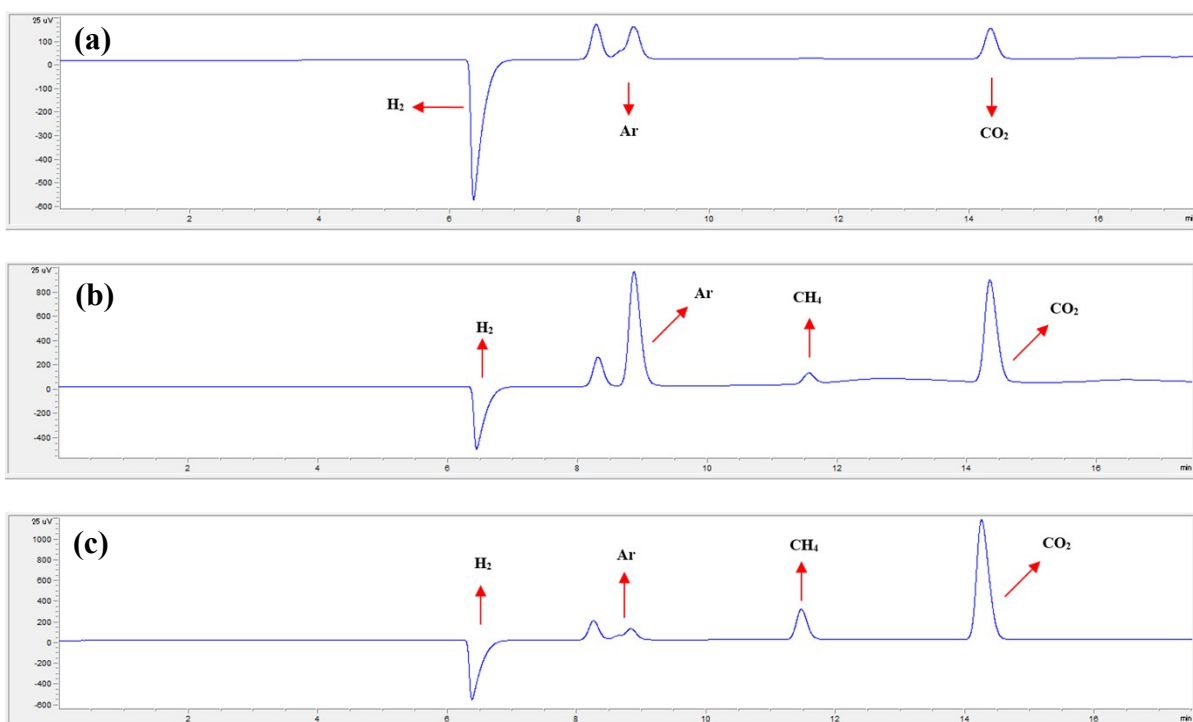


Figure S5. GC chromatogram of the gas phase products from the APHDO of pure PC pellets over the H-USY (a), Rh/C (b) and Rh/C + H-USY (c) catalysts. Reaction conditions: 473 K, 3.5 MPa H_2 , 12 h; 1 g pure PC pellets, 0.1 g Rh/C and/or 0.1 g H-USY catalyst and 40 mL H_2O were used in the tests (Ar was used as the shielding gas).



Figure S6. Photo of the APHDO product after removal of catalyst and staying at room temperature for long time. Reaction conditions: 473 K, 3.5 MPa H₂, 12 h; 1 g pure PC pellets, 0.1 g H-USY, 0.1 g Rh/C and 40 mL H₂O were used in the test.

