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Supplementary Information for:

Upgrading of Pyrolytic Lignin into Hexamethylbenzene with High Purity: Demonstration of "All-to-One" Biochemical Production Strategy in Thermo-Chemical Conversion

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Table of contents

- 1. Materials
- 2. Experimental setups and procedures
- 3. Preparation of feedstocks
- 4. Catalyst characterization
- 5. Product analysis
- 6. Additional Figures and Tables

Figure S1. HMB as a precursor to the formation of polyimide

Table S1. Average ESP of carbon atoms in phenol based compounds corresponding to Figure 3 (for phenol)

Figure S2. Electron density of *m*-cresol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP)

Table S2. Average ESP of carbon atoms in m-cresol based compounds corresponding to Figure S2

Figure S3. Electron density of *p*-ethylphenol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP)

Table S3. Average ESP of carbon atoms in *p*-ethylphenol based compounds corresponding to Figure S3

Figure S4. Electron density of eugenol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP)

Table S4. Average ESP of carbon atoms in eugenol based compoundscorresponding to Figure S4

Figure S5. Electron density of 2-methoxy-4-*n*-propylphenol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP)

Table S5. Average ESP of carbon atoms in 2-methoxy-4-*n*-propylphenol based compounds corresponding to Figure S5

Figure S6. Reaction barriers, TS structure, and IRC plot of initial step for phenol Figure S7. Reaction barriers, TS structure, and IRC plot of initial step for *m*-cresol Figure S8. Reaction barriers, TS structure, and IRC plot of initial step for *p*-ethylphenol

Figure S9. Reaction barriers, TS structure, and IRC plot of initial step for eugenol Figure S10. Reaction barriers, TS structure, and IRC plot of initial step for 2-methoxy-4-*n*-propylphenol

- Figure S11. SEM image of γ -Al₂O₃
- Figure S12. NH₃-TPD result of γ -Al₂O₃
- Figure S13. XRD pattern of γ -Al₂O₃
- Figure S14. The schematic diagram of the fixed-bed reactor
- Figure S15. The TIC of aurantius product (*o*-hydroxydiphenyl as feedstock, T=400 °C)
- Figure S16. Chemical structures corresponding to Figure S15
- Figure S17. FT-IR spectrum of the crystalline solid
- Table S6. Elemental analysis of the crystalline solid
- Figure S18. The TIC of the crystalline solid, lignin oil as feedstock
- Figure S19. MS spectrum (time of 19.92 min) of the crystalline solid corresponding to Figure S18
- Figure S20. The TIC of water-insoluble fraction in bio-oil used
- Figure S21. The chemical structures corresponding to Figure S20
- 7. Mass balance
- 8. Identification and quantitation of HMB in crystalline solid
- Enclosed: Report of biobased carbon content analysis

1. Materials

The model compounds used, including 2-methoxy-4-*n*-propylphenol (Alfa Aesar, 99 wt%), eugenol (Aladdin, 99 wt%), *p*-ethylphenol (Aladdin, 99 wt%), cresols mixture (*ortho*, *meta* and *para*, Aladdin, 98 wt%), and phenol (Aladdin, 99.5 wt%) were used as received. Methanol (99.5 wt%) was purchased from Beijing Chemical Co. Ltd. Deionized water was used for all reactions. The bio-oil was derived from the fast pyrolysis of pine wood, produced in a commercial 5 t/h pyrolysis unit developed by BTG and operated by BTL/Empyro¹ and used as received. γ -Al₂O₃ (Φ 4 mm-6 mm) was supplied by Aladdin and used without further treatment.

Reference

1 https://www.btg-btl.com/en/company/projects/empyro, accessed in 20 Feb, 2018.

