

## Reviews

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### Review of NMR Characterization of Pyrolysis Oils

Naijia Hao, Haoxi Ben, Chang Geun Yoo, Sushil Adhikari, and Arthur J. Ragauskas\*

6881 DOI: 10.1021/acs.energyfuels.6b01051

### Understanding the Reactions of CO<sub>2</sub>, NO, and N<sub>2</sub>O with Activated Carbon Catalyzed by Binary Mixtures

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6892 DOI: 10.1021/acs.energyfuels.5b02815

### Single-Core PAHs in Petroleum- and Coal-Derived Asphaltenes: Size and Distribution from Solid-State NMR Spectroscopy and Optical Absorption Measurements

R. Dutta Majumdar, K. D. Bake, Y. Ratna, A. E. Pomerantz, O. C. Mullins,\* M. Gerken, and P. Hazendonk\*

6907 DOI: 10.1021/acs.energyfuels.6b00559

### Study of the Aggregation of Metal Complexes with Asphaltenes Using Gel Permeation Chromatography Inductively Coupled Plasma High-Resolution Mass Spectrometry

Sara Gutierrez Sama, Alain Desprez, Gabriel Krier, Charles-Philippe Lienemann, Jérémie Barbier, Ryszard Lobinski, Caroline Barrere-Mangote, Pierre Giusti, and Brice Bouyssiere\*

6913 DOI: 10.1021/acs.energyfuels.6b00614

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D. Reyes-Gonzalez, E. Ramirez-Jaramillo, O. Manero, C. Lira-Galeana,\* and J. M. del Rio\*

6923 DOI: 10.1021/acs.energyfuels.6b00841


### Molecular Transformation of Crude Oil in Confined Pyrolysis System and Its Impact on Migration and Maturity Geochemical Parameters

Yahé Zhang, Yuhong Liao,\* Shaohui Guo, Chunming Xu, and Quan Shi\*

6933  DOI: 10.1021/acs.energyfuels.6b00952  
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6947 DOI: 10.1021/acs.energyfuels.6b00996  
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6968 DOI: 10.1021/acs.energyfuels.6b01082  
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7025 DOI: 10.1021/acs.energyfuels.6b01238  
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7037 DOI: 10.1021/acs.energyfuels.6b01241  
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7065 DOI: 10.1021/acs.energyfuels.6b01286  
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7100 DOI: 10.1021/acs.energyfuels.6b01341  
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- 7108 DOI: 10.1021/acs.energyfuels.6b01366  
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- 7118 DOI: 10.1021/acs.energyfuels.6b01377  
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- 7125 DOI: 10.1021/acs.energyfuels.6b01403  
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- 7134 DOI: 10.1021/acs.energyfuels.6b01419  
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- 7158 DOI: 10.1021/acs.energyfuels.6b01424  
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- 7173 DOI: 10.1021/acs.energyfuels.6b01441  
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- 7187 DOI: 10.1021/acs.energyfuels.6b01512  
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- 7196 DOI: 10.1021/acs.energyfuels.6b01534  
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- 7206 DOI: 10.1021/acs.energyfuels.6b01544  
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- 7214 DOI: 10.1021/acs.energyfuels.6b01552  
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- 7221 DOI: 10.1021/acs.energyfuels.6b01567  
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- 7229 DOI: 10.1021/acs.energyfuels.6b01583  
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- 7236 DOI: 10.1021/acs.energyfuels.6b01590  
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- 7241 DOI: 10.1021/acs.energyfuels.6b00333  
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- 7256 DOI: 10.1021/acs.energyfuels.6b00372  
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- 7268 DOI: 10.1021/acs.energyfuels.6b00583  
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- 7277 DOI: 10.1021/acs.energyfuels.6b00765  
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7284 **5** DOI: 10.1021/acs.energyfuels.6b00890  
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7291 DOI: 10.1021/acs.energyfuels.6b00978  
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7298 **5** DOI: 10.1021/acs.energyfuels.6b00971  
Nitrogen-Doped Carbon Foams Synthesized from Banana Peel and Zinc Complex Template for Adsorption of CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>  
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7310 **5** DOI: 10.1021/acs.energyfuels.6b01011  
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7319 DOI: 10.1021/acs.energyfuels.6b01064  
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7326 DOI: 10.1021/acs.energyfuels.6b01097  
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7331 DOI: 10.1021/acs.energyfuels.6b01114  
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7342 DOI: 10.1021/acs.energyfuels.6b01157  
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7357 DOI: 10.1021/acs.energyfuels.6b01183  
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7367 DOI: 10.1021/acs.energyfuels.6b01220  
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7379 DOI: 10.1021/acs.energyfuels.6b01229  
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7387 **5** DOI: 10.1021/acs.energyfuels.6b01269  
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7400 DOI: 10.1021/acs.energyfuels.6b01334  
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7410 DOI: 10.1021/acs.energyfuels.6b01522  
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7419 **5** DOI: 10.1021/acs.energyfuels.6b01568  
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7428 DOI: 10.1021/acs.energyfuels.6b01586  
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7435 DOI: 10.1021/acs.energyfuels.6b01634  
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7452 DOI: 10.1021/acs.energyfuels.6b01992  
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7460 DOI: 10.1021/acs.energyfuels.6b00246  
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7465  DOI: 10.1021/acs.energyfuels.6b00426  
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7474 DOI: 10.1021/acs.energyfuels.6b00129  
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7481 DOI: 10.1021/acs.energyfuels.6b00671  
**Effect of Amine Activators on Aqueous *N,N*-Diethylethanolamine Solution for Postcombustion CO<sub>2</sub> Capture**  
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7489 DOI: 10.1021/acs.energyfuels.6b00692  
**Evaluation of the Multi-amine Functionalized Ionic Liquid for Efficient Postcombustion CO<sub>2</sub> Capture**  
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7496  DOI: 10.1021/acs.energyfuels.6b00793  
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7524 DOI: 10.1021/acs.energyfuels.6b01126  
**Reducing Gas Flaring in Oil Production from Shales**  
 Richard Roehner, Palash Panja, and Milind Deo\*

