Chemistry Seminar

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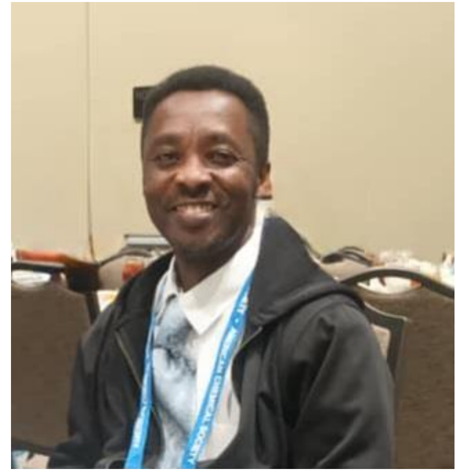

Monday, 28 October 2024
4:00 pm in 303 Schrenk Hall

Design and Synthesis of Organocatalysts for Effective Decontamination of Organophosphate-Based Pesticides and Nerve Agents

Abstract: Exposure to organophosphate-based nerve agents and pesticides poses significant health and security threats to civilians, soldiers, and first responders. In spite of the extensive efforts in developing chemical detoxification agents of the nerve agents and pesticides that could be used in the topical administration on exposure to the exposed skin-surfaces and intravenous injections, there remains unmet need to develop effective decontaminating agents that are non-hazardous to human health. The current state-of-the-art decontaminating agent, Dekon-139 (2,3-butanedione oxime, potassium salt), shows adverse effects when applied on the skin surfaces making it of great interest to develop safer and effective decontaminating agents for neutralizing nerve agent and pesticide exposed skin surface areas.

Thus, we propose to use the pharmaceutically relevant aminoguanidine-derived aldimines that are relatively non-toxic and substantially more effective in decontamination of the nerve agents and pesticides compared to the state-of-the-art decontaminating agents and they are substantially faster than Dekon-139. Our aminoguanidine based catalysts, including 2,3-butanedione aminoguanidine-imine and pyridine-4-carboxaldehyde aminoguanidine-imine, achieve near-instantaneous hydrolysis of methyl paraoxon, a nerve agent simulant, at pH ≤ 10 and the rate of hydrolysis of methyl paraoxon under these conditions is relatively faster than that of Dekon-139.

Through combined experimental multi-nuclear high-field NMR, UV-vis spectroscopy, and DFT calculations, we elucidate the pH-dependent mechanisms underlying the hydrolytic degradation of the nerve agent simulant - methyl paraoxon. Our approach and the proposed mechanism of degradation opens new avenues for the design and synthesis of effective decontamination agents that have the potential to significantly improve the safety and security of both military and civilian populations.