

## Supporting Information

### **Neutron Scattering Measurements of Carbon Dioxide Adsorption in Pores within the Marcellus Shale: Implications for Sequestration**

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Figure S1 – Schematic of the NIMROD sample environment. A null scattering  $\text{Ti}_{0.676}\text{Zr}_{0.324}$  cell (internal dimensions of 3.4 cm (width) x 5.6 cm (height) x 0.2 cm (thickness), wall thickness 0.1 cm) was used as a sample container. The sample was placed into the cell onto a shim in order to site it at the correct height, and the cell was sealed with a gasket indium seal. The top sealing flange of the cell was a 316SS plate with 1/4" tube connected with a valve and then to a 1/8" (OD) 316 SS capillary. The setup was mounted onto a candlestick with temperature control provided by a recirculating oil bath, and connected to a gas handling manifold equipped with a relief valve (80 bar), a pressure transducer (0-100 bar), and gas and vacuum connections. The gas line was connected to a high purity  $\text{CO}_2$  cylinder (99.9996%) system with the aid of a reducer.

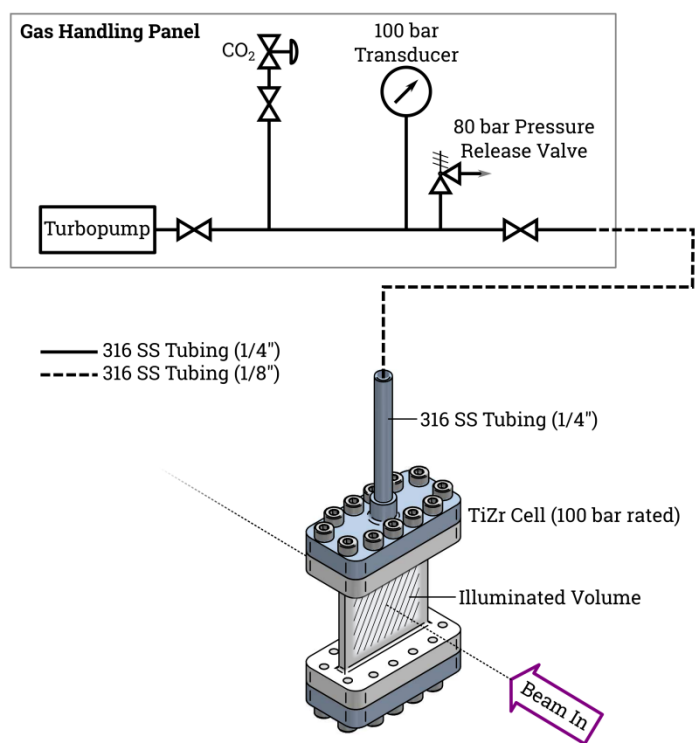


Figure S2 - Ratio of scattering intensity in CO<sub>2</sub> at 22°C and 25 and 40 bar compared to vacuum (SANS and NIMROD) for the Marcellus Shale after subtraction of flat background and showing error bars. Inset: Ratio of scattering intensity in CO<sub>2</sub> at 60°C and 25 and 40 bar (SANS) compared to vacuum showing error bars. NIMROD data of  $Q > 1 \text{ \AA}^{-1}$  were not used because the flat background was the dominant source of scattering at high  $Q$ : once it was removed, the remaining signal was very small and the errors in the ratios were very large at high  $Q$ .

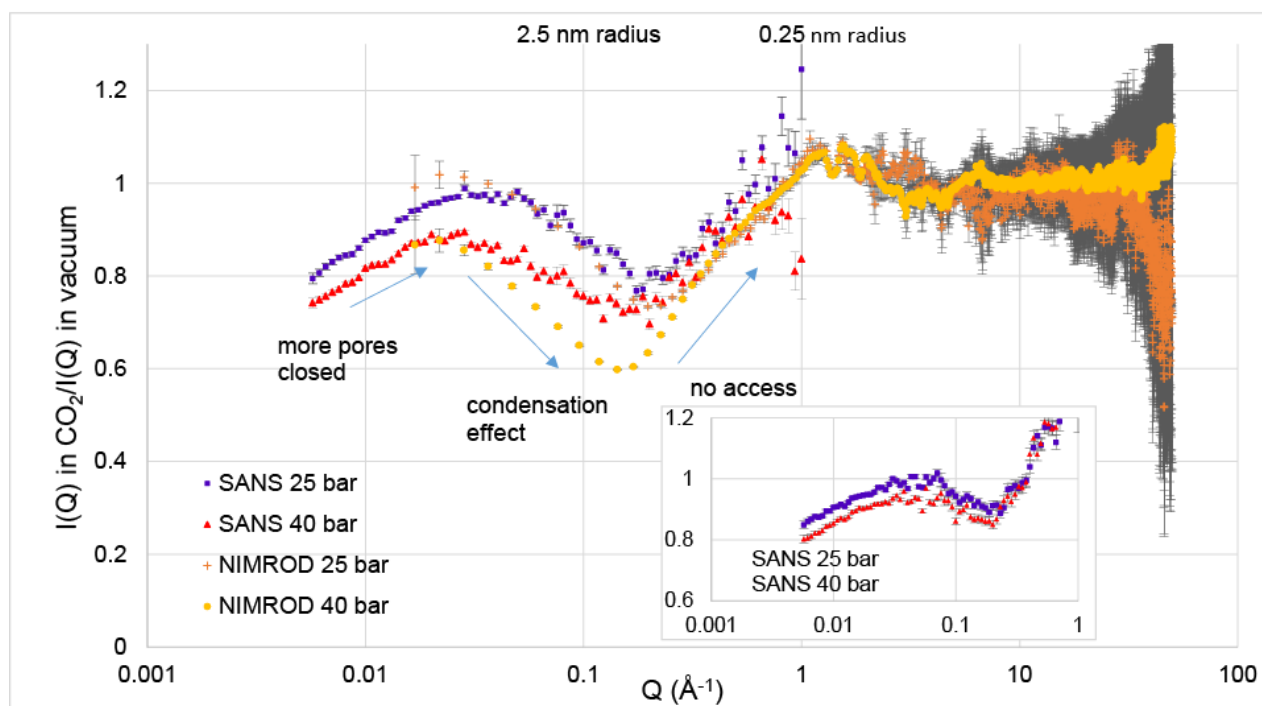


Table S1 - Expected fraction of SANS scattering intensity compared to vacuum for shale pressurized with CO<sub>2</sub> at our operating conditions. Comparison of expected scattering intensity and measured scattering intensity is used to estimate densification of CO<sub>2</sub> in pores and the percentage of open and closed micropores in the sample.

Conditions	CO <sub>2</sub> density (g/cm <sup>3</sup> )	Expected fraction of scattering intensity
22°C 25 bar	0.052	0.94
22°C 40 bar	0.095	0.88
60°C 25 bar	0.043	0.95
60°C 40 bar	0.074	0.91