International Symposium on
Chemistry of Reductases

March 11–12, 2008

Nagoya, Japan

Chairman *Kazuyuki Tatsumi (Nagoya University)*

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Grant-in-Aid for Creative Scientific Research
"Organometallic and Cluster Chemistry in Metalloenzymes with Reducing Activities"

Kyoto University/Nagoya University/Kyushu University
Joint Project of Chemical Synthesis Core Research

Nagoya University Global COE Program
"Elucidation and Design of Materials and Molecular Functions"

Under the Auspices of

Research Center for Materials Science, Nagoya University
The Chemical Society of Japan

Scientific Program

March 11 (Tuesday)

9:30 **Opening Remarks**: Kazuyuki Tatsumi (Nagoya University)

Chair: Yoshihito Watanabe (Nagoya University)

9:45 **Lance C. Seefeldt (**Utah State University**)**
Insights Into the Nitrogenase Reaction Mechanism

10:30 **Dimitri Coucouvanis** (The University of Michigan)
A Quest for a Synthetic Analog for the Fe/Mo/S Center in Nitrogenase. Collateral Progress in the Systematic Synthesis of Heterometallic Clusters.

11:15 Lunch

Chair: Kazuyuki Tatsumi (Nagoya University)

13:00 **Award Ceremony of Honorary Degree from Nagoya University to Professor Robert Huber**

Chair: Bernt Krebs (The University of Münster)

13:45 *– Keynote Lecture –*
Robert Huber (Max-Planck-Institut für Biochemie)
Life on Carbon Monoxide.

14:45 Coffee Break

Chair: Hiroyuki Kawaguchi (Institute for Molecular Science)

15:05 **Yasushi Mizobe** (The University of Tokyo)
Cubane-Type Metal Sulfido Clusters with N_2 Ligand as the New Model of the Active Site of Nitrogenase.

15:50 **Hisaaki Mihara** (Kyoto University)
Sulfur Trafficking in Biosynthesis of Iron-Sulfur Cluster.

16:35 **Poster Session**

March 12 (Wednesday)

Chair: Hideki Masuda (Nagoya Institute of Technology)

9:30 **Yuichi Fujita** (Nagoya University)
Characterization of Nitrogenase-like Enzymes in Chlorophyll and Bacteriochlorophyll Biosynthesis Pathways.

10:15 **Yoshiki Higuchi** (University of Hyogo)
Recent Progress of the Structural Study of [NiFe] Hydrogenase.

11:00 **Juan Carlos Fontecilla-Camps**
(Institut de Biologie Structurale Jean – Pierre Ebel)
Structural Bases of Catalysis by NiFeS-containing Enzymes

11:45 Lunch

Chair: Kazunari Yoshizawa (Kyushu University)

13:00 **Martin Schröder** (University of Nottingham)
Modelling Hydrogenase Enzymes: Structure, Redox and Function.

13:45 **Kazuyuki Tatsumi (**Nagoya University**)**
S-Donor/O-Donor-Bridged Heterodinuclear Complexes
Modelling the Active Site Structure and Function of [NiFe] Hydrogenase.

14:30 **Michael B. Hall (**Texas A&M University**)**
Modelling Metalloenzymes: Nickel-iron and Di-iron Hydrogenases.

15:15 Coffee Break

Chair: Kazuyuki Tatsumi (Nagoya University)

15:40 **Panel Discussion**

17:10 **Closing Remarks**

Poster Session

March 11 (Tuesday) 16:35-

P-01 Synthetic Analogues of the [4Fe-4S]$^{3+}$ Cluster in HiPIP and the Histidine-Bound [4Fe-4S]$_{dist}$ Cluster in Hydrogenases. Norihiro Yamada, Tomoyuki Tajima, Motosuke Imada, Yasihiro Ohki, Kazuyuki Tatsumi (Nagoya University)

P-02 Construction of a Novel Biocatalytic System Using the Substrate Misrecognition of Cytochrome P450$_{BS\beta}$. Takashi Fujisiro, Osami Shoji, Hiroshi Nakajima, Isamu Matsunaga, Shingo Nagano, Yoshitsugu Shiro, Yoshihito Watanabe (Nagoya University, Kyoto University, RIKEN SPring-8 Ctr)

P-03 Thiolate-Bridged Dinuclear Nickel-Iron(Carbonyl/Cyano) Complexes Modeling the [NiFe] Hydrogenase Active Site. Soichiro Tanino, Zilong Li, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

P-04 Synthesis of Dinuclear Fe-Ni Complexes Bridged by Thioether-thiolate Hybrid Ligands as Structural Models for the [NiFe] Hydrogenase Active Site. Satoko Shimokata, Frank M. A. Geilen, Soichiro Tanino, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

P-05 Polyene Assemblies by Using Protein Tubules as a Template. Cheng-yuan Huang, Tomomi Koshiyama, Norihiko Yokoi, Yuki Miura, Takafumi Ueno, Syuji Kanamaru, Fumio Arisaka, Yoshihito Watanabe (Nagoya University, PRESTO, Tokyo Institute of Technology).

