

Scientific Program

January 15 (Thursday)

9:45 **Opening Remarks:** Kazuyuki Tatsumi (Nagoya University)

Chair: Bernt Krebs (The University of Münster)

10:00 **William E. Newton** (Virginia Polytechnic Institute and State University)
Insight into the Role of the P Cluster during Substrate Reduction Catalyzed by
Wild-type and Variant *Azotobacter vinelandii* Nitrogenase MoFe Proteins.

10:45 **Ian Dance** (University of New South Wales)
A Mechanism for the Catalysed Reduction of N₂ to NH₃ at the Active Site of
Nitrogenase.

11:30 Lunch

Chair: Kazunari Yoshizawa (Kyushu University)

13:00 **Kazuyuki Tatsumi** (Nagoya University)
Synthesis of Iron-Sulfur Clusters Relevant to the Active Sites of Nitrogenase.

13:35 **Yuichi Fujita** (Nagoya University)
Structural Aspects of Dark-operative Protochlorophyllide Reductase.

14:10 Coffee Break

Chair: Yoshiki Higuchi (University of Hyogo)

14:40 **Hiroshi Nakajima** (Nagoya University)
Functional Analysis of Fe₃S₄ Cluster Involved in Nitrogenase Regulatory Protein,
VnfA from *A. vinelandii*.

15:15 **Richard A. Henderson** (Newcastle University)
Protonation of Synthetic Fe-S-Based Clusters.

16:00 **Kazunari Yoshizawa** (Kyushu University)
QM/MM Study of Tyrosinase: Structure and Catalytic Mechanism.

16:35 **Poster Session**

January 16 (Friday)

Chair: Yasuhiro Ohki (Nagoya University)

- 9:30 **Michael Fryzuk** (The University of British Columbia)
Activation and Functionalization of Molecular Nitrogen.
Abiological Approaches to Nitrogen Fixation.
- 10:15 **Hiroyuki Kawaguchi** (Tokyo Institute of Technology)
Activation of Small Molecules by Niobium and Tantalum Complexes Bearing
Phenoxide Ligands.
- 10:50 **Yasushi Mizobe** (The University of Tokyo)
Reactions of Small Molecules on the Low-Valent Mo Center Surrounded by the
Linear Tetraphosphine Ligand *meso-o*-C₆H₄(PPhPCH₂CH₂PPh₂)₂.
- 11:25 Lunch

Chair: Tsukasa Matsuo (RIKEN)

- 13:00 **Yasuhiro Arikawa** (Nagasaki University)
NO Reduction Cycle on Dinuclear Ruthenium Complexes Based on Nitric Oxide
Reductase..
- 13:35 **Holger Dobbek** (Bayreuth University)
Carbon Monoxide Dehydrogenases –Insights from Structural Biochemistry–.
- 14:20 Coffee Break

Chair: Kazuyuki Tatsumi (Nagoya University)

