

Supplementary Materials: Selective Desulfonation of Oxidized Sulfur Compounds in Crude Oil by Alcohol-Mediated Nucleophilic Attack Studied by XANES and XRF Spectroscopy

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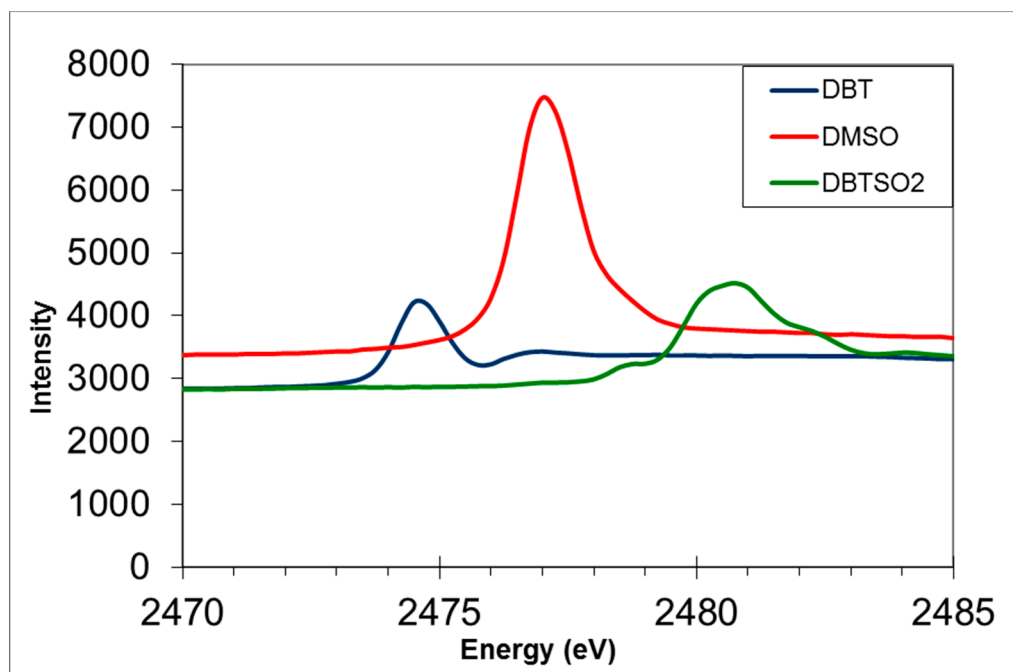


Figure S1. XANES Spectra of sulfur standards: dibenzothiophene (DBT), dimethyl sulfoxide (DMSO) and dibenzothiophene sulfone (DBTSO₂).

Table S1. Feed oil properties.

Oil	Density (g/mL at 15°C)	Viscosity (cP)	Sulfur (wt%)	Nitrogen (ppm)	Vanadium (ppm)	Nickel (ppm)	Iron (ppm)
US Gulf Coast Diesel	N/A	N/A	2.00%	N/A	N/A	N/A	N/A
Athabasca Bitumen #1	1.0355	699.7 (100°C)	6.50%	4900	240	90	24
US Gulf Coast Gas Oil	0.9206	103.8 (21°C)	1.20%	2300	<1	<1	<1
Arabian Whole Crude	0.8956	41.9 (21°C)	3.15%	1500	56	16	<1
Athabasca Bitumen #2	0.9930	180.1 (100°C)	4.37%	3300	137	54	11
Athabasca Bitumen #3	1.0090	N/A	4.80%	3900	236	93	4