7532 DOI: 10.1021/acs.energyfuels.6b01205  
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7543  DOI: 10.1021/acs.energyfuels.6b01223  
**Synthesis of Efficient CaO Sorbents for CO<sub>2</sub> Capture Using a Simple Organometallic Calcium-Based Carbon Template Route**  
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7551 DOI: 10.1021/acs.energyfuels.6b01297  
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7560  DOI: 10.1021/acs.energyfuels.6b01323  
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7571 DOI: 10.1021/acs.energyfuels.6b01328  
**Effect of Coal Combustion on the Reactivity of a CaO-Based Sorbent for CO<sub>2</sub> Capture**  
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7579  DOI: 10.1021/acs.energyfuels.6b01423  
**The Structure of Adsorbed Species on Immobilized Amines in CO<sub>2</sub> Capture: An In Situ IR Study**  
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7588 DOI: 10.1021/acs.energyfuels.6b01431  
**Stabilization of Heavy Metals in Municipal Solid Waste Incineration Fly Ash in Circulating Fluidized Bed by Microwave-Assisted Hydrothermal Treatment with Additives**  
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7596 DOI: 10.1021/acs.energyfuels.6b01433  
**Mechanically Stable Mixed Metal Oxide of Cu and Mn as Oxygen Carrier for Chemical Looping Syngas Combustion**  
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7604 DOI: 10.1021/acs.energyfuels.6b01647  
Highly Selective CO<sub>2</sub> Extraction from a Mixture of CO<sub>2</sub> and H<sub>2</sub> Gases Using Hydroquinone Clathrates  
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### Efficiency and Sustainability

7610 DOI: 10.1021/acs.energyfuels.6b01105  
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A. M. Al-Sabagh, M. A. Betiha,\* D. I. Osman, A. I. Hashim, M. M. El-Sukkary, and Tahany Mahmoud\*

7622 DOI: 10.1021/acs.energyfuels.6b01415  
Efficiency and Mechanism of Demulsification of Oil-in-Water Emulsions Using Ionic Liquids  
Xiaohua Li, Sascha R. A. Kersten, and Boelo Schuur\*

7629 DOI: 10.1021/acs.energyfuels.6b01418  
Energy and Exergy Analyses of Fluidized-Bed Municipal Solid Waste Air Gasification  
Yuanjun Tang, Jun Dong, Yong Chi,\* Zhaozhi Zhou, and Mingjiang Ni

7638 DOI: 10.1021/acs.energyfuels.6b01435  
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Georg Kreisberger,\* Christian W. Klampfl, and Wolfgang W. Buchberger

### Catalysis and Kinetics

7646 DOI: 10.1021/acs.energyfuels.6b01321  
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7656 DOI: 10.1021/acs.energyfuels.6b01397  
Modeling Growth Kinetics of Gas Hydrate in Porous Media: Experimental Validation  
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### Combustion

