

## Supporting information

### *tert*-Butylation of naphthalene by tertiary butanol over HY zeolite and cerium-modified HY catalysts

Zihua Huang<sup>ab</sup>, Jie Zhang<sup>ab</sup>, Peidong Li<sup>ab</sup>, Lanjian Xu<sup>ab</sup>, Xiaomin Zhang<sup>a</sup>, Yangyang Yuan<sup>\*a</sup> and Lei Xu<sup>\*a</sup>

<sup>a</sup> National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, People's Republic of China

<sup>b</sup> University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China

\*E-mail addresses: xulei808@dicp.ac.cn, yuanyangyang@dicp.ac.cn

Fig. S1 HRTEM images of cerium modified HY catalysts.

Fig. S2 SEM images of the parent HY and cerium modified HY catalysts.

Fig. S3 N<sub>2</sub> adsorption-desorption isotherms of the parent and cerium modified HY catalysts.

Fig. S4 The Horvath-Kawazoe micropore distribution of the parent and cerium modified HY catalysts.

Fig. S5 IR spectra in the pyridine vibration region of HY (A), Ce(5%)/HY (B), Ce(10%)/HY (C), Ce(20%)/HY (D) catalysts after pyridine adsorption and then desorption at 150 °C (i), 350 °C (ii), 450 °C (iii) for 1 h, respectively.

Fig. S6 TBN and DTBN isomers distribution for naphthalene *tert*-butylation over HY and cerium modified HY catalysts.

Fig. S7 XRD patterns of synthetic CeO<sub>2</sub> (S-CeO<sub>2</sub>) and commercial CeO<sub>2</sub> (C-CeO<sub>2</sub>).

Fig. S8 NH<sub>3</sub>-TPD profile of synthetic CeO<sub>2</sub>.

Fig. S9 Comparison of 2,6-/2,7-DTBN in products encapsulated in the pores and that in the bulk products with reaction periods.

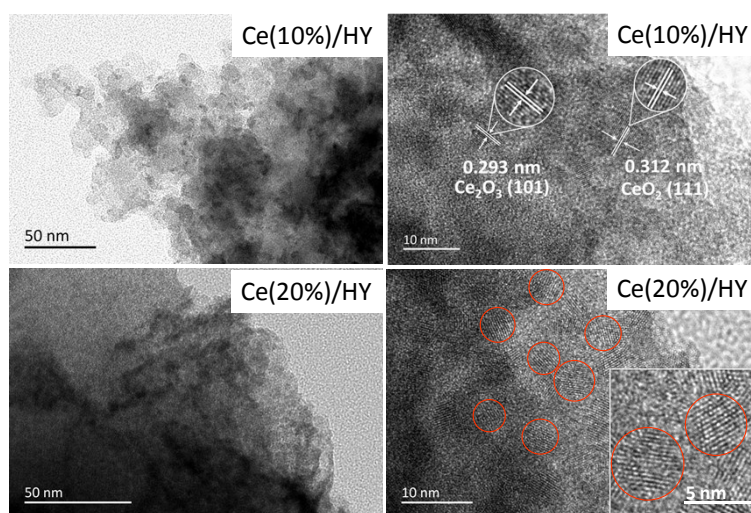


Fig. S1 HRTEM images of cerium modified HY catalysts.

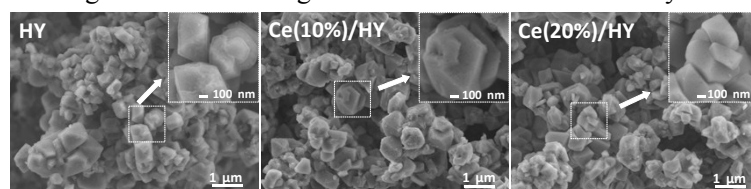


Fig. S2 SEM images of the parent HY and cerium modified HY catalysts.

