

International Symposium on *Chemistry of Reductases IV*

January 20–21, 2011

Nagoya, Japan

Chairman Kazuyuki Tatsumi (Nagoya University)

Organizing Committee

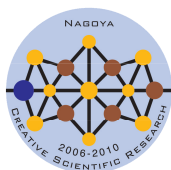
Yoshiki Higuchi (Univ of Hyogo)

Hiroyuki Kawaguchi (Tokyo Tech)

Kazuynari Yoshizawa (Kyushu Univ)

Tsuyoshi Matsumoto (Nagoya Univ)

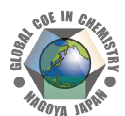
Yasuhiro Ohki (Nagoya Univ)



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



*MEXT Project of Integrated Research on
Chemical Synthesis*



*Nagoya University Global COE Program
“Elucidation and Design of Materials and Molecular Functions”*



Under the Auspices of

Research Center for Materials Science, Nagoya University

Scientific Program

January 20 (Thursday)

9:50 **Opening Remarks:** Kazuyuki Tatsumi (Nagoya University)

Chair: Yoshiki Higuchi (University of Hyogo)

10:00 **Douglas C. Rees** (California Institute of Technology)
Structural Biology of Nitrogenase.

10:45 **Kazuyuki Tatsumi** (Nagoya University)
Chemical and Biological Synthesis of Iron-Sulfide Clusters by Tinker-Toy
Construction or by Self-Assembly.

11:30 Lunch

Chair: Yuichi Fujita (Nagoya University)

13:00 **Markus W. Ribbe** (University of California, Irvine)
Unique Features of the Nitrogenase VFe Protein from *Azotobacter*
vinelandii.

13:45 **Kazunari Yoshizawa** (Kyushu University)
Theoretical Studies on Dinitrogen Fixation by Cubane-Type Clusters.

14:30 Coffee Break

Chair: Hiroshi Nakajima (Nagoya University)

14:50 **Hideki Sugimoto** (Osaka University)
Coordination Chemistry of Bis(dithiolene)metal Complexes Related to
the Reaction Centers of Molybdenum and Tungsten Enzymes.

15:35 **Hiroyuki Kawaguchi** (Tokyo Institute of Technology)
Niobium and Tantalum Hydride Complexes Bearing Triphenoxide
Ligands.

16:20 **Poster Session**

January 21 (Friday)

Chair: Kazunari Yoshizawa (Kyushu University)

- 9:40 **John W. Peters** (Montana State University)
Insights into Complex Iron-Sulfur Cluster Assembly and
Hydrogenase and Nitrogenase Maturation.
- 10:25 **Seiji Ogo** (Kyushu University)
Electron from Hydrogen – A Remarkable Insight into Hydrogenase.
- 11:10 Short Break
- 11:20 **Yasuhito Shomura** (University of Hyogo)
Structural Basis for the Reaction Mechanism of Dissimilatory Sulfite
Reductase.
- 12:05 Lunch and Poster

Chair: Bernt Krebs (The University of Münster)

- 13:30 **Yoshihito Watanabe** (Nagoya University)
Construction of Organometalloenzyme
- 14:15 **Shinnichiro Suzuki** (Osaka University)
Structure-Function Relationships of Copper Reductases in Denitrification.
- 15:00 Coffee Break
- 15:20 **Rudolf K. Thauer** (Max Planck Institute for Terrestrial Microbiology
Marburg)
Flavin-Based Electron Bifurcation: A Novel Mechanism of Energy
Coupling.
- 16:05 Short Break

Chair: Kazuyuki Tatsumi (Nagoya University)