2. Experimental setups and procedures

Catalytic experiments were carried out in a continuously operated fixed-bed reactor, which was comprised of a high temperature resistance quartz tube (inner diameter, 28 mm; length, 800 mm), furnace, temperature control system, and carrier gas system. The schematic diagram of the fixed-bed reactor is shown in Figure S14. Typically in each run, about 15 g inert ceramic balls were first padded on the bottom of the quartz tube, then 100 g catalyst (*i.e.*, γ -Al₂O₃) was loaded into the quartz tube. The reactor was heated to the desired temperature (400-500 °C) under a N₂ flow of 100 ml/min. When the temperature stays stable, the feedstock was pumped into the reaction tube at a rate of 4.0 ml/min. The atmospheric pressure of N₂ (flow of 100 ml/min) was kept in all catalytic processes. A simple isolation of produced solid crystalline was needed, which was implemented by washing with small amount of methanol.

3. Preparation of feedstocks

For model compounds feeding:

The feedstocks were prepared by well blending the model compound and methanol with molar ratio being 1:8. Then leave the mixture at room temperature for 2 h with rapid agitation.

The real bio-oil feedstock was prepared as follows:

Deionized water was added into bio-oil with slow agitation at a mass ratio of 2:1, and the mixture was set a duration of 24 h at room temperature. After adequate extraction, the aqueous soluble phase of the mixture was carefully separated from the water-insoluble fraction. Then the feedstock was obtained by intensive blending above mentioned water-insoluble fraction (25 wt%) with methanol (75 wt%).

4. Catalyst characterization

Transmission electron microscopy (TEM) was achieved with a FEI Tecnai G2 20 S Twin microscope operated at 200 kV. The samples were prepared by dispersing a small amount of catalyst powder in ethanol by sonication. The dispersion was transferred to a copper grid coated with lacey carbon film before subjected to TEM analysis.

Scanning electron microscopy (SEM) was implemented on a HITACHI S-4700 microscope.

Temperature-programmed desorption of ammonia (NH₃-TPD) was carried out in an Autochem 2920 II instrument from micromeritics. The γ -Al₂O₃ samples (0.1 g) were pretreated at 500 °C in He flow (20 cm³ min⁻¹) for 2 h. Afterward, 10 vol.% NH₃ in He (20 cm³ min⁻¹) was adsorbed at 110 °C for 30 min followed by He purging at the same temperature for 1 h. Desorption of NH₃ was monitored in the range of 110-650 °C at a heating rate of 10 °C min⁻¹.

 N_2 adsorption-desorption measurements were performed on a Micromeritics ASAP 2020 HD 88 surface area and porosity analyzer. The calcined samples were degassed at 350 °C in a vacuum of 1.33×10^{-3} Pa for 10 h and then switched to the analysis station for adsorption-desorption analysis at liquid nitrogen temperature.

X-ray diffraction (XRD) measurements were carried out using a Bruker diffractometer with Cu radiation (40 kV, 120 mA). Data were recorded in the 2 θ range of 5-80 ° with an angular step size of 0.05 ° and a counting time of 8 s per step.

5. Product analysis

¹H and ¹³C nuclear magnetic resonance (NMR) measurements were acquired at 25 °C in chloroform-d with a Bruker AVANCE spectrometer (600 MHz). The spectral widths of ¹H- and ¹³C- dimensions were 20 ppm by using 2048 data points for an acquisition time (AQ) of 128 ms and 219 ppm by using 512 increments (AQ of 11.6 ms), respectively.

GC/MS analysis of the solid and liquid products was performed with the Agilent 7890A/5975C system equipped with a HP-5 MS column. The temperature program of the column was as follow: temperature holding at 50 $^{\circ}$ C for 1 min, heating to 300 $^{\circ}$ C at a rate of 5 $^{\circ}$ C/min, and temperature holding at 300 $^{\circ}$ C for 4 min. The interpretation of the mass spectra was mainly based on an automatic library search (NIST11, version 2.0).

Fourier transform infrared spectroscopy (FT-IR) was obtained on a Nicolet Magna-IR 750 spectrometer in KBr pellets.

Elemental analysis was determined using a Vario EL III elemental analyzer.

The biobased carbon content (as a fraction of total organic carbon) in the crystalline solid is quantified by using the radiocarbon isotope (also known as 14 C) with the standard of ASTM D6866-16 Method B utilizes AMS along with Isotope Ratio Mass Spectrometry (IRMS) techniques and accomplished by American Beta Analytic Inc. (laboratory number Beta-490580).

