



UMD Department of Chemistry & Biochemistry
Fall 2021 Seminar Series
Friday, November 19, 2021
3:00 p.m. ~ Chem 200

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HOST ~ DR. MELISSA MAURER-JONES

***Assessing the Degradation of Munitions Compounds by
Compound Specific Isotope Analysis in Natural and
Engineered Environments***

Iron-bearing minerals are important reductants in the contaminated subsurface, but their availability for the reduction of anthropogenic pollutants is often limited by competition with other electron acceptors including microorganisms and poor accessibility to Fe(II) in complex hydrogeologic settings. The supply of external electron donors through in situ chemical reduction (ISCR) has been proposed as one remediation approach, but the quantification of pollutant transformation is complicated by the perturbations introduced to the subsurface by ISCR. Here, we evaluate the application of compound specific isotope analysis (CSIA) for monitoring the reduction of 2,4-dinitroanisole (DNAN), a component of insensitive munitions formulations, by mineral-bound Fe(II) generated through ISCR of subsurface material from two field sites. Electron balances from laboratory experiments in batch and column reactors showed that 3.6% to 11% of the total Fe in the sediments was available for the reduction of DNAN and its partially reduced intermediates after dithionite treatment. The extent of DNAN reduction was successfully quantified from its N isotope fractionation measured in the column effluent based on the derivation of a N isotope enrichment factor, ϵ_N , derived from a comprehensive series of isotope fractionation experiments with numerous Fe(II)-bearing minerals as well as dithionite-reduced subsurface materials. Our observations illustrate the utility of CSIA as a robust approach to evaluate the success of in situ remediation through abiotic contaminant reduction.