EXTENDED ABSTRACT

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Novel applications of bioinorganic chemistry

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Abstract:

Catalysis has been an extremely important area within Chemistry and Bio catalysis is a more recent branch of Catalysis in which the catalyst and the process originate from the biological sciences and deals with enzymes. The research programs in Inorganic chemistry, Biochemistry and Catalysis have only recently met one another, and the results are very exciting.

In many Biocatalytical systems, the metal plays an important role at the active site and usually the reaction intermediates reside on the metal ion in the enzyme. Bioinorganic catalysis deals with the processes performed with the aid of metalloenzymes, modified enzymes and synthetic metal containing molecules resembling the active sites of metalloproteins. Biomimetic oxidation catalysis aims at achieving the efficiencies and selectivity of Enzymes, such as monooxygenases and peroxidases, with lower molecular weight compoundsThe design of biomimetic oxidation catalyst is based on the active-site structure and function of oxidation enzymes. For the sake of atom economy and sustainability ,terminal oxidants such as molecular oxygen or dihydrogen peroxide are employed preferentially. It is an intrinsic feature of biomimetic oxidation catalysts that they aim at initiating soluble enzymes, which means that they are generally homogeneous in nature. The majority of the homogeneous and biomimetic oxidation catalysts being investigated to date fall into two classes: 1. Metal-ligand (peptidic or non peptidic combinations, 2) Metal – free organic catalysts Biomimetic Oxidation Catalysts based on metal complexes find application in

A] Asymmetric epoxidation of Olefins

B] Asymmetric Sulfoxidation of Thioethers

C] Baeyer- Veliger Oxidation of ketones

D[Air oxidation of Alcohols

Interesting oxidation reactions in fine chemistry are the epoxidation reactions, because the resulting materials can be used for the synthesis of a wide variety of products. In these processes, the use of iron and manganese catalysts with dioxygen and dihydrogen peroxide as primary oxidant is required because of environmental reasons.

Metal ions occurring in, or applied on, living systems, have either a crucial/beneficial role, a toxic/medicinal role, or an inert/diagnostic role. To understand these roles, and make use of it in detoxification, catalysis, design of new drugs, or design of diagnostic agents, it is required to have a good knowledge of inorganic and coordination chemistry. One hundred years after the Nobel Prize in Chemistry was given to Alfred Werner, for his breakthrough in realizing that the coordination number can be larger than the oxidation state of a metal, bioinorganic chemistry also obeys to this principle, and several papers in this special issue have a strong link with fundamental coordination chemistry. We have tried to bring together, in a single issue, a collection of articles written by scientists worldwide covering a variety of subtopics, dealing with metal ions in living systems, as well as biomimetic studies inspired by metal ions in biology. The interplay between inorganic chemistry on one hand, and medicine and biology on the other hand is visible in several papers. Although we realize that nowadays many readers refrain from browsing hard copies of journal issues, and rather use the internet and search the journals by key words, we encourage the readers to spend some time on (electronic) browsing of this special issue. It is for sure worth the effort to observe the broadness of this discipline, but also to observe the interrelationships between the several subdisciplines. It is fascinating to realize that the first International Conference on Bioinorganic Chemistry was held just 30 years ago (ICBIC 1, Florence, organized by the late IvanoBertini); the 16th ICBIC is scheduled for 2013, Grenoble. Meanwhile also conferences on the European level (EUROBIC, since 1992) have emerged, and a successful International Symposium on Applied Bioinorganic Chemistry, started by John Webb and Kui Wang, later chaired by the late David R. Williams, has been in operation since 1990. We have decided not to create subsections in the issue, but rather rank the manuscripts in a gradual fashion, from biological to biomimetic, and from biomimetic to metals in medicine. As a start four research reports cover a broad range of relevant topics from the probing of metal ion binding in nucleic acids by NMR, chelating agents for the treatment of metal overload, a historic review on nitrosyl metal halides to a comprehensive report on synthetic routes to nitrogenase model clusters. After three communications, i.e. on a dinuclear iron complex and on the role of histidine in Cu-metallothionein, 41 full articles follow. This long section, which constitutes the major part of the volume, starts with a few papers on proteins and artificial proteins, followed by several biomimetic studies focused on structures and is concluded by some chapters on reactivities. A paper on a diagnostics Bernt Krebs, Münster Jan Reedijk, Leiden 1296 www.zaac.wiley-vch.de © 2013 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim Z. Anorg.Allg. Chem. 2013, 12951296 Re compound is the bridge to anticancer studies on coordination compounds; the volume is concluded by a number of papers on metal-DNA and metal-RNA binding.

Role of the metallic elements .The metallic elements playa variety of roles in biochemistry. Several of the most important roles are the following: 1. Regulatory action is exercised by Na+, K+, Mg2+, and Ca2+. The flux of these ions through cell membranes and other boundary layers sends signals that turn metabolic reactions on and off. y2. The structural role of calcium in bones and teeth is well known, but many proteins owe their structural integrity to the presence of metal ions that tie together and make rigid certain portions of these large molecules, portions that would otherwise be only loosely linked. Metal ions particularly known to do this are Ca2+and Zn2+. y 3. An enormous amount of electron-transfer chemistry goes on in biological systems, and nearly all of it critically depends on metal-containing electron- transfer agents. These include cytochromes (Fe), ferredoxins (Fe), and a number of copper-containing "blue proteins," such as azurin, plastocyanin, and stellacyanin.

The Bioinorganic chemistry of Cobalt .The best-known biological function of cobalt is its intimate involvement in the coenzymes related to vitamin B12 It consists of four principal components: 1. A cobalt atom. 2. A macrocyclic ligand called the corrin ring, which bears various substituents. The essential corrin ring system is shown in bold lines. It resembles the porphine ring, but differs in various ways, notably in the absence of one methine (=CH-) bridge between a pair of pyrrole rings. 3. A complex organic portion consisting of a phosphate group, a sugar, and an organic base, the latter being coordinated to the cobalt atom. 4. A sixth ligand may be coordinated to the cobalt atom. This ligand can be varied, and when the cobalt atom is reduced to the oxidation state +1, it is evidently absent.