

Supporting Information

Efficient and high *para*-selective conversion of toluene with NO₂ to *para*-nitrotoluene in an O₂-Ac₂O-HβD4 composite catalytic system

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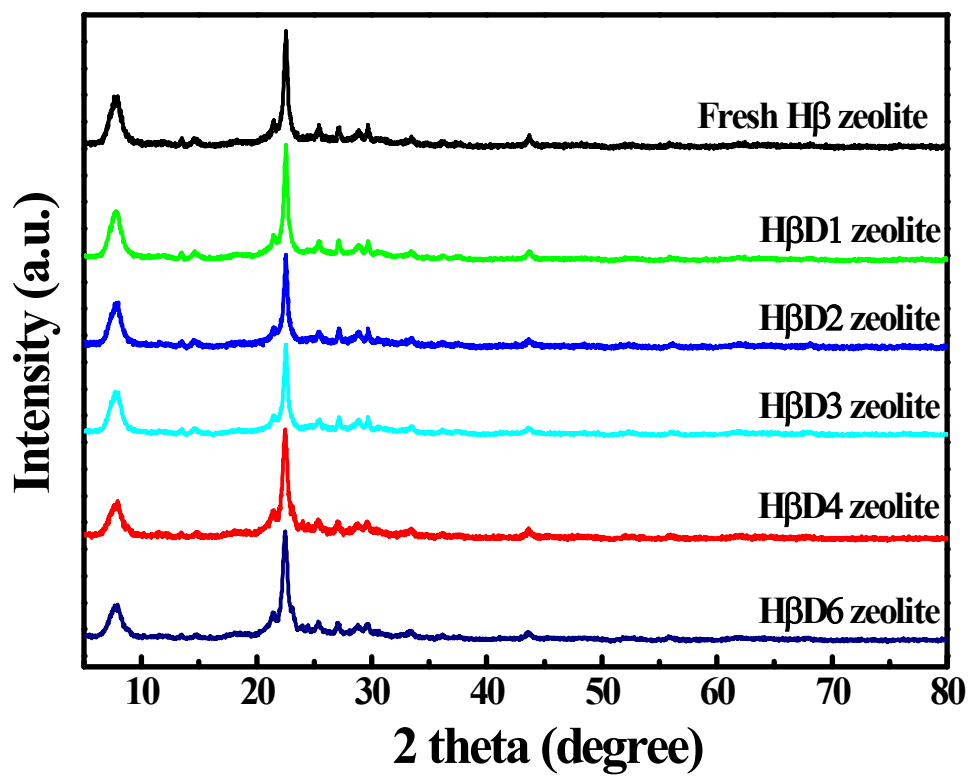


Figure S1. XRD patterns of samples.

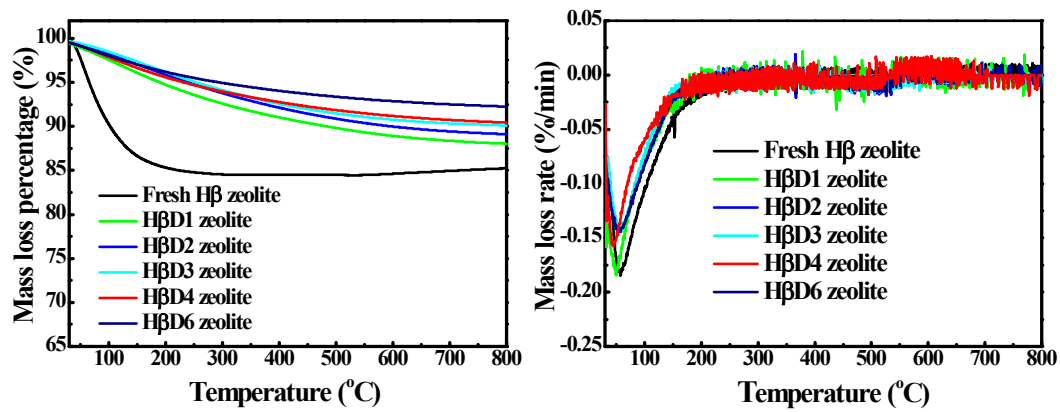


Figure S2. TG/DTG curves of samples.

