Round Table: Are Synchrotron Radiation Studies (including EXAFS) Breakthroughs in Structural Studies of Metalloproteins?

Convener: E. I. STIEFEL; Linden, N.J., U.S.A.

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Are Synchrotron Radiation Studies (including EXAFS) Breakthroughs in Structural Studies of Metalloproteins?

E. I. STIEFEL

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Electrons travelling around storage rings in vacuum at close to the speed of light are being exploited to an increasing extent by bioinorganic chemists. These electrons emit intense radiation ranging from the infrared through X-ray regions. The radiation is continuous in energy, pulsed, polarized, and of intensity not otherwise obtainable for comparable time periods. The availability of the synchrotron radiation has elicited an increasing variety of absorption and scattering techniques. The absorption edge, the X-ray Absorption Near Edge Structure (XANES) and the Extended X-ray Absorption Fine Structure (EXAFS) have each been exploited as have scattering techniques. This discussion brings together from four countries (and four synchrotron sources) some of the major proponents and users of synchrotron radiation.

The round table will entail short (20–25 minutes) formal presentations by each of the 5 participants in which they will seek not only to expose their own work but also to put it in the context of the full impact of synchrotron radiation studies. Short question periods will follow each talk and a final period will be left for discussion among the panelists, further questions from the audience and summing up.

To start the session, Cramer will introduce the synchrotron sources and radiation characteristics, discuss absorption applications to nitrogenase, hemoglobin and cytochrome oxidase and describe some of the future novel ways of exploiting the characteristics of the radiation. Stuhrmann will continue this line by describing the hierarchy of information one gets from absorption and scattering experiments and he will review applications of scattering to such systems as ferritin, hemoglobin and t-RNA. Teo will emphasize the detailed information obtainable from EXAFS and will discuss its application to Fe systems in nitrogenase and 3Fe–3S cluster systems. Bianconi will focus on the information attainable from XANES as compared to EXAFS and will discuss applications of XANES to hemoglobin and calmodulin structure. Finally, Garner will discuss some of the EXAFS analysis protocols and their limits and will analyze recent data from superoxide dismutase and metallothionein.

Between them our distinguished panelists should cover many of the established and emerging synchrotron techniques as well as their application to systems containing Fe, Cu, Zn, Mo, Ca, Mg, Cs, I and Tb. The panelists and convener are committed to pedagogical presentations, lacking in undefined jargon and abbreviations. We will endeavor to convey an appreciation for the powers and limits of the various techniques. If we do our job well, the answer to the question posed in the title of the Round Table should become obvious to the audience.

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Synchrotron Sources, EXAFS Applications and Future Directions

S. P. CRAMER

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Synchrotron radiation has opened up a wide range of the electromagnetic spectrum for bioinorganic applications. This presentation will begin with a brief summary of the properties of synchrotron radiation, the sources currently available, and the developments envisioned for future beam lines and storage rings based on 'wiggler' and 'undulator' devices. A short history of the development of EXAFS for biological applications will follow, using as examples hemoglobin, cytochrome oxidase, and molybdenum enzymes. Data acquisition and analysis problems will be discussed. Finally, an overview will be presented of the other X-ray techniques which have significant bioinorganic impact including rapid X-ray diffraction and polarized absorption spectroscopy on oriented samples.
