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Reaction of μ -oxo-bis [trichloroferrate(III)] ion with L-ascorbic acid in relation to reaction of oxygen with iron(II)-ascorbate

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ELSEVIER

- L036 SPECTROSCOPIC CHARACTERIZATION OF A BINUCLEAR IRON PEROXIDE COMPLEX.** Bridget Brennan, Qiu hao Chen, and Lawrence Que, Jr., Department of Chemistry, University of Minnesota, Minneapolis, MN 55455, USA.
Model compounds can provide insight into the structural features of binuclear iron-oxo sites which are found in a number of proteins. The binuclear iron complex, $\text{Fe}_2(\text{HPTB})(\text{NO}_3)_5$ (HPTB = N,N,N',N'-tetrakis(2-benzimidazolyl-methyl)-2-hydroxy-1,3-diaminopropane) (1) forms a metastable complex (2) with hydrogen peroxide. This complex, 2, is characterized by a new charge transfer band near 600 nm ($\epsilon = 1500 \text{ cm}^{-1} \text{ M}^{-1}$). Laser excitation into this band reveals resonance enhanced Raman vibrations near 880 cm^{-1} and 480 cm^{-1} , tentatively assigned to O-O and Fe-O stretches, respectively. The ^1H NMR and Mössbauer spectra of 1 and 2 will also be discussed.

- ** L037 REACTION OF μ -OXO-BIS [TRICHLOROFERRATE(III)] ION WITH L-ASCORBIC ACID IN RELATION TO REACTION OF OXYGEN WITH IRON(II)-ASCORBATE.** M. Y. HAMED, CHEM. DEPT., BIRZEIT UNIV., WEST BANK-via ISRAEL.

pH studies, electronic absorbance and Mössbauer spectroscopic studies on the reaction of $[\text{Fe}_2\text{OCl}_6]^-$ ion with ascorbate are reported in both aqueous and methanolic solutions. A purple complex is detected under inert atmosphere at pH5 which has a stoichiometry of two monoprotonated ascorbates per $[\text{Fe}_2\text{OCl}_6]^-$ ion. Kinetic difference spectra are constructed for the complex by rapidly mixing the metal ion and ascorbate in a stopped flow apparatus (a broad band with $\lambda_{\text{max}} = 500 \text{ nm}$, $\epsilon = 300 \text{ M}^{-1} \text{ cm}^{-1}$). Mössbauer parameters indicate the presence of iron in the +3 oxidation state. Reaction of the complex with Oxygen and its decay in the absence of Oxygen was monitored spectrophotometrically and a similar behavior was observed in relation to [1]. A mechanism for the reaction is proposed.

[1] M. Y. Hamed *et al.* *Inorganic chim. acts* 152, 227 (1988).

- L038 UNIQUE REACTIVITY OF PEROXIDE ION TRAPPED BY BINUCLEAR METAL COMPLEXES.** Y. Nishida, Yamagata University, Yamagata 990, JAPAN

The binuclear iron(III) complex with N,N,N',N'-tetrakis(2-benzimidazolylmethyl)-2-hydroxy-1,3-diaminopropane reacts with hydrogen peroxide to yield a blue (1:1) adduct. This blue species can catalyze the transformation of phenol to catechol, and exhibits high reactivity toward 1,3-diphenylisobenzofuran (scavenger of singlet oxygen) [1]. The activation of the peroxide ion in this molecule was discussed in relation to the monooxygenase function and the ability of degradation of DNA of this blue species, and also the analogous metal complexes containing peroxide ion.

[1] Y. Nishida, *Z. Naturforsch.*, 42B, 52 (1987).