Nickel Complexes for Reducing Nitric Oxide and Implications for Agricultural Denitrification

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Impact on California Agriculture: Agricultural fertilizer use is a highly inefficient practice, with up to 55% of nitrogen applied as fertilizer lost into the environment as reactive nitrogen species. Reactive nitrogen species include NO_3^{1-}, N_2O, NH_3, and NO_x (x = any number of O atoms), and are a significant contributor to climate change, ozone depletion, air pollution, and water pollution. Approximately 80% of these are produced through agricultural activities, creating significant costs and negative environmental impacts resulting from agriculture.

Rationale/Introduction: Ideally, NO_x species could be reintroduced into fertilizers for a fully sustainable and atom economical cycle. The challenge is that the chemistry of these small molecules is very complex, and in particular, NO and N_2O are difficult to chemically "activate" or react to make other molecules. There is significant interest in developing new catalysts with Earth-abundant transition metals to utilize NO-containing small molecules to counteract agricultural pollution and take advantage of underutilized nitrogen sources as potential for new fertilizers.

Experimental Approach: Bidentate N-heterocyclic carbene ligands were synthesized with varying wingtips and bite angles, and complexed with Ni(0). The products were characterized by single crystal X-ray diffraction and reacted with NOx sources. The nickel NOx complexes were chemically reduced to form reduced complexes, which were characterized by infrared spectroscopy.

Major Conclusion: Bidentate N-heterocyclic carbene nickel complexes with varying ligand motifs were synthesized and reacted with NOx sources. The new nickel nitrosyl complexes were characterized by infrared spectroscopy, with a shift in stretching frequency observed upon reduction. This demonstrates that nickel complexes could be useful for reducing NOx.