- 16:15 **Panel Discussion**
- 17:45 **Closing Remarks**

Poster Session

January 20 (Thursday) 16:20, 21 (Friday) lunch time

- P-01 The Role of the Fe-S Cluster Involved in Nitrogenase Transcriptional Activator, VnfA.** Hiroshi Nakajima, Kyohei Yoshimitsu, Yoshihito Watanabe (Nagoya University)
- P-02 The Host Legume *FEN1* Gene Required for Symbiotic Nitrogen Fixation.** Tsuneo Hakoyama^{1,2}, Kaori Niimi², Hirokazu Watanabe², Ryohei Tabata², Junichi Matsubara², Shusei Sato³, Yasukazu Nakamura³, Satoshi Tabata³, Li Jichun⁴, Tsuyoshi Matsumoto⁴, Kazuyuki Tatsumi⁴, Mika Nomura⁵, Shigeyuki Tajima⁵, Masumi Ishizaka⁶, Koji Yano¹, Haruko Imaizumi-Anraku¹, Masayoshi Kawaguchi⁷, Hiroshi Kouchi¹, Norio Suganuma (1National Institute of Agrobiological Sciences, 2Aichi University of Education, 3Kazusa DNA Research Institute, 4Nagoya University, 5Kagawa University, 6National Institute of Agro-Environmental Sciences, 7National Institute of Basic Biology)
- P-03 Characterization of a Nitrogenase-like Protochlorophyllide Reductase Encoded by Chloroplast DNA from *Physcomitrella patens*.** Haruki Yamamoto¹, Shohei Kurumiya¹, Rie Ohashi¹, Yuichi Fujita^{1,2} (1Nagoya University, 2PRESTO, JST)
- P-04 Thiolate, Carboxylate, and Imidazole Coordinated [4Fe-4S] Clusters Carrying Tridentate Thiolate Ligand TempS₃³⁻.** Tamaki Terada, Tomohiko Nakamura, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)
- P-05 Ligand Exchange Reactions of Highly Oxidized [Fe₄S₄] Clusters and Formation of an [Fe-Fe₄S₄] Cluster.** Kazuki Tanifuji, Norihiro Yamada, Yomoyuki Tajima, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-06 CH₃-S Bond Cleavage of Ni(I) Cyclam Complexes Having Thioether Pendants: A Model Reaction of Methyl Coenzyme M Reductase.** Jun-ichi Nishigaki, Tsuyoshi Matsumoto, Kazuyuki Tatsumi
- P-07 Dinuclear Ni(II)-Ni(II/I/0) Complexes Coordinated by Diaminedithiolate (dadt^{Et})²⁻ and Diamidodithiolate (mbpa)⁴⁻: Active Site Models of Acetyl CoA Synthase.** Ayaka Oana, Tsuyoshi Matsumoto, Sachie Arae, Mikinao Ito, Kazuyuki Tatsumi (Nagoya University)
- P-08 A Functional [NiFe] Hydrogenase Model: Dihydrogen Activation by Hetero-dinuclear Ru/Ge Complexes Bridged by S/OH and S/SH.** Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)
- P-09 Modeling the Active Site of the [NiFe] Hydrogenase in the Reduced Form.** Zilong Li, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

- P-10 Thiolate-Bridged Dinuclear (CO)₃Fe-Ni Complexes Relevant to the Active Site of [NiFe] Hydrogenase.** Yasuhiro Ohki, Kazunari Yasumura, Katsuaki Kuge, Soichiro Tanino, Masaru Ando, Zilong Li, Kazuyuki Tatsumi (Nagoya University)
- P-11 Synthesis and Properties of [8Fe-7S] Clusters Modeling the Nitrogenase P-Cluster.** Yasuhiro Ohki,¹ Motosuke Imada,¹ Ayuro Murata,¹ Yusuke Sunada,¹ Shun Ohta,¹ Masaru Honda,¹ Motomi Katada,² Kazuyuki Tatsumi¹ (¹Nagoya University, ²Tokyo Metropolitan University)
- P-12 Self-Assembly of [Fe₆S₃], [Fe₈S₇], and [Fe₈S₈] Clusters by the Reactions of Fe{N(SiMe₃)₂}₂, Elemental Sulfur, and Various Bulky Thiols.** Yiming Xie, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-13 Synthesis of an [8Fe-7S] Cluster from Fe₂Me₄.** Takayoshi Hashimoto, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-14 Synthesis and Reactions of a [6Fe-5S]-3{Fe} Cluster Having a Trigonal-Prismatic Core.** Miku Miki, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University).
- P-15 An [8Fe-6S-O] Cluster Structurally Relevant to the FeMo-cofactor of Nitrogenase.** Shun Ohta, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-16 Dinitrogen Fixation by Mononuclear Molybdenum Diphosphinoamine Complexes and Their Silylations.** Takahiko Ogawa, Yuji Kajita, Hideki Masuda (Nagoya Institute of Technology)
- P-17 Synthesis of a Siloxy-Bridged Dicubane Cluster from [MoFe₃S₄] Clusters Carrying an O,N,N-Tridentate Ligand on Molybdenum.** Shunsuke Senda, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-18 Syntheses and Structures of Novel Molybdenum Complexes with SNS Thioamide Pincer Type Ligand.** Tatsuya Suzuki, Jun Matsumoto, Yuji Kajita, Hideki Masuda (Nagoya Institute of Technology)
- P-19 Theoretical Study on Mo-Catalyzed Conversion of Dinitrogen into Silylamine.** Hiromasa Tanaka,¹ Akira Sasada,¹ Tomohisa Kouno,¹ Masahiro Yuki,² Yoshihiro Miyake,² Yoshiaki Nishibayashi,² Kazunari Yoshizawa¹ (¹Kyushu University, ²The University of Tokyo)
- P-20 Synthesis of V(III) Thiolate Complexes Bearing a Tridentate O-Donor Ligand or an O- and P-Donor Hybrid Ligand and Their Reactions with S₈ and Iron-Thiolate Complexes.** Nobuhiro Taniyama, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)

