

Curriculum Vitae

Hideaki Takano

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ORCID: <https://orcid.org/0000-0003-0744-9292>

1. Education

- Apr. 2011 – Mar. 2015: **B.Sc.**, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University (Prof. Takanori Shibata)
- Apr. 2015 – Mar. 2017: **M. Sc.**, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University (Prof. Takanori Shibata)
- Apr. 2017 – Mar. 2020: **PhD. Sc.**, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University (Prof. Takanori Shibata)

2. Career

- Apr. 2020 – Sep. 2021: **Postdoctoral Researcher**, WPI-ICReDD, Hokkaido University (JST-ERATO Maeda Artificial intelligence for Chemical Reaction Design and Discovery Project)
- Oct. 2021 – Nov. 2022: **Specially Appointed Assistant Professor**, WPI-ICReDD, Hokkaido University (JST-ERATO Maeda Artificial intelligence for Chemical Reaction Design and Discovery Project)
- Dec. 2022 – **Assistant Professor**, Institute for Advanced Research and Graduate School of Engineering, Nagoya University (Organic Material Chemistry, Shinokubo lab.)

3. Fellowship

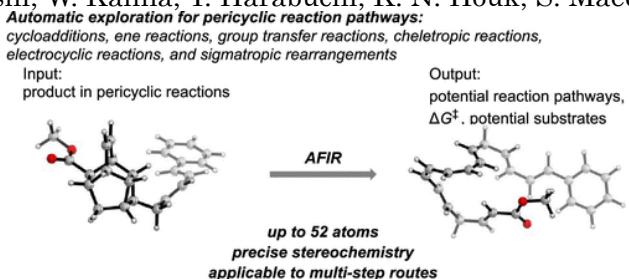
- Dec. 2022 – **Leading Initiative for Excellent Young Researchers**, Japan Society for the Promotion of Sciences (JSPS)
- Apr. 2018 – Mar. 2020: **Research Fellowship for Young Scientists (DC2)**, Japan Society for the Promotion of Sciences (JSPS)
- Apr. 2018 – Mar. 2019: **Visiting Student**, Department of Chemistry, University of Cambridge (Prof. Robert J. Phipps), supported by Overseas Challenge Program for Young Researchers of JSPS

4. Publication

- 1). Prediction of High-Yielding Single-Step or Cascade Pericyclic Reactions for the Synthesis of Complex Synthetic Targets

J. Am. Chem. Soc. **2022**, *144*, 22985-23000.

T. Mita, H. Takano, H. Hayashi, W. Kanna, Y. Harabuchi, K. N. Houk, S. Maeda

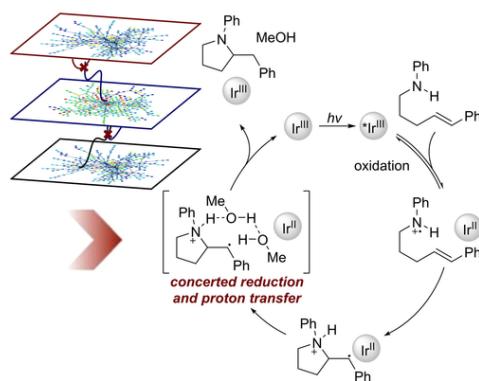


2). Oxidation and Reduction Pathways in the Knowles Hydroamination via a Photoredox-Catalyzed Radical Reaction

Angew. Chem. Int. Ed. **2022**, DOI: 10.1002/anie.202211936

Y. Harabuchi, H. Hayashi, H. Takano, T. Mita, S. Maeda

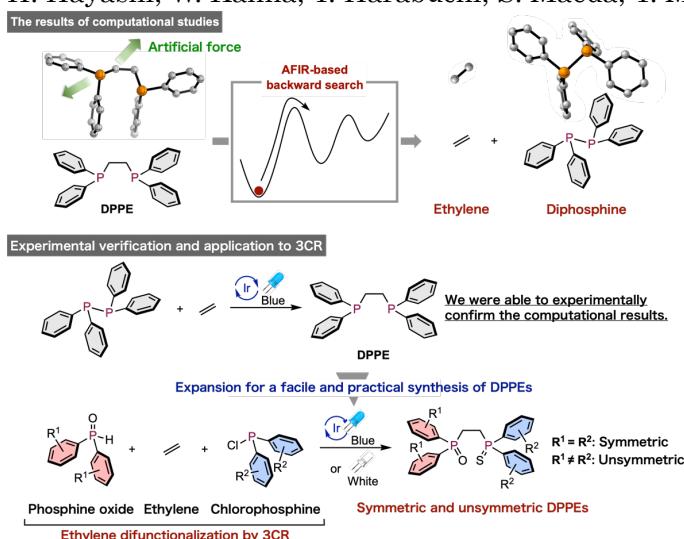
Crossings connect
Reaction Path Networks Entire mechanism of
Knowles hydroamination



3). A theory-driven synthesis of symmetric and unsymmetric 1,2-bis(diphenylphosphino)ethane analogues via radical difunctionalization of ethylene

Nat. Commun. **2022**, *13*, 7034.

