Supplementary Material For:

Insights into the Nature of the Chemical Bonding in Thiophene-2-Thiol from X-ray Absorption Spectroscopy

Julien J. H. Cotelesage,[†] M. Jake Pushie,[†] Linda Vogt,^{†,¶} Monica Barney,[‡] Andrew Nissan,[‡] Ingrid J. Pickering,^{†,¶} and Graham N. George^{*†,¶}

[†] Molecular and Environmental Sciences Group, Department of Geological Sciences, University of Saskatchewan, Saskatchewan, Saskatchewan S7N 5E2, Canada

[¶] Department of Chemistry, University of Saskatchewan, Saskatchewan, Saskatchewan, S7N 5C9, Canada

[‡]Chevron Energy Technology Company, Richmond, California 94802 USA

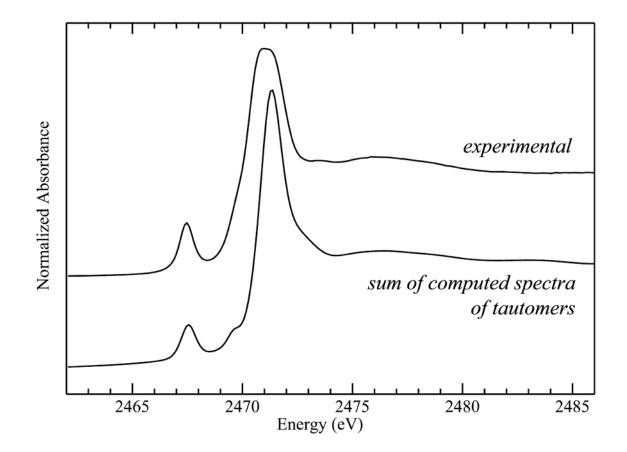


Figure S1. Comparison of sum of StoBe-DeMon DFT simulated spectra (68% 1 + 32% 2) with the experimental spectra for thiophene-2-thiol in toluene solution.