**Proposal: Metal catalyzed Si-C bond cleavage of DMSD**

Broadly speaking, my research interests involve understanding the mechanistic processes that cleave methyl group carbon bonds (–CH3) to high-valent main group elements, specifically silicon (Si) and sulfur (S).

I’m interested in silicon–carbon bonds (Si–CH3) of the molecule dimethylsilanediol (abbreviated DMSD) because this specific molecule has been detected in environmental matrices. One source of DMSD in the environment is from chemical additives in personal care and other down-the-drain household products. Because no naturally occurring organosilicon compounds have been reported, chemical species containing silicon–carbon bonds, such as DMSD, are anthropogenic. The impacts of organosilicon xenobiotics are not entirely clear, but there is evidence for Si–CH3 catabolism in mammals. The long-term goal of my research is the identification of a catalytic system that can efficiently break the Si–CH3 bonds of DMSD under mild conditions and physiological pH. Neither a chemical nor a biological catalytic system has yet been identified. The identification of a catalyst capable of breaking a Si–CH3 bond would be a significant advancement in the field and applicable to the design of systems engineered to treat environmental pollutants.

You will propose a metal-catalyzed cycle that ultimately cleaves at least one Si–CH3 bond in DMSD using fundamental reaction steps introduced in CHEM 375. There are no restrictions upon the other reagents used or products formed. However, your proposed catalytic cycle must produce a balanced chemical reaction (both mass and charge) and reagents must be known molecules with structures consistent with chemical theory. Proposed intermediates must be clearly depicted in your catalytic cycle. There are no restrictions to the number of steps you propose.

The completed proposal must be submitted via Blackboard no later than May 8th at 1:30 p.m. Proposals must reflect individual work, but you will have the opportunity to give and receive feedback from your peers (and your instructor) prior to the due date. You must use ChemDraw to create your proposed catalytic cycle (.docx documents only).

A detailed rubric will be provided and explained during lecture 22, April 18th.

***VIII. Your Grade:***

Reading Comprehension Tests (average of 7): 35%

Quizzes (average of 3): 15%

Take home exams (average of 3): 30%

**Final written proposal:**  **20%**

100%

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| **Proposal Rubric** | | |
| **Item** | **Description** | **Points** |
| Title | The given title was *Metal catalyzed Si–C bond cleavage of dimethylsilanediol (DMSD).* You may amend that title to provide a more descriptive title consistent with your specific proposed catalytic cycle. | 10 |
| Balanced Chemical Reaction | A good example of a balanced chemical reaction followed by a proposed catalytic cycle is question 4 from reading comprehension test #5. | 10 |
| Catalytic Cycle | Using ChemDraw, depict your proposed balanced chemical reaction.  Importantly, your proposed intermediates can be generic, i.e. M for a transition metal and L for ancillary ligands not directly involved in your chemistry. | 60 |
| Written Description | Using full sentences, describe the proposed catalytic cycle, being as specific as possible. A good example is provided by C&W in your textbook for Rh-catalyzed hydroformylation (starting at the bottom of page 202) | 20 |
| **total** | | **100** |

For additional points

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| **Item** | **Description** | **Points** |
| Assign a specific metal and ancillary ligands | Determine the oxidation state of the metal, the *d*-electron count, the total electron count (metals and ligands) and propose a reasonable structure for each intermediate, clearly depicting the stereochemistry at the metal center. | 10 |
| Include reference(s) from peer-reviewed literature as precedent for a proposed intermediate | Describe the search process (i.e. Scifinder, google scholar, ACS e-journals, etc.) and the queries used to find the literature precedent. Describe in a short paragraph how the specific reference relates to your proposed process. | 10 |
| Estimate overall G of the reaction | You may use tabulated bond dissociation energies to estimate the overall enthalpy. You may make reasonable assumptions about the entropy of your balanced chemical reactions. Ideally, Gf values for the products and the reactants can be used to calculate the overall G of the reaction. | 10 |