Observation of CO release reaction in a crystalline Lysozyme-$Mn(CO)_3$ scaffold

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Direct observation of a chemical reaction is important to explore the mechanism of the reaction. Current studies on this includes spectroscopy, structure determination and isolation of intermediates. However, it becomes complicated if the intermediate is transient or short-lived. Although ultrafast spectroscopic studies provide information about such species, structural assignments in those studies are mostly based on the theoretical spectrum of the model structures. Therefore, a suitable methodology is needed to see the reaction dynamics in real time and space. Recently, serial femtosecond crystallography has attracted significant attention for its ability to capture structural changes of proteins/enzymes up to femtosecond time intervals.[1-3] Such time-resolved serial crystallography has potential to study a chemical reaction with capturing short-lived intermediates or transient structural changes. However, the methodology has been applied mostly to explore the mechanism of natural protein/enzymes reactions and not extended to any synthetic chemistry reactions due to less diffraction spots, low solvent content, rigidity etc. of the small-molecules crystals. In order to overcome such issues associated with small-molecule reactions, we have fixed the reaction into a porous protein crystal to study their reactions by time-resolved serial crystallography. This presentation will describe the structural changes during the progress of a CO release reaction from an organometallic Mn-carbonyl complex fixed into the lysozyme protein crystal (Figure 1). Such methodology is expected to be applied to study the mechanism of less-explored reactions involved in synthetic chemistry as well as artificial metalloenzyme reactions.

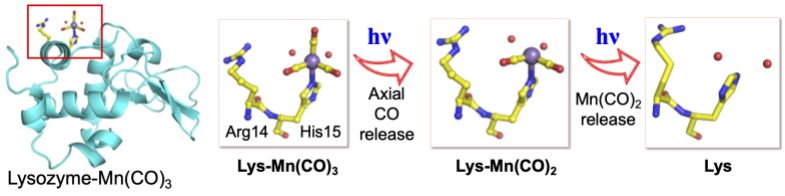

Figure 1: Structure of Lys-$Mn(CO)_3$ and CO release reaction pathway.

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