- P-21 Synthesis of [Mo-5Fe-9S] and [2Mo-4Fe-9S] Clusters from [Cp*MoS₃]⁻, FeCl₂, and NEt₄SH.** Kosuke Miyazaki, Takayuki Nagasawa, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-22 Reactivities of Mononuclear Cobalt(II) Complexes with Tripodal Ligands Bearing Noncovalent Interaction Sites.** Jun Matsumoto, Yuji Kajita, Hideki Masuda (Nagoya Institute of Technology)
- P-23 Structural Basis for the Apparent Lack of Stereospecificity in Coenzyme B₁₂-Dependent Radical Enzyme Ethanolamine Ammonia-Lyase.** Naoki Shibata,¹ Tetsuo Toraya,² Yoshiki Higuchi¹ (¹University of Hyogo, ²Okayama University)
- P-24 Crystallization and X-ray Analysis of ATP-Sulfurylase from Sulfate-Reducing Bacteria.** Midori Taketa,¹ Yasuhito Shomura,^{1,2} Yoshiki Higuchi^{1,2} (¹University of Hyogo, ²RIKEN Harima Institute/SPring-8)
- P-25 Expression and Purification of the Rab GTPase-Effector Complex.** Shin-ichi Terawaki, Yoshiki Higuchi (University of Hyogo)
- P-26 Structure and Molecular Evolution of Multicopper Blue Proteins.** Hirofumi Komori, Yoshiki Higuchi (University of Hyogo, RIKEN SPring-8 Center)
- P-27 Synthesis of a Substrate-binding Dicopper-dioxygen Complex for Investigating the Reaction Mechanism of Tyrosinase.** Yasuhiro Funahashi, Tomoaki Toyama, Kotaro Yoshii, Tomohide Nishikawa, Yuko Wasada-Tsutsui, Yuji Kajita, Tomohiko Inomata, Tomohiro Ozawa, Hideki Masuda (Nagoya Institute of Technology)
- P-28 Biomimetic Study of Multicopper Oxidases Using Tricopper Complexes with a Cage-type Ligand.** Kojiro Nagata, Kensuke Fukui, Yuji Kajita, Yuko Wasada-Tsutsui, Tomohiko Inomata, Tomohiro Ozawa, Yasuhiro Funahashi, Hideki Masuda (Nagoya Institute of Technology)
- P-29 Synthesis and Structures of Homoleptic Fe(I) and Fe(0) Complexes Bearing N-Heterocyclic Carbenes.** Ryoko Hoshino, Takayoshi Hashimoto, Tsubasa Hatanaka, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-30 Synthesis and Reactions of Iron Complexes having Tridentate Bisaryloxy Ligands.** Tsubasa Hatanaka, Hiroyuki Kawaguchi (Tokyo Institute of Technology)