

Undergraduate Colloquium in Mathematics

Thursday, November 29th 1:00 PM-1:50 PM

STV 131

Investigations into the coordination geometries of oxovanadates and enzymes

Craig C. McLauchlan, Ph.D.

Department of Chemistry, ISU

Vanadate and vanadium compounds are known for their roles as both enzyme active sites and as inhibitors of enzymes. For example, vanadium is found in the active site of vanadium-dependent haloperoxidases, yet a range of vanadium complexes have been shown to inhibit phosphatases. Both species include vanadium in a five-coordinate geometry. Five-coordinate geometries for transition metal ions such as vanadium, however, are often found to be between the idealized square planar and trigonal bipyramidal geometries, the latter being more in line with the five-coordinate exploded transition-state geometry of phosphate ester hydrolysis. However, other coordination geometries and other metal complexes have been characterized as inhibitors, suggesting that the structural features are not the sole reason for the observed potency in the complexes. Here we present an analysis of the structural parameters from X-ray crystallography of five-coordinate vanadium complexes with a VO₄X core geometry (X = C, N, O, Cl, F, S) and comparing this to the vanadium-based inhibitors crystalized inside various phosphorylases and the known structures of vanadium-dependent haloperoxidases. We will examine the catalytic cycles for both classes of enzymes and comment on implications in the mechanism of each. Intentional emphasis will be placed on the mathematics associated with aspects of the data collection and analysis.