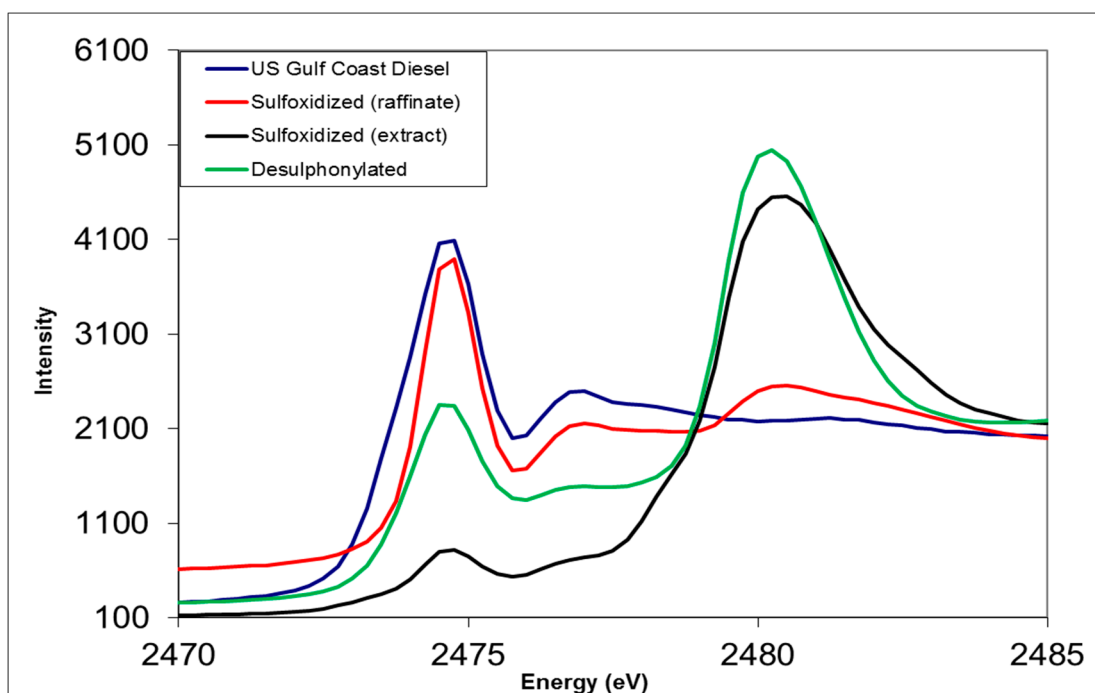


Figure S2. XANES spectra of US Gulf Coast Diesel.