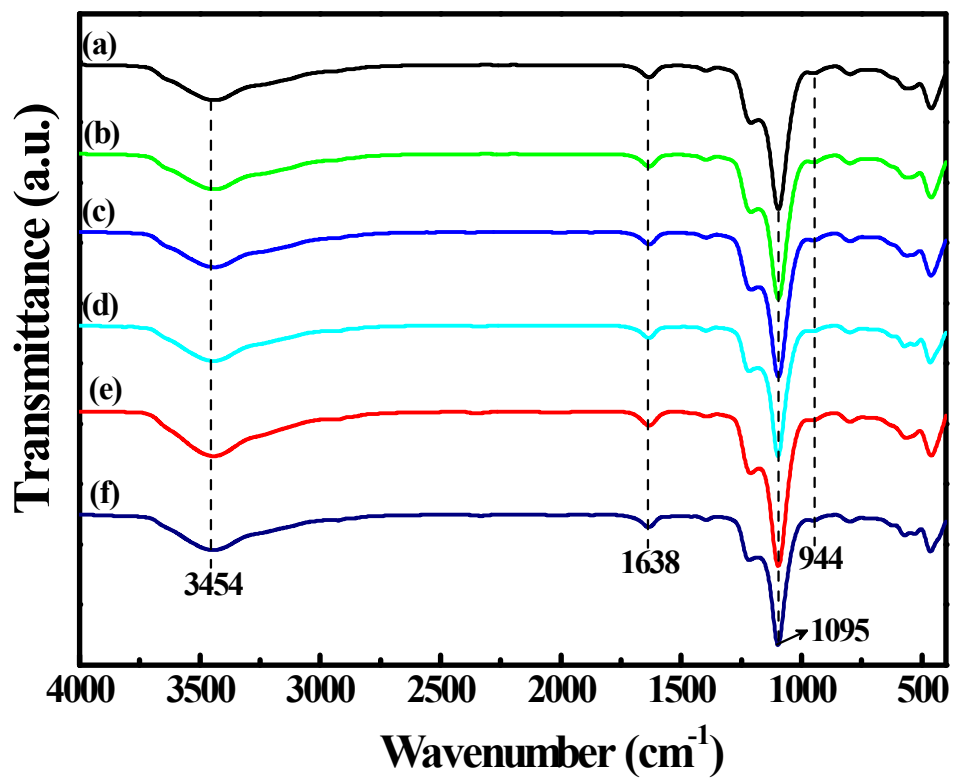


Figure S3. FT-IR spectra of (a) fresh H β (40), (b) H β D1, (c) H β D2, (d) H β D3, (e) H β D4, (f) H β D6 samples.

Table S1. Effect of catalyst amount on the nitration reaction ^a.

Amount of H β D4 (g)	Conversion (%)	Selectivity (%)			The ratio of <i>p/o</i>
		<i>o</i> -NT	<i>m</i> -NT	<i>p</i> -NT	
0.5	69.8	27.7	5.9	66.4	2.4
1	70.1	25.7	5.6	68.7	2.7
1.5	78.1	22.5	5.7	71.8	3.2
2	78.3	22.9	5.5	71.6	3.1
2.5	78.5	22.5	5.6	71.9	3.2

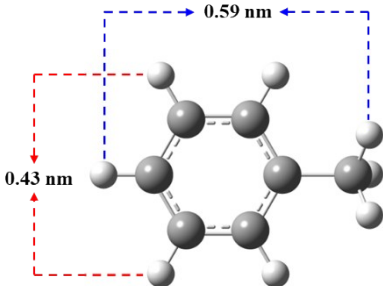
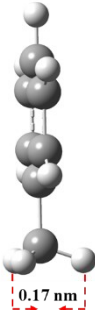
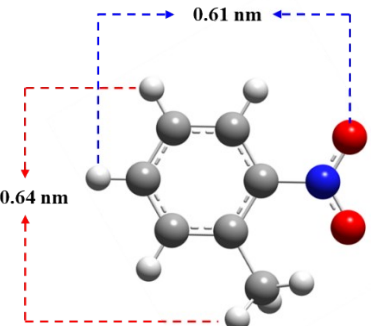
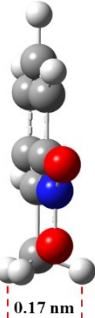
^a Reaction conditions: reaction temperature was 35 °C, the toluene:NO₂ molar ratio was 1:2, reaction time was 4 h, O₂ pressure was 0.5 MPa, and the amount of Ac₂O was 10.0 g.

Table S2. Effect of the amount of Ac₂O in the catalytic nitration reaction^a.

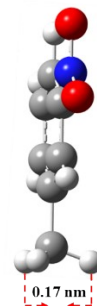
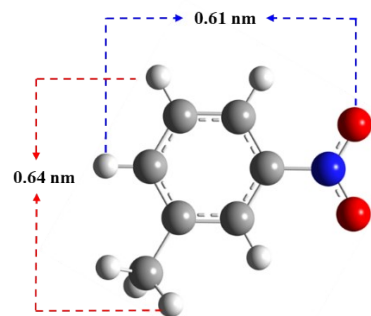
Amount of Ac ₂ O (g)	Conversion (%)	Selectivity (%)			p/o ratio
		o-NT	m-NT	p-NT	
1.0	65.3	25.7	6.1	68.2	2.7
5.0	71.4	23.8	5.9	70.3	3.0
10.0	78.1	22.5	5.7	71.8	3.2
15.0	72.3	22.5	5.8	71.7	3.2
20.0	68.5	22.8	5.7	71.5	3.1

^a Reaction conditions: reaction temperature was 35 °C, toluene:NO₂ molar ratio was 1:2, reaction time was 4 h, O₂ pressure was 0.5 MPa, and the amount of HβD4 was 1.5 g.

Table S3 Schematic diagram and size of and various nitration produces and the pore diameter of treated catalyst

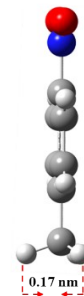
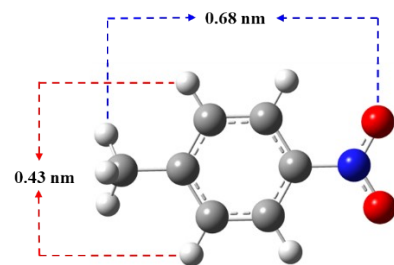
Subtract	Front view	Side view	Minimum diameter of cross section (nm)	Pore diameter of treated catalyst (nm)
Toluene			0.43	0.55
<i>o</i> -NT			0.61	

m-NT



0.61

p-NT



0.43
