INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study	:	**Ph.D.**
Thesis Title: .		**Metal nitrosyl and dinitrosyl complexes as small molecule models for NOD and FNOR**
Name of Thesis Supervisor(s)	:	**Prof. Biplab Mondal**
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The PhD dissertation entitled, "**Metal nitrosyl and dinitrosyl complexes as small molecule models for NOD and FNOR"** contains five chapters on the topic of mainly the non-heme iron nitrosyls and dinitrosyls and a chromium nitrosyl. The reactivity of these metal nitrosyls with dioxygen (O_2) and other reactive oxygen species such as H_2O_2 have been described in this thesis. Chapter 1 provides a review of recent literature on Fe, Co, Cu, Mn, and Cr nitrosyls, focusing on their reactivity with dioxygen and other reactive oxygen species. The reactivity of the metal nitrosyls with O_2 and H_2O_2 was explored with an aim to understand the mechanism of the nitric oxide dioxygenase (NOD) enzyme, as discussed in chapters 2 to 4. For instance, in chapter 2, the formation of Fe(III)-peroxynitrite intermediate was observed, which decomposes to $[Fe^{IV}=O]$ and NO_2, leading to the ligand modification. In chapter 3, study of the dioxygen reactivity of two iron-nitrosyls having same ligand framework but different spin-states suggest that the reaction proceeds through different pathways based on M-NO bond strength. In chapter 4, a $[Cr^{V}=O]$ intermediate was observed in the reaction of chromium nitrosyl with H_2O_2. These findings definitely enhance our current understanding of NOD chemistry and make a substantial contribution to the field of metalloenzyme chemistry. In chapter 5, a diiron dinitrosyl complex was synthesized as a model complex of flavodiiron nitric oxide reductase (FNOR). This diiron dinitrosyl complex promotes N–N bond formation leading to transient hyponitrite species through a $\{Fe(NO)_2\}^9$ intermediate to result in the spontaneous release of N_2O.