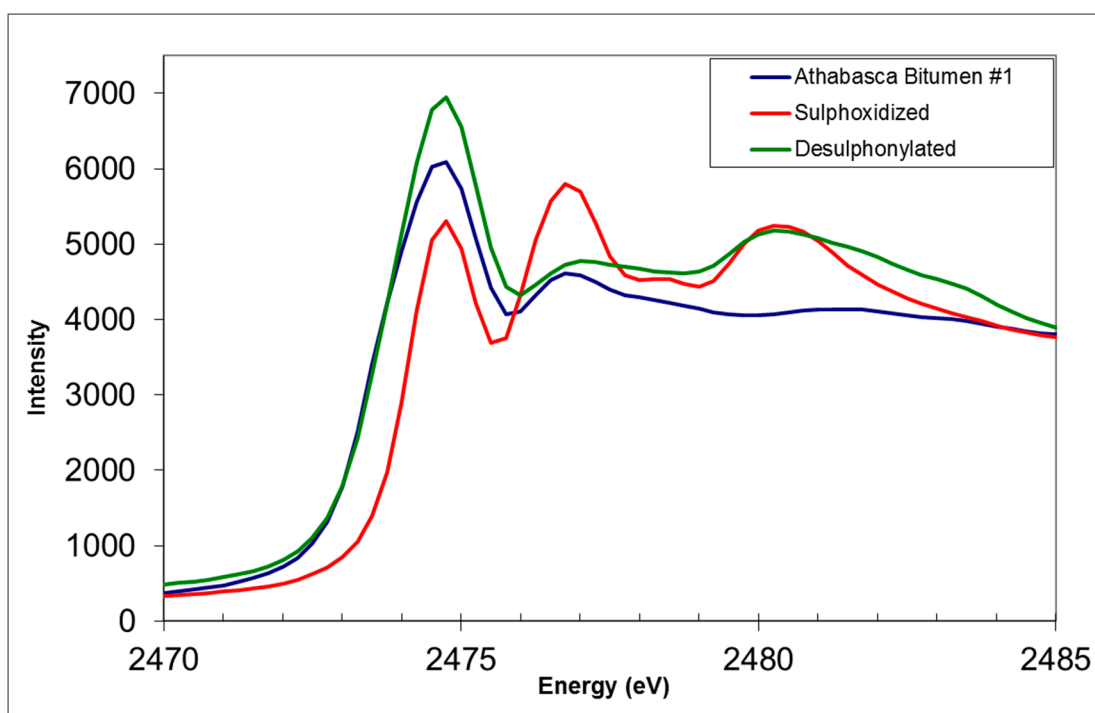


Figure S3. XANES Spectra of Athabasca Bitumen #1.

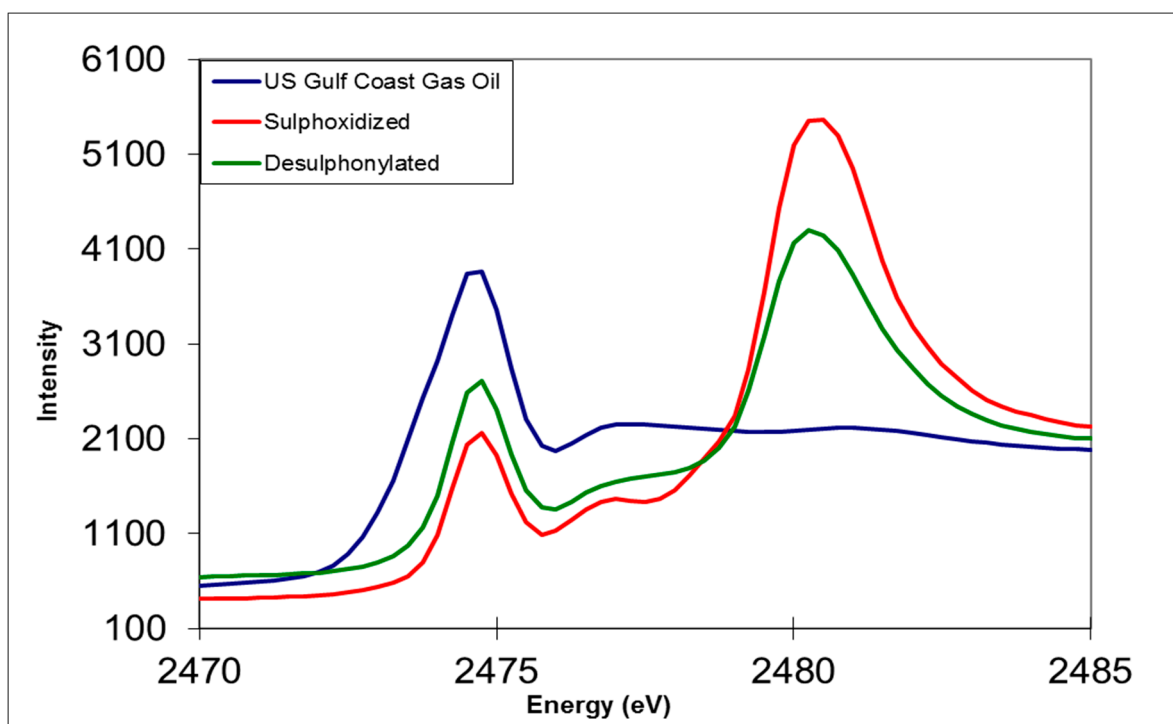


Figure S4. XANES Spectra of US Gulf Coast Gas Oil.