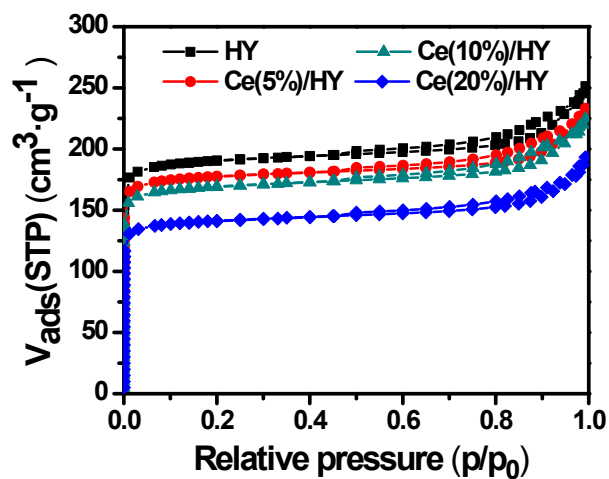


Fig. S3  $N_2$  adsorption-desorption isotherms of the parent and cerium modified HY catalysts.

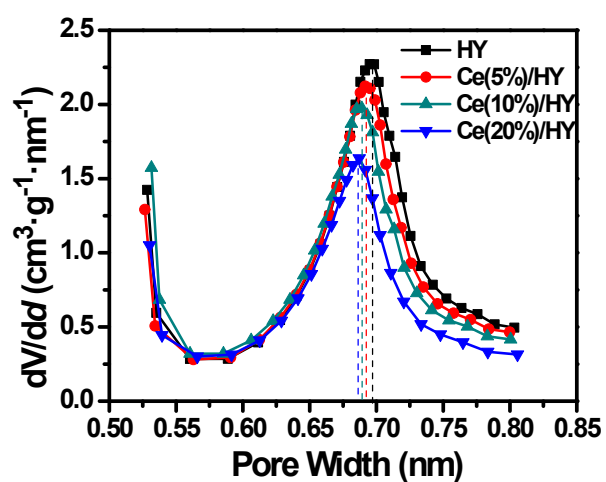


Fig. S4 The Horvath-Kawazoe micropore distribution of the parent and cerium modified HY catalysts.

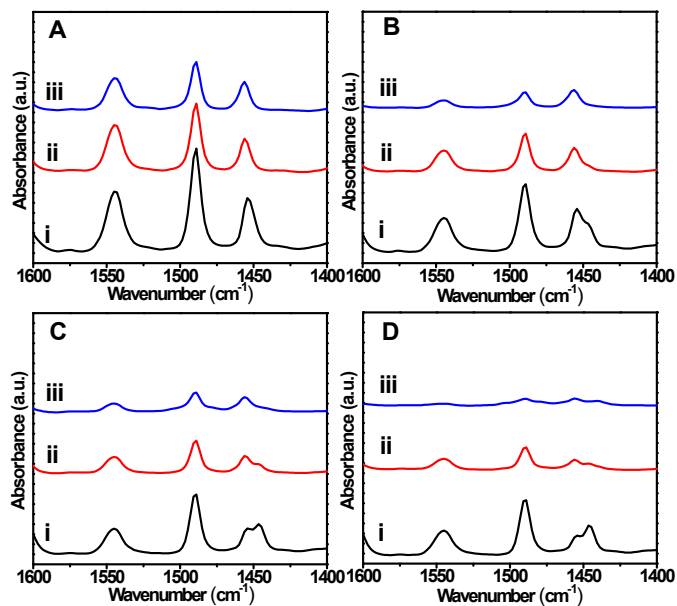


Fig. S5 IR spectra in the pyridine vibration region of HY (A), Ce(5%)/HY (B), Ce(10%)/HY (C), Ce(20%)/HY (D) catalysts after pyridine adsorption and then desorption at 150 °C (i), 350 °C (ii), 450 °C (iii) for 1 h, respectively.