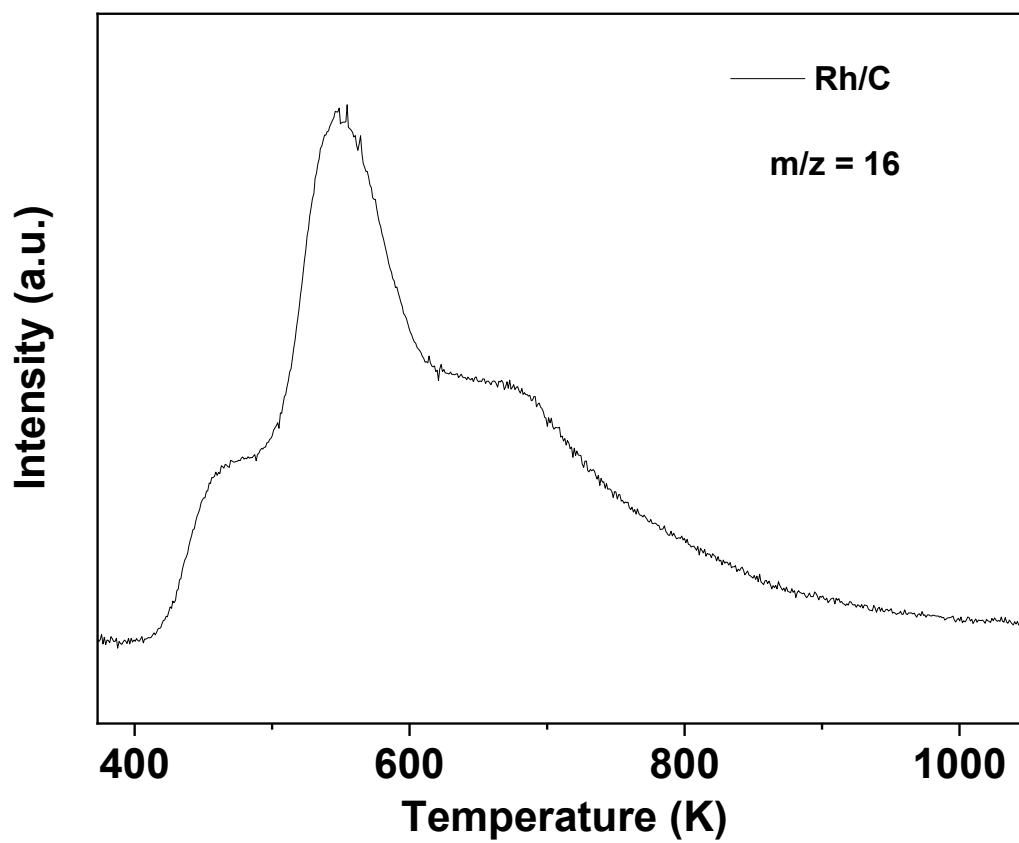


Figure S7. NH_3 -TPD profile of the Rh/C catalyst.

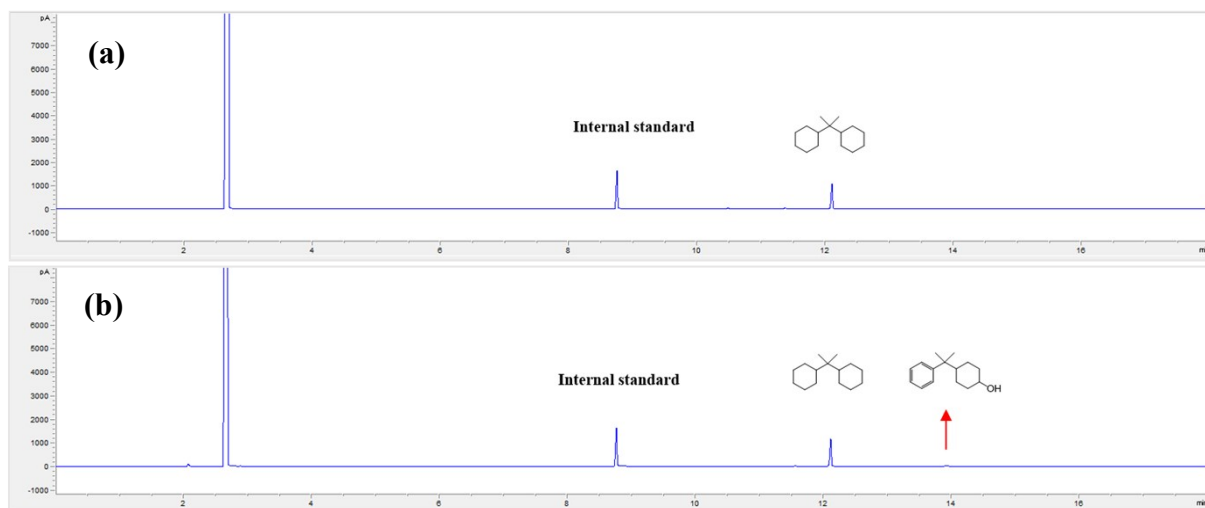


Figure S8. GC chromatograms of the products obtained the APHDO of pure PC pellets over the Ru/C + H-USY (a) and Pd/C + H-USY (b) catalysts. Reaction conditions: 473 K, 3.5 MPa H₂, 12 h; 1 g pure PC pellets, 0.1 g M/C (M = Ru or Pd), 0.1 g H-USY and 40 mL H₂O were used in the tests.