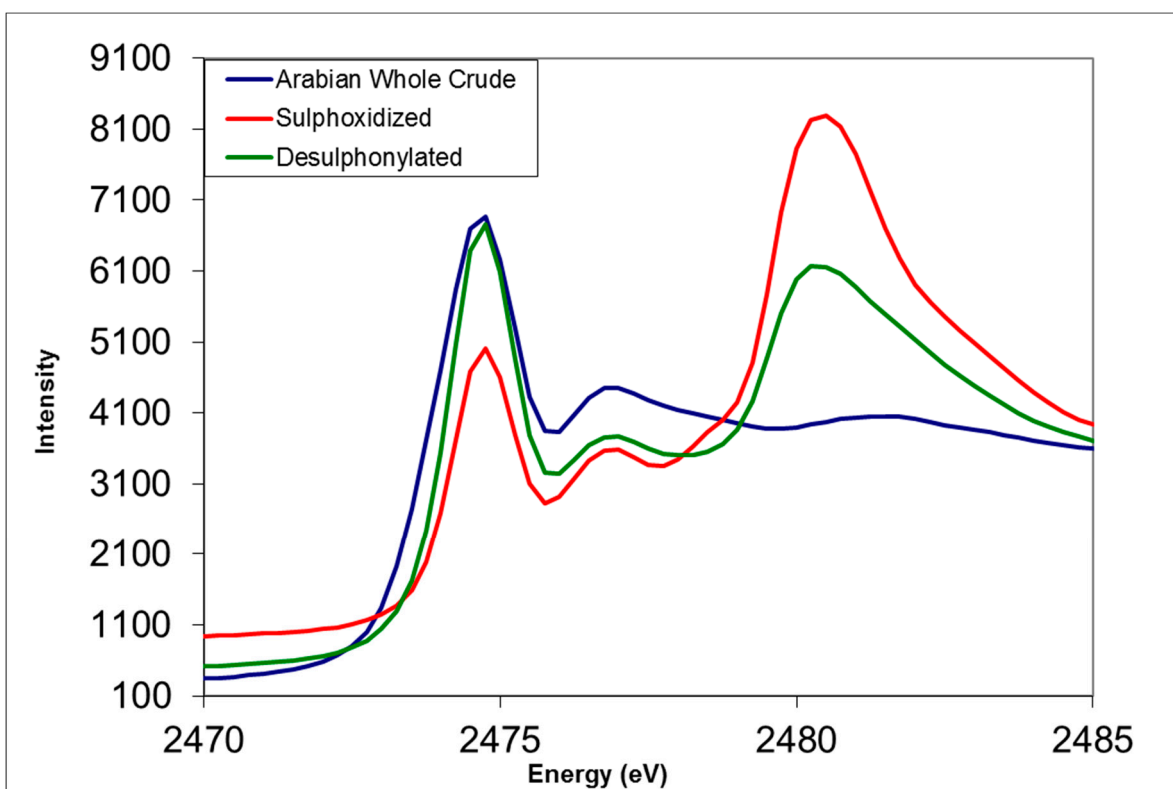
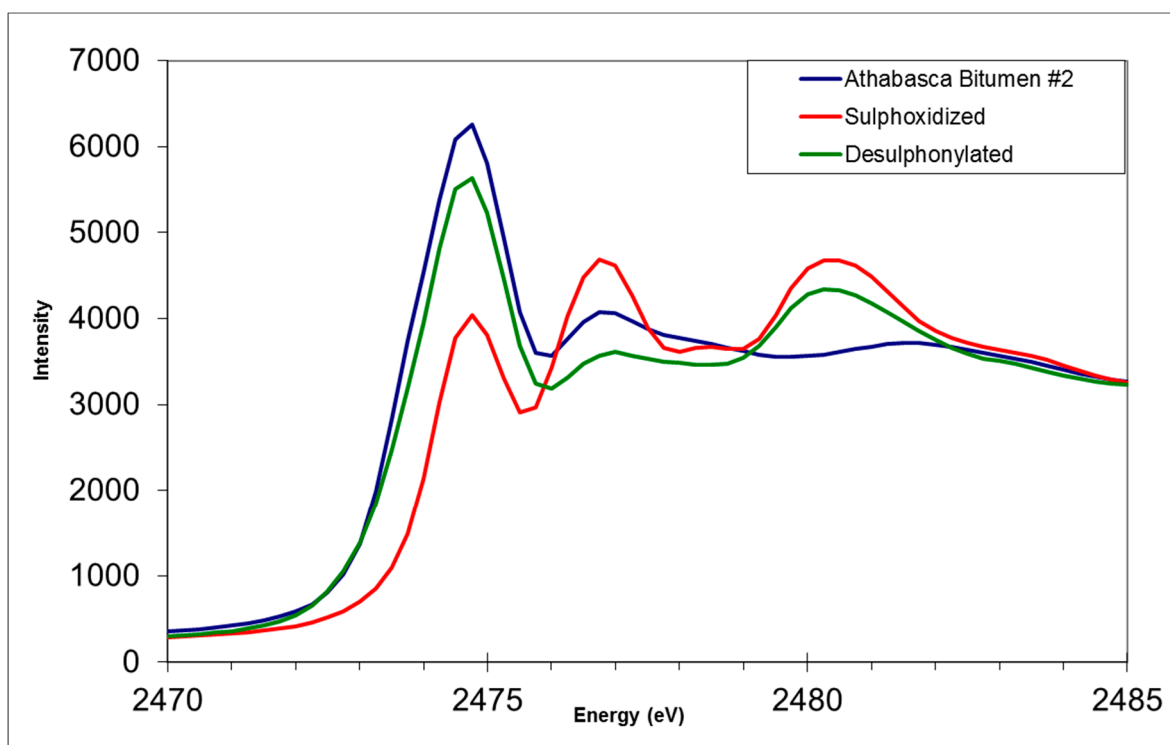
