Targeted Substituted-Phenol Production by Strategic Hydrogenolysis of Sugar-Cane Lignin

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1. Supplementary Information

1.1. Thermogravimetric Analysis

The temperature programmed oxidation analysis of Al2O3 and Ni/Al2O3 are shown in Figure S1 and Figure S2. It can be seen that the weight loss was between 15-20 %, which about 8-10 % corresponded to the loss of carbon. The Ion current plot revealed that the main event between 550 K and 800 K was regarded to CO_2 evolution. For both catalysts there was not only one type of carbon species due to small events from 600 K to 700 K.

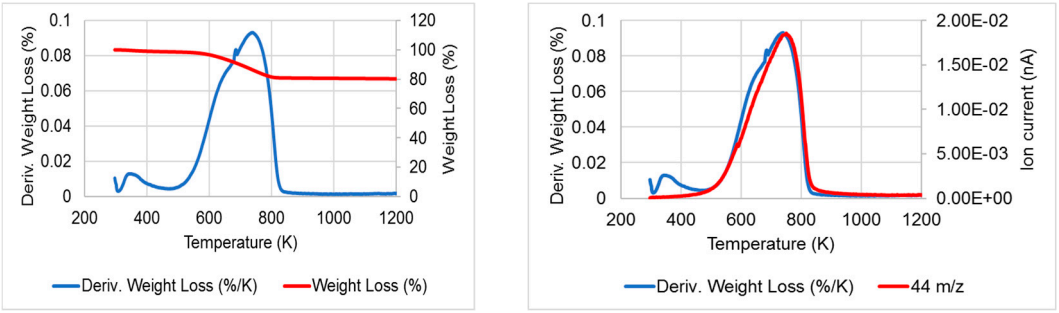


Figure S1. TPO plot (left) and derivative weight loss (right) with CO_2 m/z 44 evolution of spent Al_2O_3 catalyst after acetone/H_2O reaction with the sugar-cane lignin

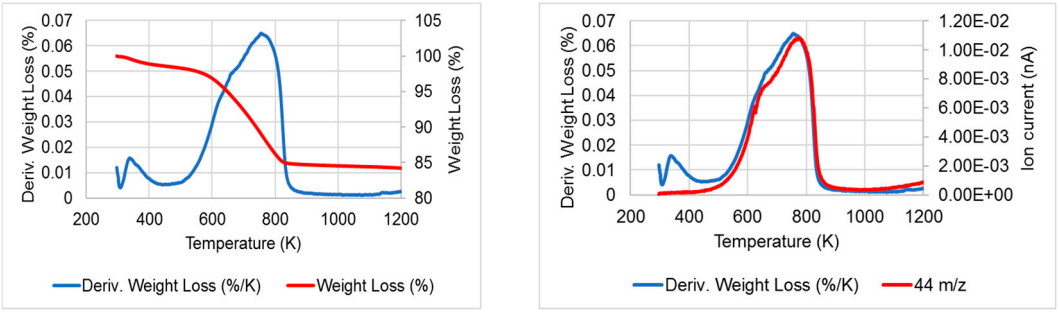


Figure S2. TPO plot (left) and derivative weight loss (right) with CO_2 m/z 44 evolution of spent Ni/Al_2O_3 catalyst after acetone/H_2O reaction with the sugar-cane lignin

1.2. CHN analysis

Table S1 presents the carbon, hydrogen and nitrogen content in the post reaction catalysts. Nitrogen was present in the initial SCL, hence, its detection in the analysis indicated the interaction between SCL and the catalyst ocurred.

Table S1. Elemental analysis of spent alumina catalysts in SCL depolymerisation

Spent Catalyst	C (%)	H (%)	N (%)
Spent Al_2O_3	8.9	0.9	0.08
Spent Pt/Al_2O_3	8.3	0.8	0.05

Spent Ni/Al_2O_3	10.7	1.0	0.05

1.2. Raman Analysis

The Raman for SCL are shown in Figure S3. It were found bands at ~ 1380 cm^{-1} and ~ 1600 cm^{-1}, corresponding to disordered and ordered carbon species[1,2].

