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Project Title: Characterization of Copper Hyponitrite Complexes using X-ray Absorption Spectroscopy

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Abstract: Nitrous oxide (N2O) is the main contributor to the ozone layer depletion, has almost 300 times the warming potential of carbon dioxide, and lingers in the atmosphere for an average of 114 years. Biological systems can both produce N2O via NO reductive coupling and reduce N2O through reactions at copper and iron centers, but not at sufficient rates to mitigate pollution. The mechanisms are not fully understood, and a more complete understanding would benefit pollution remediation efforts. Hyponitrite (O2N22-) intermediates are proposed, but there are few isolated examples. In the current work, discrete ?-diketiminate (iPrNNF6) copper complexes formed in solution from NO coupling were analyzed by X-ray absorption spectroscopy (XAS) to determine the metal oxidation state, coordination environment, and assess hyponitrite formation. The X-ray absorption near edge structure (XANES) analysis determined the oxidation state of the complexes [(iPrNNF6)CuO2N2][CoCp2] and (iPrNNF6)CuO2N2 to be +1, while (iPrNNF6)CuO2N2Ph has an oxidation state of +2. The [(iPrNNF6)CuO2N2][CoCp2] complex had a lower rising edge feature making the oxidation state assignment more nuanced. The extended X-ray absorption fine structure (EXAFS) allowed for the copper coordination environment to be determined, using (iPrNNF6)CuO2N2Ph as a comparison for which the 3-D atomic structure is reported. The EXAFS for [(iPrNNF6)CuO2N2][CoCp2] suggest dimer formation. The EXAFS for (iPrNNF6)CuO2N2 are consistent with O2N2 bound to copper, and suggest that the hyponitrite complex was synthesized and isolated. This has implications for understanding reactivity and reduction of N2O and NO and is one of the first examples of an isolated copper hyponitrite complex. Future work includes understanding the mechanism by studying other intermediates formed in NO coupling reactions and has implications for understanding pollutant reduction. This work was