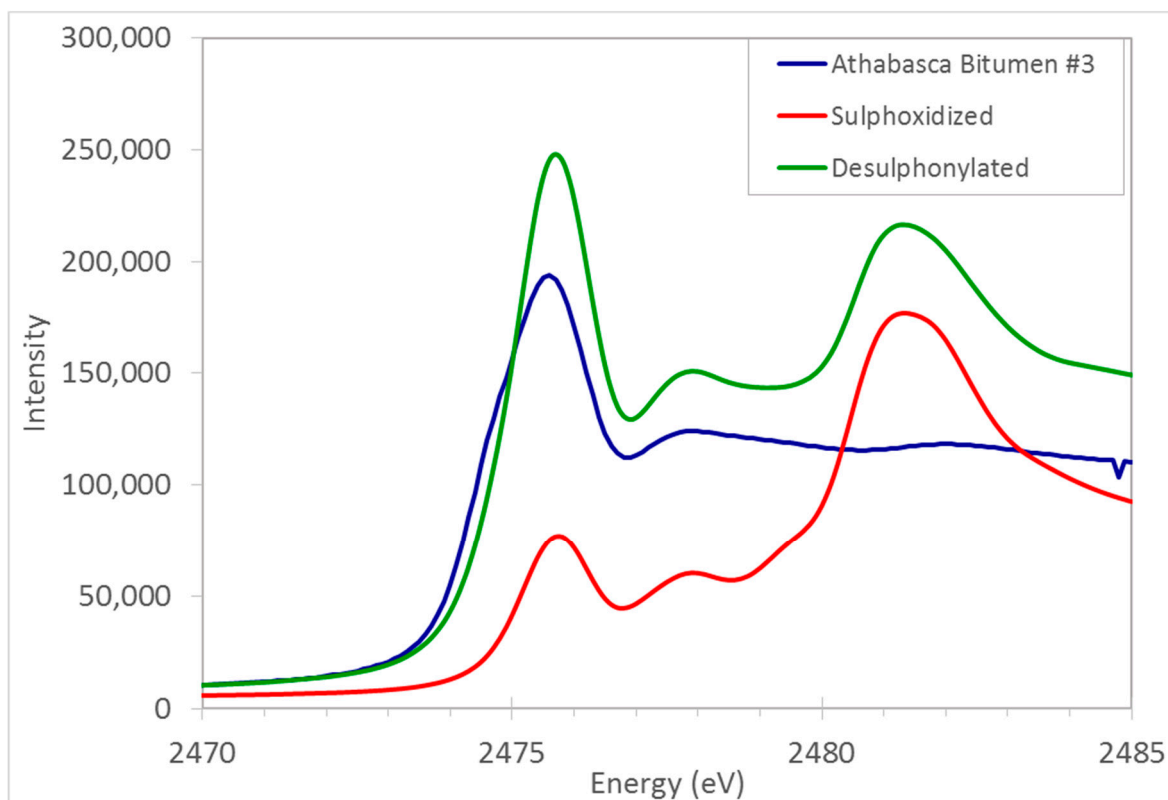