P-06 Arene-Bridged Dizirconium Complexes Supported by Bulky Aryloxide Ligands. Takahito Watanabe, Tsukasa Matsuo, Hiroyuki Kawaguchi (Institute for Molecular Science)

P-07 Synthesis and Reactions of the Dinuclear Iron(tris-carbonyl)-Nickel Complexes Bridged by *tert*-Butanethiolates: Models for the [NiFe] Hydrogenase Active Site. Masaru Ando, Soichiro Tanino, Kazunari Yasumura, Katsuaki Kuge, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

P-08 Structural Transformation of O_2-Adducts in Distorted Dicopper Complex Systems. Kotaro Yoshii, Tomohide Nishikawa, Yuji Kajita, Tomohiro Ozawa, Yasuhiro Funahashi, Hideki Masuda (Nagoya Institute of Technology)

P-09 Artificial Beta-helical Tube Protein as a Template of Molecular Modifications. Norihiko Yokoi, Yuki Miura, Chen-Yuang Huang, Tomomi Koshiyama, Takafumi Ueno, Shuji Kanamaru, Fumio Arisaka, Katsuhide Yutani, and Yoshihito Watanabe (Nagoya University, PRESTO, Tokyo Institute of Technology, RIKEN)

P-10 **Synthesis and Structures of Anionic and Neutral [$MoFe_3S_4$] Cubane Clusters with Tripodal O,N,N-Heteroscorpionate Ligands.** Shunsuke Senda, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

P-11 **Synthesis and Site Selective Substitution of [4Fe-4S] Clusters Bearing the Tridentate Ligand Composed of Fluorobenzenethiolate.** Takuya Wakimoto, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)

P-12 **Metal Bipyridine Complexes Aligned on a Beta-helical Scaffold Derived from Bacteriophage T4.** Yuki Miura, Norihiko Yokoi, Cheng-yuan Huang, Tomomi Koshiyama, Kanamaru Shuji, Fumio Arisaka, Takafumi Ueno, Yoshihito Watanabe (Nagoya University, Tokyo Institute of Technology, PRESTO)

P-13 **Synthesis of [8Fe-7S] Clusters Analogous to the FeMo-cofactor in Nitrogenases.** Shun Ohta, Yohei Ikagawa, Rie Suizu, Won-seok Han, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

P-14 **Synthesis and Structure of a Diethyldihydroborate Zirconium Complex with Aryloxide Ligands.** Yutaka Ishida, Fumio Akagi, and Hiroyuki Kawaguchi (Institute for Molecular Science)

P-15 **Molecular Design of Protein Assemblies Providing a Bio-nanocup as a Catalytic Reaction Space.** Tomomi Koshiyama, Norihiko Yokoi, Takafumi Ueno, Shuji Kanamaru, Shingo Nagano, Yoshitsugu Shiro, Fumio Arisaka, Yoshihito Watanabe (Nagoya University, PRESTO, Tokyo Institute of Technology, RIKEN SPring-8 Ctr.)

P-16 **Synthesis, Properties, and Reactivity of [8Fe-7S] Models for Nitrogenase P-cluster.** Ayuro Murata, Motosuke Imada, Yusuke Sunada, Masaru Honda, Motomi Katada, Yasuhiro Ohki, and Kazuyuki Tatsumi (Nagoya University, Tokyo Metropolitan University)

P-17 **Coordination Modes of Ni(II/III) Complexes Mimicking an Active Center of NiSOD.** Daisuke Nakane, Tatsuya Fujii, Yasuhiro Funahashi, Tomohiro Ozawa, Hideki Masuda (Nagoya Institute of Technology)

P-18 **Crystal Structure of a Hydrogenase Maturation Protein HypE.** Yasuhito Shomura, Yoshiki Higuchi (University of Hyogo)

P-19 **Artificial Metalloproteins Exploiting Apo-Myoglobin Cavity.** Satoshi Abe, Takafumi Ueno, Seiji Okazaki, Takashi Yamane, and Yoshihito Watanabe (Nagoya University)

P-20 **Synthesis and Reactions of Tetraazamacrocyclic Nickel(I) Complexes Modeling Methyl Coenzyme M Reductase.** Jun-ichi Nishigaki, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)

P-21 **Theoretical Study on Nitrogen Fixation Catalyzed by a Cubane-Type $RuIr_3S_4$ Cluster and Unique Ru−N−N Geometries in Intermediates.** Hiromasa Tanaka, Hiroyuki Mori, Hidetake Seino, Masanobu Hidai, Yasushi Mizobe, Kazunari Yoshizawa (Kyushu University, The University of Tokyo, Tokyo University of Science)

