

Supporting Information

Selective catalytic degradation of lignin model compound into phenol over transition metal sulfates

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Materials

Benzyl phenyl ether (BPE, GC), chromium sulfate ($\text{Cr}_2(\text{SO}_4)_3 \cdot 6\text{H}_2\text{O}$, AR), manganese sulfate ($\text{MnSO}_4 \cdot \text{H}_2\text{O}$, AR), ferrous sulfate ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$, AR), cobaltous sulfate ($\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$, AR), nickel sulfate ($\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$, AR), copper sulfate ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, AR), zinc sulfate ($\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$, AR), nickel chloride ($\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, AR), nickel nitrate ($\text{NiNO}_3 \cdot 6\text{H}_2\text{O}$, AR), nickel carbonate (NiCO_3 , AR), phenol (GC), benzyl methyl ether (GC), benzyl alcohol (GC) were supplied by Aladdin bio-chem technology Co., Ltd. (Beijing, China). Methanol (GC) and tetrahydrofuran (GC) were purchased from Merck (Germany).

Characterization

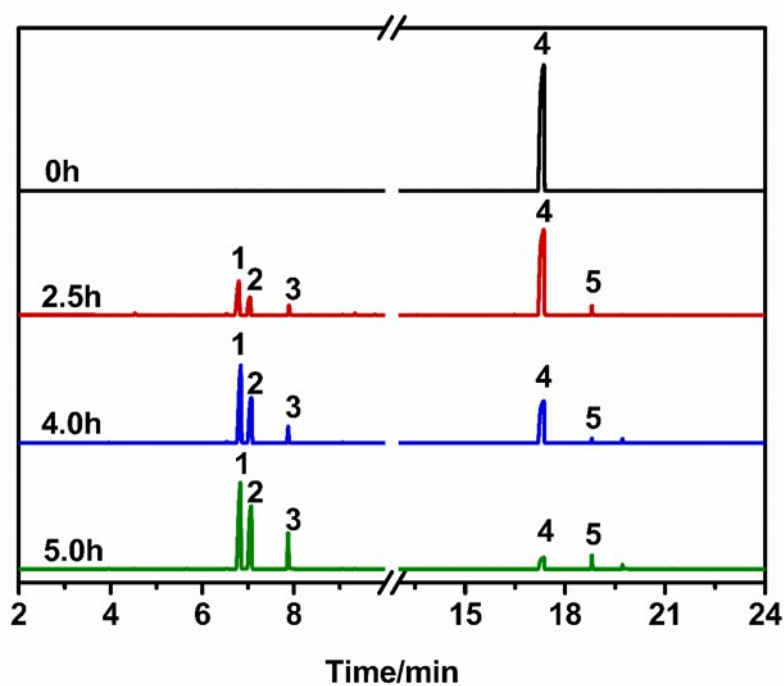


Fig. S1 GC-MS spectra of BPE degradation products. Condition: 0.3000 g BPE, 1.4 mmol $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$, 200 °C.