6. Additional Figures and Tables



Figure S1. HMB as a precursor to the formation of polyimide.

	Average electrostatic potential (ESP), kcal/mol						
Atom#	Phenol	<i>p</i> -cresol	2,4-dimethylphenol	2,3,4-trimethylphen ol	2,3,4,5-tetramethyl phenol	2,3,4,5,6-pentamet hylphenol	Hexamethylbenzen e
1	-14.44243	-13.37755	-14.63306	-14.83316	-14.93961	-15.84443	-16.27657
2	-14.26604	-14.33476	-14.95195	-13.85694	-14.74042	-16.09292	-16.24581
3	-14.28229	-15.08989	-13.98427	-14.38687	-15.44877	-16.82456	-16.26555
4	-10.29141	-11.55336	-11.45781	-12.93028	-13.89955	-14.38549	-16.22759
5	-11.15402	-12.15821	-13.1983	-14.30423	-14.63308	-13.70023	-16.24737
6	-13.17189	-13.51535	-14.94772	-15.79882	-14.78038	-14.81421	-16.21874

Table S1. Average ESP of carbon atoms in phenol based compounds corresponding to Figure 3 (for phenol).



Figure S2. Electron density of *m*-cresol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP).

	Average electrostatic potential (ESP), kcal/mol						
Atom#	<i>m</i> -cresol	3,4-dimethylphenol	2,3,4-trimethylphen ol	2,3,4,5-tetramethyl phenol	2,3,4,5-tetramethyl phenol	2,3,4,5,6-pentamet hylphenol	Hexamethylbenzen e
1	-14.93651	-13.89669	-14.85285	-14.96613	-14.96613	-15.84374	-16.23336
2	-13.44674	-13.45468	-13.83592	-14.73414	-14.73414	-16.07681	-16.23139
3	-14.66112	-15.50122	-14.40428	-15.51018	-15.51018	-16.77907	-16.24597
4	-11.60391	-12.70354	-12.96793	-13.90615	-13.90615	-14.3465	-16.22196
5	-12.43308	-13.43051	-14.31747	-14.6231	-14.6231	-13.71509	-16.25514
6	-14.37051	-14.66855	-15.77472	-14.745	-14.745	-14.79755	-16.26992

Table S2. Average ESP of carbon atoms in *m*-cresol based compounds corresponding to Figure S2.



Figure S3. Electron density of *p*-ethylphenol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP).

	Average electrostatic potential (ESP), kcal/mol						
Atom#	<i>p</i> -ethylphenol	4-ethyl-2-methylph enol	2,4-dimethylphenol	2,3,4-trimethylphen ol	2,3,4,5-tetramethyl phenol	2,3,4,5,6-pentamet hylphenol	Hexamethylbenzen e
1	-13.97565	-15.22137	-14.62805	-14.81681	-14.96583	-15.83506	-16.26122
2	-14.57988	-15.18895	-14.95218	-13.87625	-14.71181	-16.07696	-16.29084
3	-15.00934	-13.82205	-13.98364	-14.4065	-15.51031	-16.7753	-16.18757
4	-11.39404	-11.20754	-11.45816	-12.89112	-13.90622	-14.35601	-16.29539
5	-11.866	-12.92889	-13.19601	-14.33932	-14.62028	-13.71318	-16.29149
6	-13.47284	-14.82198	-14.94702	-15.80131	-14.7488	-14.79947	-16.30532

Table S3. Average ESP of carbon atoms in *p*-ethylphenol based compounds corresponding to Figure S3.



Figure S4. Electron density of eugenol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP).