P-22 **Manganese Cluster as OEC Model of Photosystem II: Synthesis, Structure, and Characterization of the Manganese Core.** Yoshiki Naganuma, Beibei Yang, Kensuke Fukui, Tomohiro Ozawa, Yasuhiro Funahashi, Hideki Masuda (Nagoya Institute of Technology)

P-23 **Crystallographic Study of H_2O_2 Reductase, Rubperoxin.** Koji Nishikawa, Yasuhito Shomura, Shinji Kawasaki, Yu Sakai, Youichi Niimura, Hirofumi Komori, Naoki Shibata, Yoshiki Higuchi (University of Hyogo, Tokyo University of Agriculture)

P-24 **Dinitrogen Cleavage by a Diniobium(IV) Tetrahydride Complex: Formation of a Nitride and Its Reaction with Methyl Iodide.** Fumio Akagi, Tsukasa Matsuo, Hiroyuki Kawaguchi (Institute for Molecular Science)

P-25 **A Functional Hydrogenase Model: Dihydrogen Activation by Hetero-dinuclear Ru/Ge Complexes.** Tsuyoshi Matsumoto, Yukiko Nakaya, Kazuyuki Tatsumi (Nagoya University)

P-26 **Theoretical Study of Dinitrogen Activation by a Diniobium Complex.** Yoshihito Shiota, Kenichiro Takahashi, Hiromasa Tanaka, Tsukasa Matsuo, Hiroyuki Kawaguchi, Kazunari Yoshizawa (Kyushu University, Institute for Molecular Science)

P-27 **Synthesis and Reactions of Dinuclear Fe-Ni Complexes Having Bis(trimethylsilyl)amide on Fe.** Dong Liu, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)

P-28 **A Role of Cys Residues Integrated in N-Terminal Region of VnfA, a Transcriptional Regulator of Nitrogenase.** Nobuyuki Takatani, Mitsuko Itoh, Hiroshi Nakajima, Shigetoshi Aono, Yoshihito Watanabe (Nagoya University, Institute for Molecular Science)

P-29 **X-Ray Crystal Structure Analysis of the Engineered Multicopper Oxidase CueO.** Hirofumi Komori, Kunishige Kataoka, Yusaku Ueki, Yusuke Konno, Yuji Kamitaka, Shinji Kurose, Seiya Tsujimura, Kenji Kano, Daisuke Seo, Takeshi Sakurai, Yoshiki Higuchi (University of Hyogo, Kanazawa University, Kyoto University)

P-30 **Comparative Analysis of Two Nitrogenase-like Enzymes, Protochlorophyllide Reductase and Chlorophyllide *a* Reductase.** Jiro Nomata, Masaharu Kitashima, Takuro Ogawa, Kazuhito Inoue, Yuichi Fujita (Nagoya University, Kanagawa University, The University of Tokyo)

P-31 **Synthesis of a New Trinuclear Pd(II) with a Cage-type Ligand, Including a Small Guest Molecule.** Beibei Yang, Kensuke Fukui, Tomohiro Ozawa, Yasuhiro Funahashi, Hideki Masuda (Nagoya Institute of Technology)

P-32 **Dicarboxyamido-dithiolato Bridged Dinuclear Nickel Complexes: Modeling the Active Site of Acetyl Coenzyme A Synthase.** Yumei Song, Mikinao Ito, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)

P-33 **Synthesis and Characterization of N3-type Metal(II) Complexes with a Calix[6]arene.** Takumi Higa, Tatsuya Fujii, Yuji Kajita, Yasuhiro Funahashi, Tomohiro Ozawa, Hideki Masuda (Nagoya Institute of Technology)

P-34 **Snapshot Analyses of Pd Ion Uptake into the apo-Fr Cavity.** Mizue Abe, Satoshi Abe, Masako Suzuki, Takafumi Ueno, Kunio Hirata, Nobutaka Shimizu, Masaki Takata, Yoshihito Watanabe (Nagoya University, PRESTO, RIKEN JASRI/SPring-8)

P-35 **Dinuclear Ni(II)-Ni(I) Complex Modeling the Active Site of Acetyl-CoA Synthases.** Mikinao Ito, Mai Kotera, Yumei Song, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)

P-36 **Controlling Diastereoselectivity in the Organocatalyzed Formation of γ-Butyrolactones.** Keiichi Hirano, Frank Glorius (The University of Münster)

P-37 **Titanium and Zirconium Complexes pf Preorganized Tripodal Triphenoxide Ligands.** Fumio Akagi, Tsukasa Matsuo, Hiroyuki Kawaguchi (Institute for Molecular Science)

P-38 **Synthesis and Reactions of a Coordinatively Unsaturated Cp*Fe Complex Having a 2,6-Dimesitylbenzenethiolate.** Tomomi Yasuda, Yuko Takikawa, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)