

Supporting Information

Preparation and Catalytic Performance of a Novel Organometallic CoH/H β catalyst for n-hexane isomerization

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S1. Characterization of Catalysts

A series of samples was synthesized following the foregoing procedure. The phase structure of the samples was analyzed on Japanese D/max-III A powder X-ray diffraction (XRD) equipment with a Cu-K α radiation source working at 35kV and 40 mA and scanning from 5° to 75° at a speed of 8° min⁻¹. The surface morphology of the catalyst was investigated by scanning electronic microscopy (SEM, Hitachi, S-4800). The surface acidity was measured by Fourier transformed infrared (Py-FTIR) spectroscopy by A Nicolet 6700 FTIR Fourier. Temperature programmed desorption of H₂ (H₂-TPR) and temperature programmed desorption of NH₃ (NH₃-TPD) were operated on TP-5076 TPD/TPR dynamic adsorption produced by Tianjin Xianquan Company. The samples (1g) were placed in a quartz reaction tube with a thermocouple built in, and followed by pretreating at 200 °C for 0.5 h in a helium gas stream (30 mL/min), and then cooled to 30°C, switched to hydrogen, and purged to make the baseline flat. Afterwards temperature programming rate achieved 10 °C/min. Sample flows into the reactor through a pump. After the reaction was completed, products were taken and analyzed using 6820 GC equipped with a FID and Al₂O₃ capillary column (50×0.32 mm).

S2. Catalytic Testing.

Catalyst performance was evaluated on a 550×8 mm fixed-bed stainless steel reactor. The temperature and pressure were adjusted to the appropriate values.

The catalyst was packed in the middle of the reaction tube, and then filled with quartz sand, and then quartz wool was stoppered at the other side of the reaction tube. The isomerization reaction was operated for 3 h and then sampled to ensure that the catalytic activity of the catalyst reached a stable period. After the isomerized product was sampled, the composition of the product was analyzed using 6820 GC equipped with a FID and Al₂O₃ capillary column (50 m × 0.32 mm).

The conversion ratio (X) of n-hexane, the selectivity and yield of i-hexane are (S) and (Y), and the calculation methods of octane number show respectively in (1), (2), (3), (4):

$$X = \frac{\sum A - A_{n-C_6}}{\sum A} \times 100\%$$

(1)

$$Y = \frac{\sum A_{isomer}}{\sum A} \times 100\%$$

(2)

$$S = \frac{Y}{X} \times 100\%$$

(3)

$$RON = \sum_{i=1}^n \times RON_i \quad (4)$$

where $\sum A$ represents the total area in the chromatogram, A_{n-C_6} represents the peak area of the raw n-hexane, $\sum A_{isomer}$ is the peak area of an i-alkane in the isomerized product, RON_i is the research octane number corresponding to the product i.

Figures:

Fig. S1. FT-IR spectras of CoH(P(OPh)₃)₄ and P(OPh)₃.

Fig. S2. The effect of temperature on n-pentane isomerization.

Fig. S3. XRD patterns of catalyst CoH/H β before and after H₂ pre-reduction, and work in N₂.

Fig. S4. The effect of carriers on n-hexane isomerization.