7666 DOI: 10.1021/acs.energyfuels.6b00314  
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7678 DOI: 10.1021/acs.energyfuels.6b00322  
Quantification of the Fraction of Particulate Matter Derived from a Range of <sup>13</sup>C-Labeled Fuels Blended into Heptane, Studied in a Diesel Engine and Tube Reactor  
Aaron Eveleigh,\* Nicos Ladammatos, Paul Heller, and Anne-Lise Jourdan

7691 DOI: 10.1021/acs.energyfuels.6b00421  
Computational Study of NO<sub>x</sub> Formation at Conditions Relevant to Gas Turbine Operation, Part 2: NO<sub>x</sub> in High Hydrogen Content Fuel Combustion at Elevated Pressure  
Sheikh F. Ahmed, Jeffrey Santner, Frederick L. Dryer, Bihter Padak, and Tanvir I. Farouk\*

7704 DOI: 10.1021/acs.energyfuels.6b01048  
Numeric Model for Assessment of Naphthalene Conversion through Ionization Reactions in a Microwave Air Plasma Torch  
A. Pilatau,\* H. S. Medeiros, A. S. da Silva Sobrinho, and G. Petraconi Filho

7713 DOI: 10.1021/acs.energyfuels.6b01080  
Sulfur and Chlorine Gas Species Formation during Coal Pyrolysis in Nitrogen and Carbon Dioxide Atmosphere  
Lorenz Frigge,\* Ghada Elserafi, Jochen Ströhle, and Bernd Epple

7721 DOI: 10.1021/acs.energyfuels.6b01193  
Evaluation of Adding an Olefin to Mixtures of Primary Reference Fuels and Toluene To Model the Oxidation of a Fully Blended Gasoline  
J. C. G. Andrae\* and T. Kovács

7731 DOI: 10.1021/acs.energyfuels.6b01234  
Mn-Catalyzed Oxidation of Heavy Oil in Porous Media: Kinetics and Some Aspects of the Mechanism  
Andrey Galukhin,\* Mohammed Amine Khelkhal, Alexander Gerasimov, Timur Biktairov, Marat Gafurov, Alexander Rodionov, and Sergei Orlinkii

7738 DOI: 10.1021/acs.energyfuels.6b01348  
Experimental and Kinetic Modeling Study of Nitroethane Pyrolysis at a Low Pressure: Competition Reactions in the Primary Decomposition  
Kuiwen Zhang,\* Peter Glarborg, Xueyao Zhou, Lidong Zhang, Lili Ye, and Guillaume Dayma

7746 DOI: 10.1021/acs.energyfuels.6b01365  
A Mechanism Study on Hydrothermal Carbonization of Waste Textile  
Yousheng Lin,\* Xiaoqian Ma, Xiaowei Peng, and Zhaosheng Yu

7755 DOI: 10.1021/acs.energyfuels.6b01370  
Synthesis and Characterization of Aviation Turbine Kerosene Nanofluid Fuel Containing Boron Nanoparticles  
Fateme Sadat Shariatmadar and Shahram Ghanbari Pakdehi\*

7763 DOI: 10.1021/acs.energyfuels.6b01525  
Experiment and Mechanism Study on the Effect of Kaolin on Melting Characteristics of Zhundong Coal Ash  
Mingqiang Li, Zhongxiao Zhang, Xiaojiang Wu, and Junjie Fan\*



- 7770 DOI: 10.1021/acs.energyfuels.6b01581  
 Demonstration of a Regulatory Method for Aircraft Engine Nonvolatile PM Emissions Measurements with Conventional and Isoparaffinic Kerosene fuels  
 Prem Lobo,\* Jamey Condevaux, Zhenhong Yu, Joshua Kuhlmann, Donald E. Hagen, Richard C. Miake-Lye, Philip D. Whitefield, and David W. Raper

- 7778 DOI: 10.1021/acs.energyfuels.6b01624  
 Elementary Reaction Modeling and Experimental Characterization on Methane Partial Oxidation within a Catalyst-Enhanced Porous Media Combustor  
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## Process Engineering

- 7786 DOI: 10.1021/acs.energyfuels.6b01279  
 Conceptual Design of an Oil Shale Comprehensive Refinery Process with High Resource Utilization  
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- 7802 DOI: 10.1021/acs.energyfuels.6b01364  
 Leaching Kinetics of Vanadium with Electro-oxidation and H<sub>2</sub>O<sub>2</sub> in Alkaline Medium  
 Hao Peng,\* Zuohua Liu, and Changyuan Tao\*