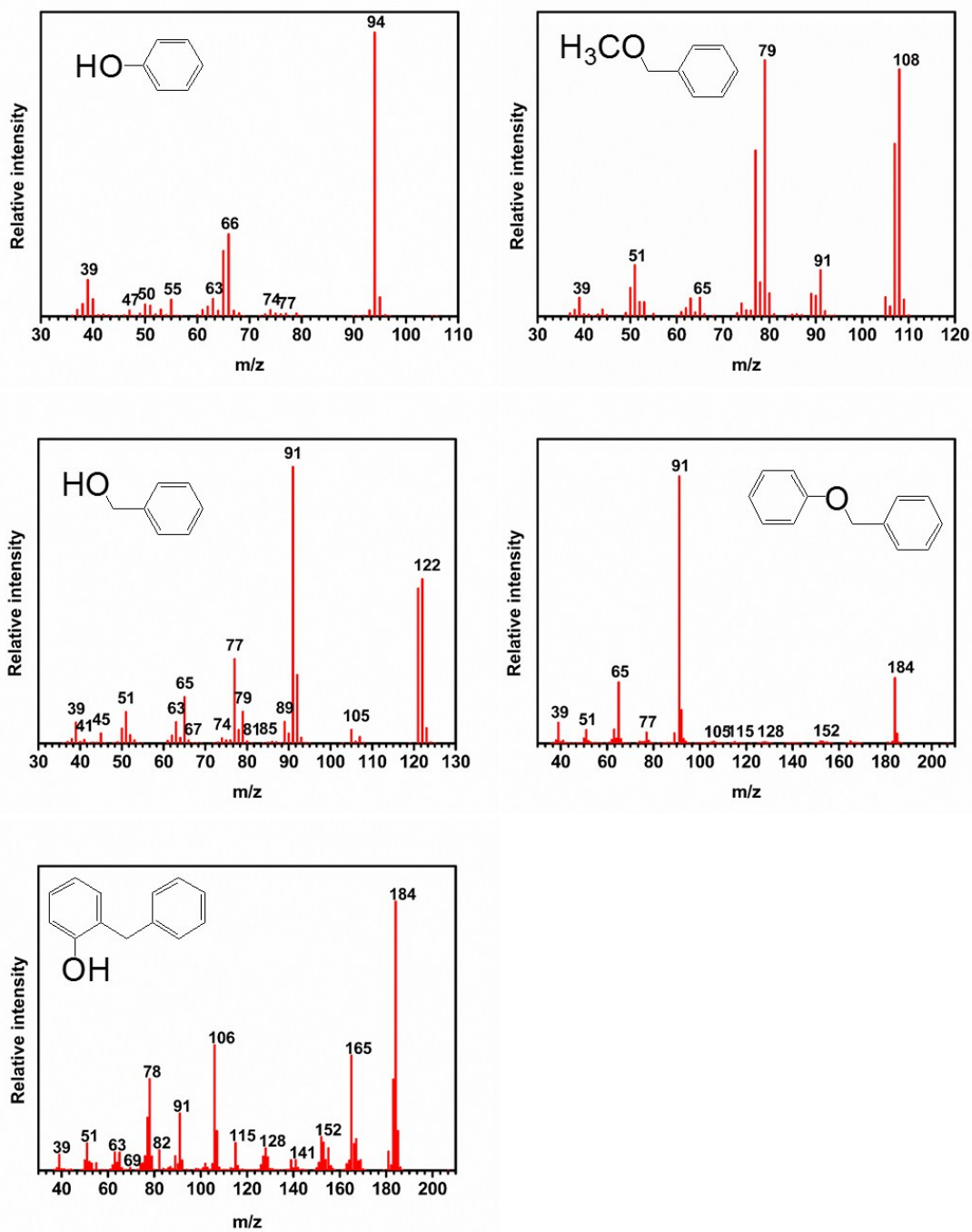


Fig. S2 MS of BPE primary degradation products. Condition: 300 mg BPE, 1.4 mmol $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$, 200 °C.


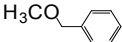

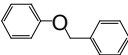
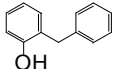
Table S1 The effect of transition metal salts on BPE degradation efficiency and phenol selectivity.

Run	Catalyst	pH	Total Degradation (%)	Phenol Selectivity (%)
1	-	-	3.6	-
2	$\text{Cr}_2(\text{SO}_4)_3 \cdot 6\text{H}_2\text{O}$	2.94	38.5	14.9
3	$\text{MnSO}_4 \cdot \text{H}_2\text{O}$	4.21	18.7	-
4	$\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$	2.16	57.2	20.1
5	$\text{CoSO}_4 \cdot 7\text{H}_2\text{O}$	3.72	28.3	12.9
6	$\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$	2.89	90.4	48.6
7	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$	2.62	65.7	24.5
8	$\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$	4.15	43.6	22.7
9	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	3.44	52.2	3.2
10	$\text{NiNO}_3 \cdot 6\text{H}_2\text{O}$	5.46	30.9	4.3
11	NiCO_3	7.96	18.8	-

Condition: 300 mg BPE, 1.4 mmol transition metal salts, 20 mL methanol, 200 °C, 5 h.

- Without catalyst.

Table S2 The component of primary degradation products.

Run	Name	Structure	Retention time(min)
1	phenol		6.810
2	benzyl methyl ether		7.048
3	benzyl alcohol		7.888
4	benzyl phenyl ether		17.235
5	2-Benzyl phenol		18.800

Condition: 300 mg BPE, 1.4 mmol NiSO₄·6H₂O, 20 mL methanol, 200 °C.

Table S3 The selectivity of each products.

R.T	BPE	Phenol	Benzyl methyl ether	Benzyl alcohol
	dep%	sel%	sel%	sel%
0.5h	5.63	16.34	9.21	1.59
1.0h	8.56	18.57	15.40	1.83
1.5h	15.62	31.03	24.76	3.69
2.0h	32.20	34.45	26.57	4.97
2.5h	37.10	41.36	31.72	8.13
3.0h	61.16	46.18	31.82	10.41
4.0h	75.60	53.14	32.10	10.84
5.0h	90.82	48.65	31.22	11.39

Condition: 0.3000 g BPE, 1.4 mmol NiSO₄·6H₂O, 20 mL methanol, 200 °C.