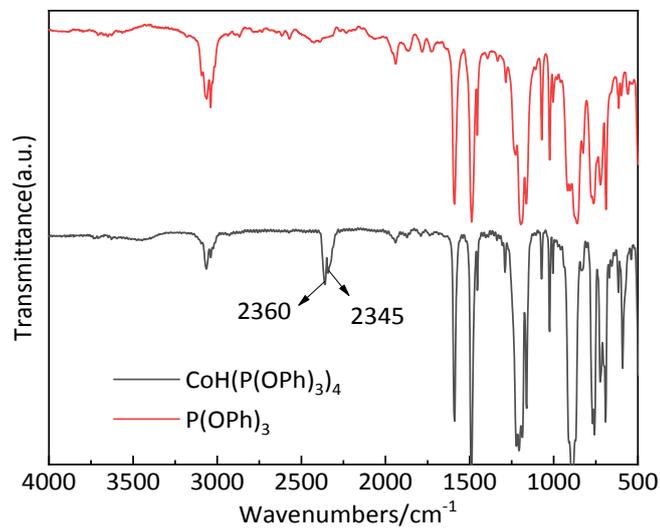


Fig S1 FT-IR spectras of CoH(P(OPh)₃)₄ and P(OPh)₃

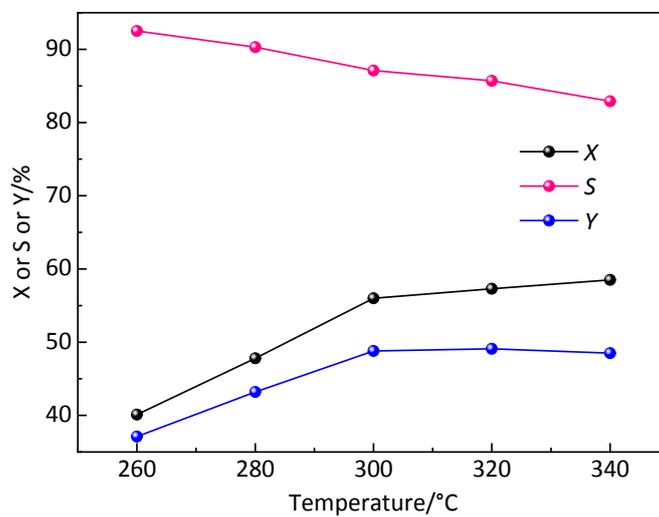


Fig. S2 The effect of temperature on n-pentane isomerization (reaction pressure, 2.0MPa; WHSV, 1.0h⁻¹; Hydrogen oil molar ratio, 4.0)

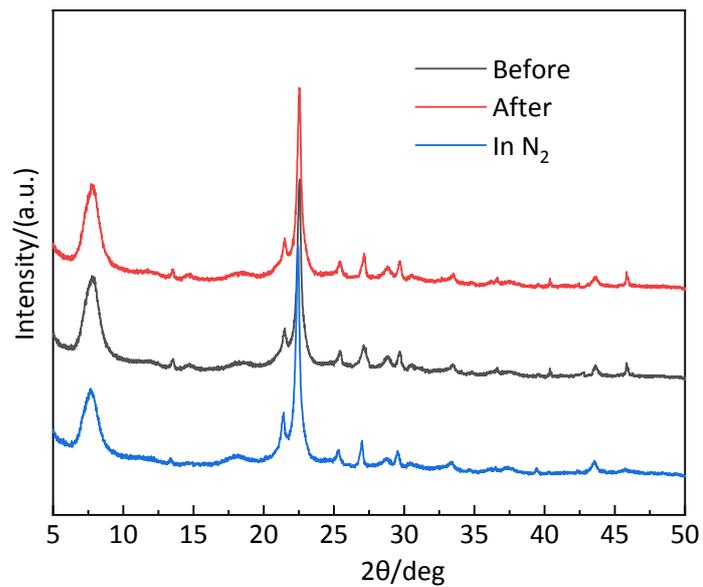


Fig. S3 XRD patterns of catalyst CoH/H β before and after H₂ pre-reduction, and after work in N₂.

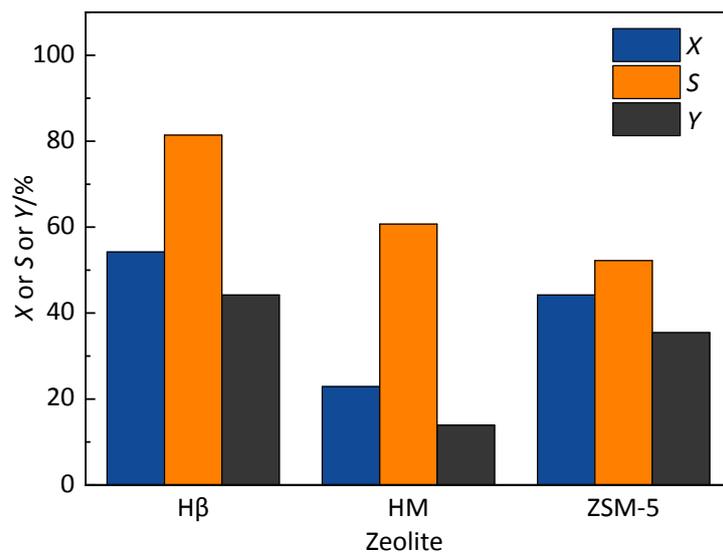


Fig.S4 The effect of carriers on n-hexane isomerization