Supporting Information available via online article

## Review of NMR Characterization of Pyrolysis Oils

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**ABSTRACT:** Pyrolysis of renewable biomass has been developed as a method to produce green fuels and chemicals in response to energy security concerns as well as to alleviate environmental issues incurred with fossil fuel usage. However, pyrolysis oils still have limited commercial application, mainly because unprocessed oils cannot be readily blended with current petroleum-based transportation fuels. To better understand these challenges, researchers have applied diverse characterization techniques in the development of bio-oil studies. In particular, nuclear magnetic resonance (NMR) is a key spectroscopic characterization method through analysis of bio-oil components. This review highlights the NMR strategies for pyrolysis oil characterization and critically discusses the applications of <sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P, <sup>19</sup>F, and two-dimensional (2-D NMR) analyses such as heteronuclear single quantum correlation (HSQC) in representative pyrolysis oil studies.

### 1. INTRODUCTION

Developing viable green energy technologies is imperative because of environmental issues related to fossil fuel usage.<sup>1–3</sup> Utilization of biomass has been introduced as a solution toward the development of sustainable and green energy platforms.<sup>4</sup> Lignocellulosic biomass is a complex composite primarily comprising three principle components: cellulose (~35–50%), hemicellulose (~20–35%), and lignin (~10–25%).<sup>5</sup> Besides these three main components, biomass also has minor components including ash, protein, and other extractives, whose concentrations widely vary depending on the feedstocks. Lignocellulosic biomass is an attractive feedstock for biofuels because it is relatively inexpensive and abundant, avoids the “food or fuel” argument, and is a renewable source of carbon. Typical bioresources for biofuels include energy crops, such as switchgrass, miscanthus, poplar, and energy cane, or biomass residues from agriculture and forestry operations.<sup>6</sup> The U.S. Department of Energy and U.S. Department of Agriculture established a national goal that lignocellulosic biomass will supply 5% of the nation's power by 2020 and 20% of its transportation fuels and 25% of its chemicals by 2030. This goal is approximately equivalent to 30% of the petroleum consumption in the year 2005.<sup>7</sup>

Biomass pyrolysis is a promising thermochemical conversion technology that involves irreversible thermochemical decomposition of lignocellulose in the absence of oxygen.<sup>8</sup> The complex polymer constituents of lignocellulose (i.e., lignin, cellulose, and hemicellulose) are depolymerized into smaller molecules upon thermal treatment. The pyrolysis products contain char, gas, and a pyrolysis oil. In particular, the pyrolysis oil has the potential to be blended in the transportation fuels even though it still has some challenges as a fuel, because of its physiochemical properties (which will be discussed in the following section).<sup>9</sup>

In addition, a number of valuable chemicals such as methanol, phenol, catechol, carboxylic acid, and furfural, can be derived from pyrolysis oils.<sup>10</sup> Thus, understanding pyrolysis oil components is an essential part of pyrolysis research, which will provide a fundamental foundation from which future chemical upgrading of bio-oils can be developed.<sup>11</sup>

Various instrumental analytical techniques including gas chromatography (GC), liquid chromatography (LC), high-resolution mass spectrometry (HRMS), Fourier transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), and NMR have been introduced for characterization of bio-oils in the previous studies.<sup>12–16</sup> One of the most comprehensive spectroscopic experiments suited for the comprehensive elucidation of bio-oil components is NMR spectroscopy. Various NMR experiments have been employed to better understand the components and structures of thermally generated bio-oils. <sup>1</sup>H and <sup>13</sup>C NMR analyses have been widely used to investigate the structural hydrogen–carbon framework of bio-oils.<sup>17</sup> Moreover, selective analysis of functional groups in the pyrolysis oils through NMR analysis techniques allows a deep understanding of the characteristics of pyrolysis oils. For instance, hydroxyl functional groups of bio-oils can be measured by phosphorylation followed by <sup>31</sup>P NMR spectroscopy.<sup>18</sup> Likewise, derivatization of bio-oils with 4-(trifluoromethyl)phenylhydrazine followed by <sup>19</sup>F NMR spectroscopy provides a quantitative and comprehensive understanding of carbonyl groups, which lead to corrosion and aging problems during upgrading.<sup>19</sup> 2D-NMR experiments, such as <sup>1</sup>H–<sup>13</sup>C HSQC, are used to

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