	Average electrostatic potential (ESP), kcal/mol						
Atom#	Eugenol	4-allyl-2-methoxy- 6-methylphenol	4-allyl-6-methoxy- 2,3-dimethylphenol	6-methoxy-2,3,4-tri methylphenol	1-methoxy-2,3,4,5- tetramethylbenzene	1-methoxy-2,3,4,5, 6-pentamethylbenz ene	Hexamethylbenzen e
1	-13.20099	-14.23203	-14.34933	-15.61275	-15.75857	-14.36115	-16.22936
2	-15.44092	-15.74521	-14.71313	-15.59099	-15.5571	-14.0892	-16.2863
3	-15.85375	-14.59671	-14.7319	-16.10319	-15.62439	-14.15143	-16.24328
4	-12.06147	-11.92436	-13.31165	-14.58176	-16.37598	-15.1268	-16.22709
5	-8.28147	-9.27615	-10.62604	-11.87716	-15.03657	-17.11735	-16.27895
6	-10.84928	-12.00589	-12.98887	-14.52361	-16.16266	-15.23725	-16.25196

Table S4. Average ESP of carbon atoms in eugenol based compounds corresponding to Figure S4.



Figure S5. Electron density of 2-methoxy-4-*n*-propylphenol and different substituted compounds from total SCF density (isoval=0.001, mapped with ESP).

	Average electrostatic potential (ESP), kcal/mol						
Atom#	2-methoxy-4- <i>n</i> -pro pylphenol	2-methoxy-6-meth yl-4-propylphenol	2-methoxy-4,6-dim ethylphenol	6-methoxy-2,3,4-tri methylphenol	1-methoxy-2,3,4,5- tetramethylbenzene	1,2,3,4,5-pentamet hylbenzene	Hexamethylbenzen e
1	-14.71569	-15.7575	-15.7655	-15.58956	-15.73515	-14.12931	-16.22352
2	-16.44189	-16.73277	-15.69906	-15.6302	-15.49977	-14.33981	-16.28872
3	-16.67922	-15.36563	-15.71964	-16.10902	-15.67821	-14.1209	-16.24531
4	-12.99823	-12.84658	-14.07442	-14.58796	-16.35543	-15.22196	-16.30007
5	-9.24843	-10.33404	-11.27977	-11.87375	-15.04723	-17.14012	-16.22481
6	-11.91149	-13.13548	-14.18023	-14.50005	-16.13763	-15.19564	-16.2336

Table S5. Average ESP of carbon atoms in 2-methoxy-4-*n*-propylphenol based compounds corresponding to Figure S5.



Geometrical structure of TS, -981.88 of imaginary frequency:







Figure S6. Reaction barriers, TS structure, and IRC plot of initial step for phenol.



Geometrical structure of TS, -1188.66 of imaginary frequency:







Figure S7. Reaction barriers, TS structure, and IRC plot of initial step for *m*-cresol.



Geometrical structure of TS, -766.47 of imaginary frequency:



Figure S8. Reaction barriers, TS structure, and IRC plot of initial step for p-ethylphenol.



Geometrical structure of TS, -757.30 of imaginary frequency:



Figure S9. Reaction barriers, TS structure, and IRC plot of initial step for eugenol.



Geometrical structure of TS, -761.75 of imaginary frequency:



Figure S10. Reaction barriers, TS structure, and IRC plot of initial step for 2-methoxy-4-*n*-propylphenol.



Figure S11. SEM image of γ -Al₂O₃.



Figure S12. NH₃-TPD result of γ -Al₂O₃.



Figure S13. XRD pattern of γ -Al₂O₃.



Figure S14. The schematic diagram of the fixed-bed reactor.



Figure S15. The TIC of aurantius product (*o*-hydroxydiphenyl as feedstock, T=400 °C).



Figure S16. Chemical structures corresponding to Figure S15.



Figure S17. FT-IR spectrum of the crystalline solid.

Table S6. Elemental analysis of the crystalline solid.

Element	1	2
C (wt%)	88.12	88.11
H (wt%)	10.96	10.99
O (wt%)	0.889	0.849
H/C (molar ratio)	0.6747	0.6728
H/C (molar ratio), in average	().6728

For HMB $C_{12}H_{18}$ -- calculated: C, 88.82%; H, 11.18% and H/C molar ratio ~ 0.6667.



Figure S18. The TIC of the crystalline solid, lignin oil as feedstock.



Figure S19. MS spectrum (time of 19.92 min) of the crystalline solid corresponding to Figure S18.



Figure S20. The TIC of water-insoluble fraction in bio-oil used.



Figure S21. The chemical structures corresponding to Figure S20.