- 14:40 **Panel Discussion**
- 16:10 **Closing Remarks**

Poster Session

January 15 (Thursday) 16:35-

- P-01 Heterolysis of H₂ Mediated by Metal-Sulfur Sites of Coordinatively Unsaturated Iridium and Rhodium-Thiolate Complexes.** Mayumi Sakamoto, Yasuhiro Ohki and Kazuyuki Tatsumi (Nagoya University)
- P-02 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)
- P-03 Ultra-High Resolution X-ray Crystallography of Tetraheme Cytochrome c₃.** Toshihiro Nagao, Koji Nishikawa, Midori Taketa, Hirofumi Komori, Hisao Kobayashi, and Yoshiki Higuchi. (University of Hyogo)
- P-04 Crystal Structure of Coenzyme B₁₂-Dependent Ethanolamine Ammonia-Lyase.** Naoki Shibata¹, Naoki Hieda², Keita Akita², Koichi Mori², Tetsuo Toraya², Yoshiki Higuchi¹ (¹University of Hyogo, ²Okayama University)
- P-05 Reaction of Ni^{II}-Ni⁰ Dinuclear Complex and Methylcobaloxime Modeling the Function of Acetyl-CoA Synthase.** Mai Kotera, Mikinao Ito, Yumei Song, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University).
- P-06 Synthesis of Iron Arylthiolate and Zirconium Aryloxy Complexes Having Bulky “Rind” Groups.** Mikinao Ito, Daisuke Hasizume, Tsukasa Matsuo, and Kohei Tamao (RIKEN)
- P-07 Synthesis and Properties of New Au(I)-Ferrocenophane Complexes.** Gerrit L bbecke, Roland Fr hlich, Gerald Kehr, Gerhard Erker (The University of M nster)
- P-08 Synthesis of Manganese(II) Complexes of N-Heterocyclic Carbene or Bulky Phenolate.** Yuko Kawato, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-09 C-H Bond Activation of Arenes by Coordinatively Unsaturated Cp*Fe-Alkyl Complexes.** Tsubasa Hatanaka, Yasuhiro Ohki, and Kazuyuki Tatsumi (Nagoya University)
- P-10 Biomimetic Studies of O₂-activating Non-heme Iron Active Centers with Tetrahedral Distortion.** Yasuhiro Funahashi, Kotaro Yoshii, Takanori Inazumi, Tomohide Nishikawa, Takeshi Okumura, Yuko Wasada-Tsutsui, Yuji Kajita, Tomohiko Inomata, Tomohiro Ozawa, Hideki Masuda (Nagoya Institute of Technology)

- P-11 Synthesis and Reactivity of Trihydride-Bridging Ditantalum Complexes.** Takahito Watanabe and Hiroyuki Kawaguchi (Tokyo Institute of Technology)
- P-12 Me-S Bond Activation by Ni(I) Model Complexes: Insight into the Function of Methyl CoM Reductase.** Jun-ichi Nishigaki, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)
- P-13 X-Ray Crystallographic Analysis of Multicopper Oxidase CueO Mutants.** Hirofumi Komori¹, Kunishige Kataoka², Yusaku Ueki², Yusuke Konno², Yuji Kamitaka³, Shinji Kurose^{2,3}, Seiya Tsujimura³, Kenji Kano³, Daisuke Seo², Takeshi Sakurai², Yoshiki Higuchi¹ (¹University of Hyogo, ²Kanazawa University, ³Kyoto University)
- P-14 Structural Studies on Dissimilatory Sulfite Reductase.** Yasuhito Shomura, Yoshiki Higuchi (University of Hyogo)
- P-15 Synthesis and Characterization of Dimolybdenum Complex Coordinated by Aromatic Compound.** Takahiko Ogawa, Jun Matsumoto, Yuji Kajita, Yasuhiro Funahashi, Tomohiro Ozawa, Hideki Masuda (Nagoya Institute of Technology)
- P-16 Effect of the Dihedral Angles of Two CuS₂ Planes of Disulfidodicopper(II) Complexes on Their Reactivity Toward Exogenous Substrates.** Jun Matsumoto¹, Yuji Kajita¹, Yuko Wasada-Tsutsui², Yasuhiro Funahashi¹, Tomohiro Ozawa¹, Hideki Masuda¹ (¹Nagoya Institute of Technology, ²Nagoya City University)
- P-17 Iron Aryl Complexes Having Bulky Thiolate Ligands and Their Application to Fe-S Cluster Synthesis.** Takayoshi Hashimoto, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-18 Synthesis of 1:3 Site-Differentiated [4Fe-4S] Clusters Modeling Aconitase Active Site and [4Fe-4S]_{dist} Cluster of Hydrogenases.** Tamaki Terada, Kiyohisa Hirabayashi, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)
- P-19 Synthetic Analogues of Histidine-Bound Distal-[4Fe-4S] Clusters in Hydrogenases.** Norihiro Yamada, Tomoyuki Tajima, Motosuke Imada, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-20 Synthesis and Reactions of [Ni(N₂S₂)Fe(N(SiMe₃)₂)₂] Complexes.** Dong Liu, Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)

