

# S1

## Supporting Information

for

Hydrothermal Reactions from Sodium Hydrogen Carbonate to Phenol

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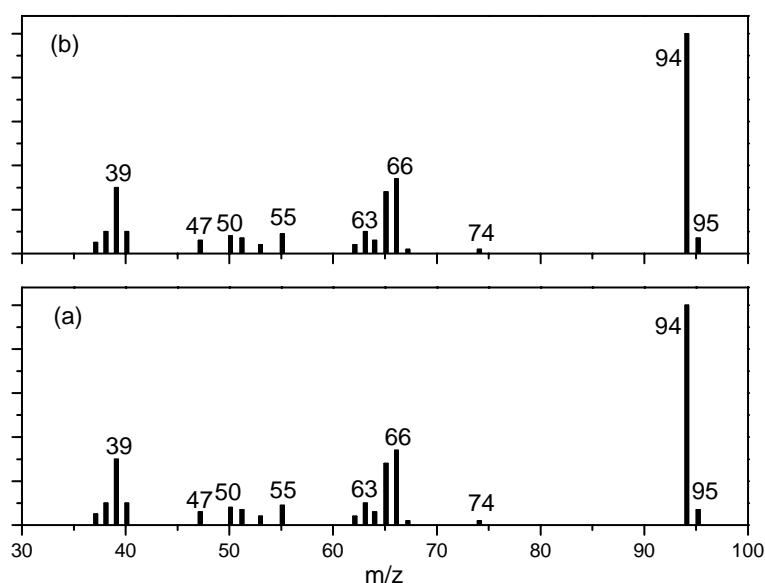
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### 1. Experimental procedure.

0.630 g NaHCO<sub>3</sub> (A.R., Beijing Chem. Reagents Co.; repurified free of the organic) and 0.5 g Fe powders (Sinopharm Chem. Reagent Co.; calcined at 500 °C for 3 h in N<sub>2</sub>(99.99%) flow) were mixed with 25 ml of pure water. The mixture was sealed in the autoclave and allowed reaction at 200 °C for 1-120 h. [The pressure was autogenic \(approximate 1.8MPa\).](#)

### 2. GC-MS characterization for product phenol.

The data were recorded on the TRACE MS GC-MS (Finnigan Co.). Temperatures: column, 80 °C for 1 min, then increased from 80 to 280 °C at 20 °C /min, final temperature 280 °C. Sample volume: 1 µl. Column type: HP-5ms. MS: EI source.



**Figure S1.** (a) Mass spectrum of standard sample phenol and (b) Mass spectrum of phenol formed via the hydrothermal reaction.

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3. Scheme S1. Formation mechanisms of phenol under hydrothermal conditions. (①

refers to the oxidative coupling reaction; ② refers to the rearrangement reaction)