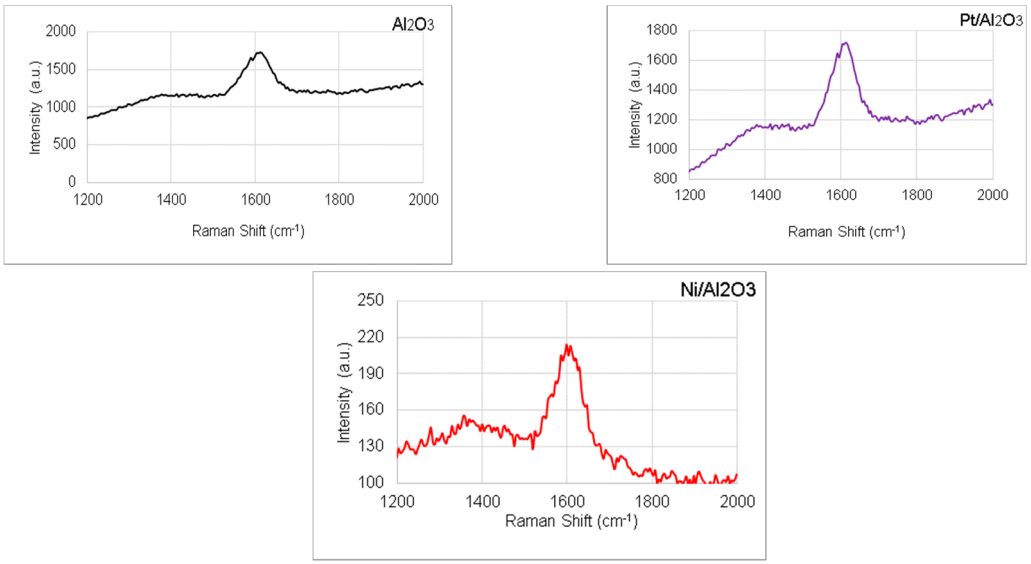


Figure S3. Raman spectrum of spent Al_2O_3 support, Pt/Al_2O_3 and Ni/Al_2O_3

1.3. BET analysis

BET analysis of spent catalysts are presented in Table S2. Before reaction, surface area (m^2/g), pore volume (cm^3/g) average pore diameter (Å) for Al_2O_3 was 104 m^2/g, 0.5 cm^3/g and 116 Å, for Pt/Al_2O_3: 124 m^2/g, 0.6 cm^3/g and 146 Å, and for Ni/Al_2O_3 106 m^2/g, 0.5 cm^3/g and 126 Å. The average pore diameter did not have significant changes.

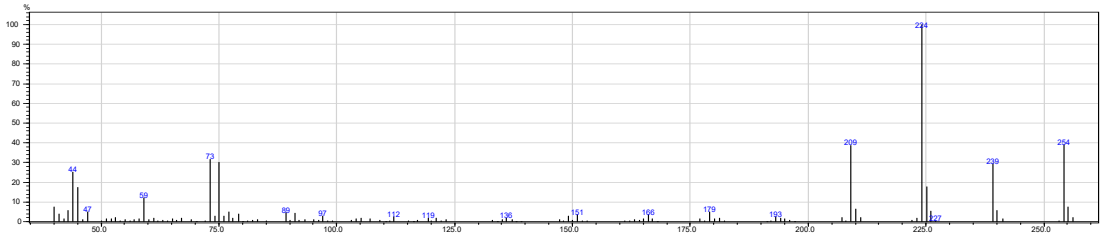
Table S2. BET analysis of spent Al2O3,Pt/Al2O3 and Ni/Al2O3

Spent Catalyst	S_{BET} (m^2/g)	V_p(cm^3/g)
Spent Al_2O_3	110	0.3
Spent Pt/Al_2O_3	140	0.4
Spent Ni/Al_2O_3	106	0.3

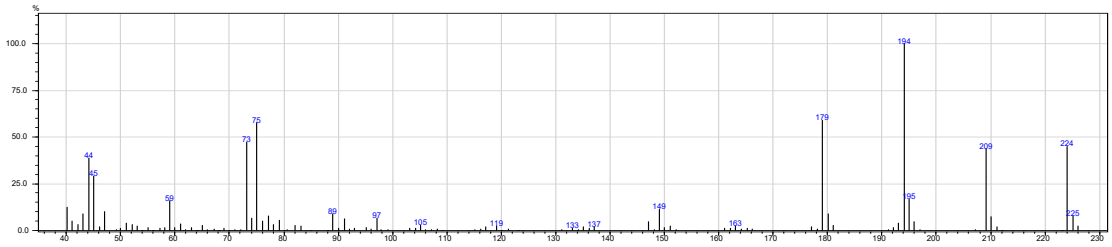
1.4. GCMS analysis

Below are the GCMS traces for 4-ethyl-2,6-methoxyphenol (compound 11) and 4-ethyl-2-methoxyphenol (compound 3) as per table 2 in the main paper.

GC-MS trace for 4-ethyl-2,6-methoxyphenol (compound 11)



GC-MS trace for 4-ethyl-2-methoxyphenol (compound 3)



References

1 J. J. H. B. Sattler, A. M. Beale and B. M. Weckhuysen, *Phys. Chem. Chem. Phys.*, 2013, **15**, 12095.

2 A. Sadezky, H. Muckenhuber, H. Grothe, R. Niessner and U. Pöschl, *Carbon N. Y.*, 2005, **43**, 1731–1742.