7. Mass balance

Yields of crystalline solid are calculated based on the quantity of model compounds or lignin oil, which is presented as follow.

Substrate	Input/g, m ₁	Produced crystalline/g, m ₂	Yield, m_2/m_1
Phenol	8.0	9.8	122.5%
Cresols	8.7	11.5	132.2%
<i>p</i> -ethylphenol	9.7	11.9	122.7%
Eugenol	12.0	10.1	84.2%
2-methoxy-4-n-propylphenol	12.2	10.3	84.4%
Lignin cil	13.7	5.3	38.7%
	11.9	4.7	39.5%
Control reaction*	26.6	Not detected	

*only methanol feed

8. Identification and quantitation of HMB in crystalline solid

The quantitation was implemented based on standard curve method, which was stated as follows.

n-tetradecane (Aladdin, \geq 99.5 wt%) as internal standard (IS), hexamethylbenzene (Dr. Ehrenstorfer, 99.5 wt%) as authentic standard. 100 µL of an internal standard solution (50 mg *n*-tetradecane in 50 mL *n*-hexane) was added to 1 mL solution. Five different solutions of authentic standard (10 mg/L, 20 mg/L, 50 mg/L, 100 mg/L, 200 mg/L) were prepared to define the standard curve. And all the resulting solutions were analyzed by GC/MS with Selected Ion Monitoring (SIM) mode. During SIM process, the characteristic peaks were respectively determined as follow: m/z ratio of 57, 99, 198 for *n*-tetradecane, and 105, 147, 162 for hexamethylbenzene.

The detailed evaluation of data was implemented as follows: the ratio of HMB response value to IS response value was recorded as y, then according to standard curve, we got the percentage of HMB (*i.e.* the value of x) in crystalline solid.



Standard curve for HMB quantitation.



Quantitation of HMB in crystalline solid produced from model compounds and lignin oil as feedstock, HMB selectivity of (a) 78.4 wt%, (b) 86.0 wt%, (c) 99.6 wt%, (d) 98.2 wt%.



(*Continued*), quantitation of HMB in crystalline solid produced from model compounds and lignin oil as feedstock, HMB selectivity of (e) 98.8 wt%, and (f) 99.9 wt%.



Biobased and Biogenic Carbon Testing Laboratory

ISO/IEC 17025:2005 Accredited

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April 01, 2018

Chenxi Wang Beijing University of Chemical Technology Beijing, China

Dear Dr. Wang

Please find enclosed your radiocarbon (C14) report for the material recently submitted. The result is reported as "% Biobased Carbon". This indicates the percentage carbon from "natural" (plant or animal by-product) sources versus "synthetic" (petrochemical) sources sources. For reference, 100 % Biobased Carbon indicates that a material is entirely sourced from plants or animal by-products and 0 % Biobased Carbon indicates that a material did not contain any carbon from plants or animal by-products. A value in between represents a mixture of natural and fossil sources.

The analytical measurement is cited as "percent modern carbon (pMC)". This is the percentage of C14 measured in the sample relative to a modern reference standard (NIST 4990C). The % Biobased Carbon content is calculated from pMC by applying a small adjustment factor for C14 in carbon dioxide in air today. It is important to note is that all internationally recognized standards using C14 assume that the plant or biomass feedstocks were obtained from natural environments.

Reported results are accredited to ISO/IEC 17025:2005 Testing Accreditation PJLA #59423 standards and all chemistry was performed here in our laboratory and counted in our own accelerators in Miami, Florida.

The international standard method utilized for this analysis is cited on your report. The report also indicates if the result is relative to total carbon (TC) or only total organic carbon (TOC). When interpreting the results, please consider any communications you may have had with us regarding the analysis. If you have any questions please contact us. We welcome your inquiries.

