

## **SUPPORTING INFORMATION**

### **Impact of Mineralogical Variation on CO<sub>2</sub> Behavior in Small Pores from Producing Intervals of the Marcellus Shale: Results from Neutron Scattering**

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#### **Additional Methods**

- Quantitative mineralogic analyses were conducted using a Panalytical x-Pert Pro diffractometer equipped with a Cu source and an X'celerator detector operating at 40kV and 40 mA over a range of 5 – 70 degrees 2 $\Theta$ .
- Mineral identification was performed with X'Pert HighScore software and the PDF4/Minerals ICDD database; quantities of crystalline phases were determined by the Rietveld method.
- Kerogen was separated from the samples with HCl/HF/HCl acid digestion followed by a Zn/Br heavy liquid separation at 1.8 and 2.0 g/cm<sup>3</sup> to obtain a high purity kerogen isolate for CHNOS analysis.
- CHN data were obtained on a Flash EA 1112 Series Analyzer using the Dumas method, following density separation of the organic material. O was determined on a Leco RO-478 Oxygen Analyzer following ASTM D5622, and S was determined on a Leco Model S-144DR Sulfur Analyzer following ASTM D4239 and D1552 methods.

#### **References**

1. ASTM, 2017, D5622 Standard Test Methods for Determination of Total Oxygen in Gasoline and Methanol Fuels by Reductive Pyrolysis, ASTM International, West Conshohocken, PA, <https://www.astm.org/Standards/D5622.htm>.
2. ASTM, 2018, D4239 Standard Test Methods for Sulfur in the Analysis Sample of Coal and Coke Using High-Temperature Tube Furnace Combustion, ASTM International, West Conshohocken, PA, <https://www.astm.org/Standards/D4239.htm>.
3. ASTM, 2016, D1552 Standard Test Methods for Sulfur in Petroleum Products by High Temperature Combustion and Infrared (IR) Detection or Thermal Conductivity Detection (TCD), ASTM International, West Conshohocken, PA, <https://www.astm.org/Standards/D1552.htm>.