- P-21 Nitrogenase Transcriptional Activator, VnfA: Identification of Signal Molecule by Using *in vivo* Activity Assay System.** Kyohei Yoshimitsu, Nobuyuki Takatani, Hiroshi Nakajima, Shigetoshi Aono, Yoshihito Watanabe (Nagoya University, Okazaki Institute for Integrative Biosciences)
- P-22 Role of the Sensory Domain in VnfA, a Transcriptional Activator of Nitrogenase.** Nobuyuki Takatani, Kyohei Yoshimitsu, Mitsuko Itoh, Hiroshi Nakajima, Shigetoshi Aono, Yoshihito Watanabe (Nagoya University, Okazaki Institute for Integrative Biosciences)
- P-23 Synthesis of Two Types of [8Fe-7S] Cores Analogous to the FeMo-cofactor and P^N-cluster.** Shun Ohta, Yohei Ikagawa, Rie Suizu, Won-seok Han, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-24 DFT Study on the Mechanism of the N≡N Bond Cleavage in a Diniohium Complex.** Hiromasa Tanaka,¹ Yoshihito Shiota,¹ Kenichiro Takahashi,¹ Tsukasa Matsuo,² Hiroyuki Kawaguchi,³ Kazunari Yoshizawa¹ (¹Kyushu University, ²RIKEN, ³Tokyo Institute of Technology)
- P-25 Synthesis of Cubane-Type Mo/Fe/S Clusters from Trithio-chloro Molybdate.** Nobuaki Sugimura, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-26 Oxygen Sensitivity of Nitrogenase-like Protochlorophyllide Reductase from the Cyanobacterium *Leptolyngbya boryana*.** Haruki Yamamoto, Shuhei Kurumiya, Rieko Ohashi, Yuichi Fujita (Nagoya University)
- P-27 Crystal Structure of NB-protein, the Catalytic Component, of Nitrogenase-like Protochlorophyllide Oxidoreductase from *Rhodobacter capsulatus*.** Jiro Nomata,¹ Norifumi Muraki,² Junpei Harimoto,¹ Tadashi Mizoguchi,³ Hitoshi Tamiaki,³ Tomoo Shiba,² Genji Kurisu,² Yuichi Fujita¹ (¹Nagoya University, ²The University of Tokyo, ³Ritsumeikan University)
- P-28 FT-IR study on [NiFe] hydrogenase from *Desulfovibrio vulgaris* Miyazaki F.** Hisao Osuka,¹ Shun Hirota,² Yoshiki Higuchi¹ (¹University of Hyogo, ²Nara Institute of Science and Technology)
- P-29 Purification and Characterization of ATP-sulfurylase from Sulfate-Reducing Bacteria.** Midori Taketa,¹ Bunsho Kure,² Seiji Ogo,² Yoshiki Higuchi¹ (¹University of Hyogo, ²Kyushu University)

- P-30 [8Fe-7S] Models of Nitrogenase P-Cluster: Synthesis, Properties, and Reactivity.** 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-31 Thiolate-Bridged Dinuclear Iron(tris-Carbonyl)-Nickel Complexes Relevant to the Active Site of [NiFe] Hydrogenase.** Yasuhiro Ohki, Kazunari Yasumura, Katsuaki Kuge, Soichiro Tanino, Masaru Ando, Zilong Li, and Kazuyuki Tatsumi (Nagoya University)
- P-32 Synthesis and Reactions of Dinuclear (tris-carbonyl)Fe-Ni Complexes Relevant to the Active Site of [NiFe] Hydrogenase.** Satoko Shimokata, Frank M. A. Geilen, Soichiro Tanino, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-33 Synthesis of Thiolate-Bridged Dinuclear Nickel-Iron(Carbonyl/Cyano) Complexes.** Soichiro Tanino, Zilong Li, Koshi Onishi, Yasuhiro Ohki, Kazuyuki Tatsumi (Nagoya University)
- P-34 A Functional Model of Hydrogenase and CO-Dehydrogenase: H₂ and CO Activation by Hetero-dinuclear Ru/Ge Complexes.** Tsuyoshi Matsumoto, Kazuyuki Tatsumi (Nagoya University)