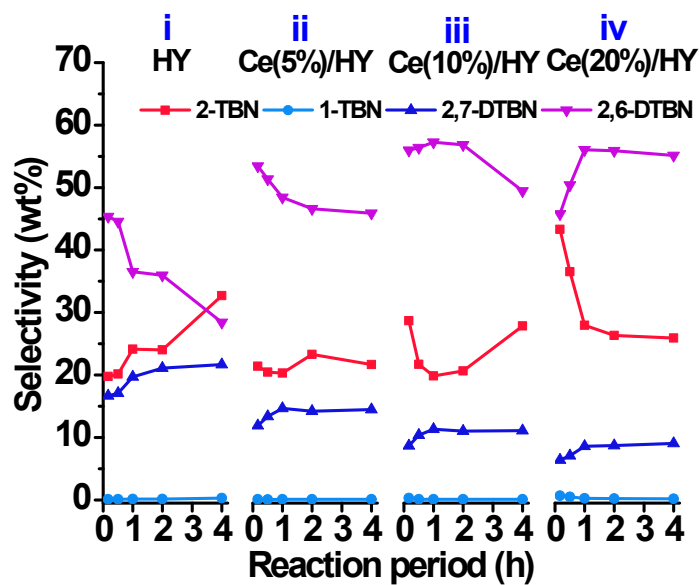


Fig. S6 TBN and DTBN isomers distribution for naphthalene *tert*-butylation over HY and cerium modified HY catalysts.

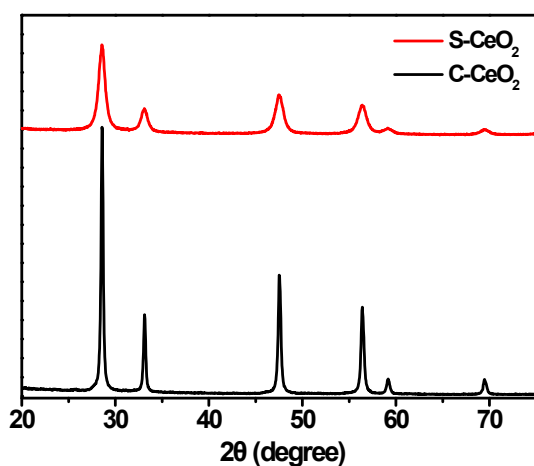


Fig. S7 XRD patterns of synthetic  $\text{CeO}_2$  (S- $\text{CeO}_2$ ) and commercial  $\text{CeO}_2$  (C- $\text{CeO}_2$ ). (CeO<sub>2</sub> was synthesized with cerium nitrate according to the calcination heating procedure that was adopted in the process of preparing modified catalysts)

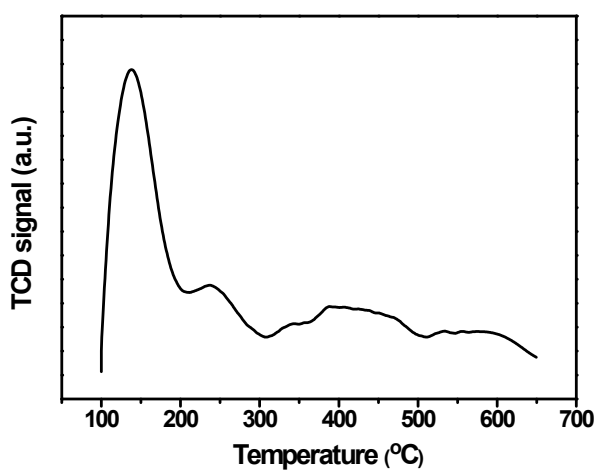


Fig. S8  $\text{NH}_3$ -TPD profile of synthetic  $\text{CeO}_2$ .

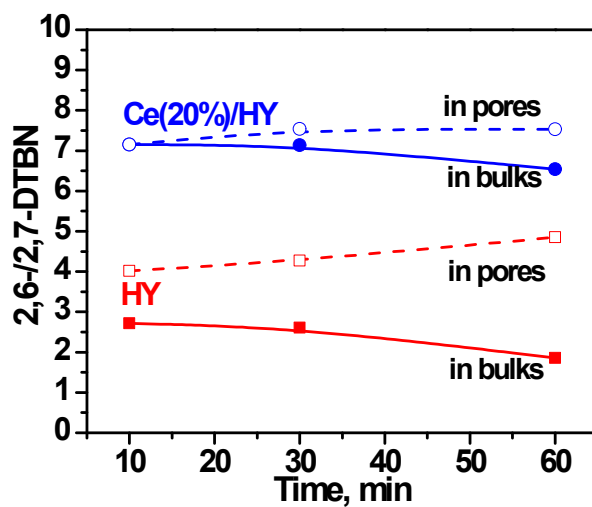


Fig. S9 Comparison of 2,6-/2,7-DTBN in products encapsulated in the pores and that in the bulk products with reaction periods.

(Reaction temperature = 160 °C, Catalyst weight = 200 mg.)