Figure S5. XANES Spectra of Arabian Whole Crude.

XANES Spectra of Athabasca Bitumen #2

**Figure S6.** XANES Spectra of Athabasca Bitumen #2.**Figure S7.** XANES Spectra of Athabasca Bitumen #3.

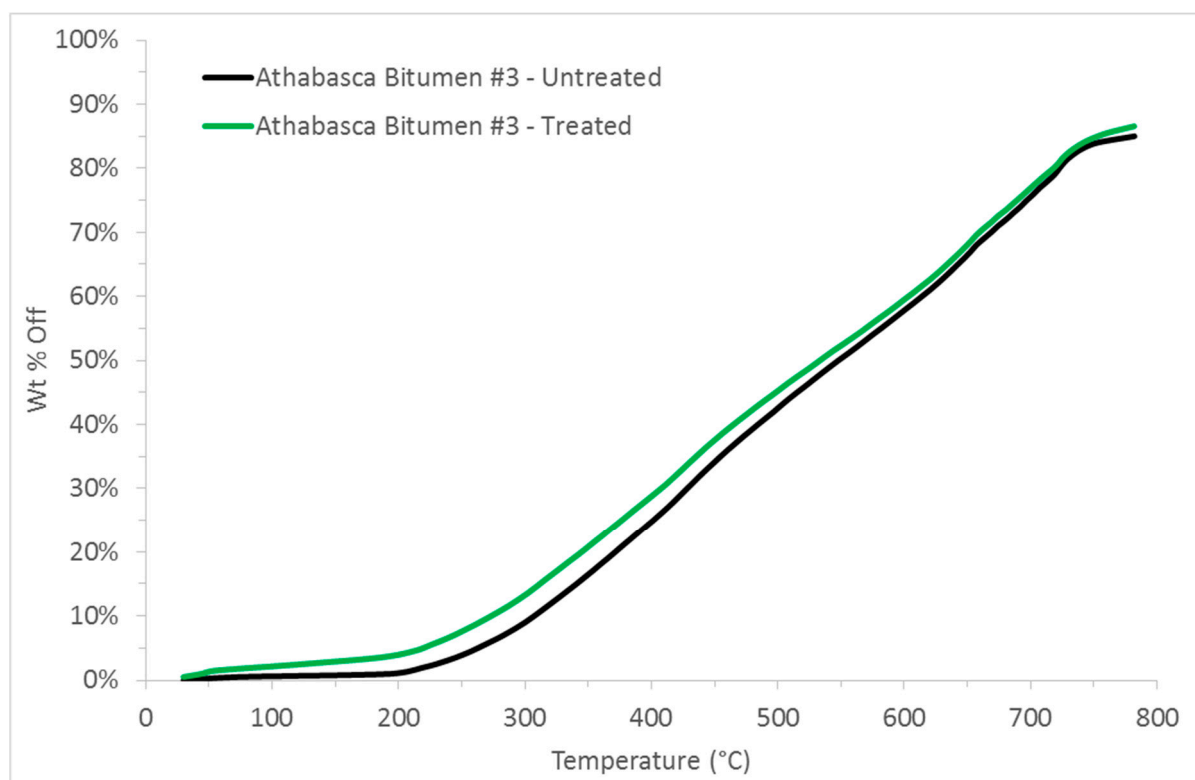


Figure S8. HT-SIMDIS (ASTM D7169) of Athabasca Bitumen #3, before treatment, and after sulfoxidation/desulfonylation.