Sincerely,

Darden Hood

Darden Hood President





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Summary of Results - % Biobased Carbon Content ASTM D6866-16 Method B (AMS)	Certificate Number: 37648949058090952 Validation: A.E. Surfiel Quality Mompu
Submitter	Chenxi Wang
Company	Beijing University of Chemical Technology
Date Received	March 27, 2018
Date Reported	April 01, 2018
Submitter Label	Biocarbon content of HMB
RESULT:	58 % Biobased Carbon Content (as a fraction of total organic carbon)
Laboratory Number	Beta-490580
Percent modern carbon (pMC)	58.71 +/- 0.18 pMC
Atmospheric adjustment factor (REF)	100.5; = pMC/1.005



Package received - labeling COC



View of content (1mm x 1mm scale)



18.3mg analyzed (1mm x 1mm scale)

Disclosures: All work was done at Beta Analytic in its own chemistry lab and AMSs. No subcontractors were used. Beta's chemistry laboratory and AMS do not react or measure artificial C 14 used in biomedical and environmental AMS studies. Beta is a C14 tracer-free facility. Validating quality assurance is verified with a Quality Assurance report posted separately to the web library containing the PDF downloadable copy of this report.

Precision on the RESULT is cited as +/- 3% (absolute). The cited precision on the analytical measure (pMC) is 1 sigma (1 relative standard deviation). The reported result only applies to the analyzed material. The accuracy of the RESULT relies on the measured carbon in the analyzed material having been in recent equilibrium with CO2 in the air and/or from fossil carbon (from living more than 40,000 years ago such as petroleum or coal. The RESULT only applies to relative carbon content, not to relative mass content. The RESULT is calculated by adjusting pMC by the applicable "Atmospheric adjustment factor (REF)" cited in this report.



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Precision on the RESULT is cited as +/- 3% (absolute). The cited precision on the analytical measure (pMC) is 1 sigma (1 relative standard deviation). The reported result only applies to the analyzed material. The accuracy of the RESULT relies on the measured carbon in the analyzed material having been in recent equilibrium with CO2 in the air and/or from fossil carbon (from living more than 40,000 years ago such as petroleum or coal. The RESULT only applies to relative carbon content, not to relative mass content. The RESULT is calculated by adjusting pMC by the applicable "Atmospheric adjustment factor (REF)" cited in this report.



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% Biobased Carbon Content ASTM D6866-16 Method B (AMS)

Explanation of Results

The result was obtained using the radiocarbon isotope (also known as Carbon-14, C14 or 14C), a naturally occurring isotope of carbon that is radioactive and decays in such a way that there is none left after about 45,000 years following the death of a plant or animal. Its most common use is radiocarbon dating by archaeologists. An industrial application was also developed to determine if consumer products and CO2 emissions were sourced from plants/biomass or from materials such as petroleum or coal (fossil-based). By 2003 there was growing demand for a standardized methodology for applying Carbon-14 testing within the regulatory environment. The first of these standards was ASTM D6866-04, which was written with the assistance of Beta Analytic. Since ASTM was largely viewed as a US standard, European stakeholders soon began demanding an equivalent CEN standard while global stakeholders called for ISO standardization.

The analytical procedures for measuring radiocarbon content using the different standards are identical. The only difference is the reporting format. Results are usually reported using the standardized terminology "% biobased carbon". Only ASTM D6866 uses the term "% biogenic carbon" when the result represents all carbon present (Total Carbon) rather than just the organic carbon (Total Organic Carbon). The terms "% biobased carbon" and "% biogenic carbon" are now the standard units in regulatory and industrial applications, replacing obscure units of measure historically reported by radiocarbon dating laboratories e.g. disintegrations per minute per gram (dpm/g) or radiocarbon age.

The result was obtained by measuring the ratio of radiocarbon in the material relative to a National Institute of Standards and Technology (NIST) modern reference standard (SRM 4990C). This ratio was calculated as a percentage and is reported as percent modern carbon (pMC). The value obtained relative to the NIST standard is normalized to the year 1950 AD so an adjustment was required to calculate a carbon source value relative to today. This factor is listed on the report sheet as the terminology "REF".

Interpretation and application of the results is straightforward. A value of 100% biobased or biogenic carbon would indicate that 100% of the carbon came from plants or animal by-products (biomass) living in the natural environment and a value of 0% would mean that all of the carbon was derived from petrochemicals, coal and other fossil sources. A value between 0-100% would indicate a mixture. The higher the value, the greater the proportion of naturally sourced components in the material.