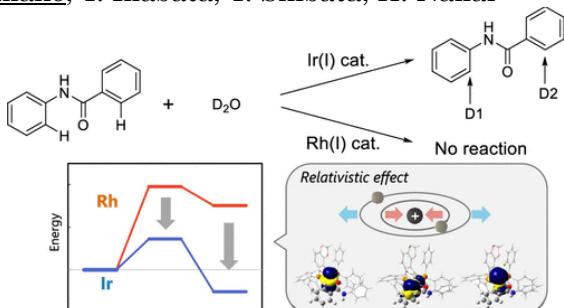
H. Takano, H. Katsuyama, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda, T. Mita



4). Experimental and Theoretical Evidence for Relativistic Catalytic Activity in C–H Activation of N-Phenylbenzamide Using a Cationic Iridium Complex

J. Phys. Chem. A **2022**, *126*, 7627-7638.

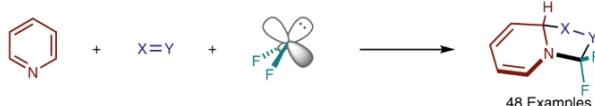
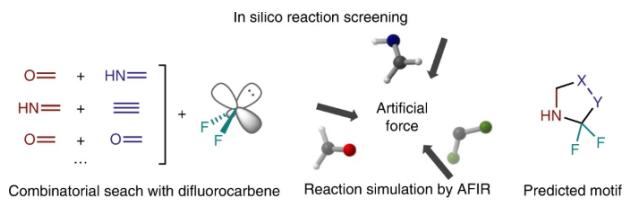
C. Takashima, H. Kurita, H. Takano, Y. Ikabata, T. Shibata, H. Nakai



5). In silico reaction screening with difluorocarbene for N-difluoroalkylative dearomatization of pyridines

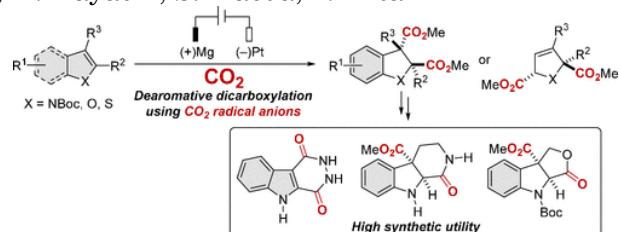
Nat. Synth. **2022**, *1*, 804-814.

H. Hayashi, H. Katsuyama, H. Takano, Y. Harabuchi, S. Maeda, T. Mita



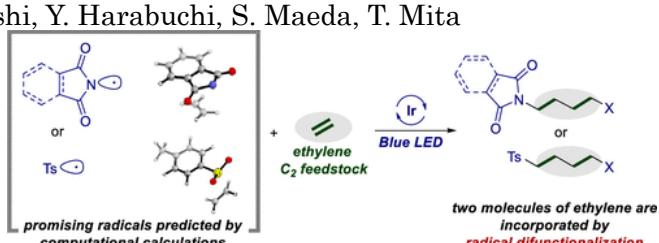
- 6). Electrochemical Dearomative Dicarboxylation of Heterocycles with Highly Negative Reduction Potentials
J. Am. Chem. Soc. **2022**, *144*, 3685-3695.

Y. You, W. Kanna, H. Takano, H. Hayashi, S. Maeda, T. Mita



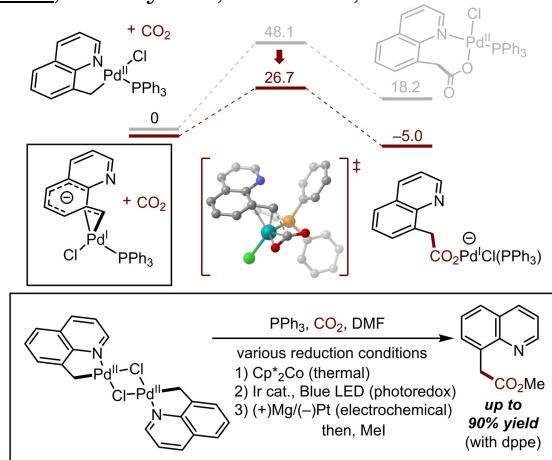
- 7). Radical Difunctionalization of Gaseous Ethylene Guided by Quantum Chemical Calculations: Selective Incorporation of Two Molecules of Ethylene
ACS Omega, **2021**, *6*, 33846-33854.

H. Takano, Y. You, H. Hayashi, Y. Harabuchi, S. Maeda, T. Mita



- 8). Carboxylation of a Palladacycle Formed via C(sp³)–H Activation: Theory-Driven Reaction Design
Chem. Asian J. **2021**, *16*, 4072-4080.

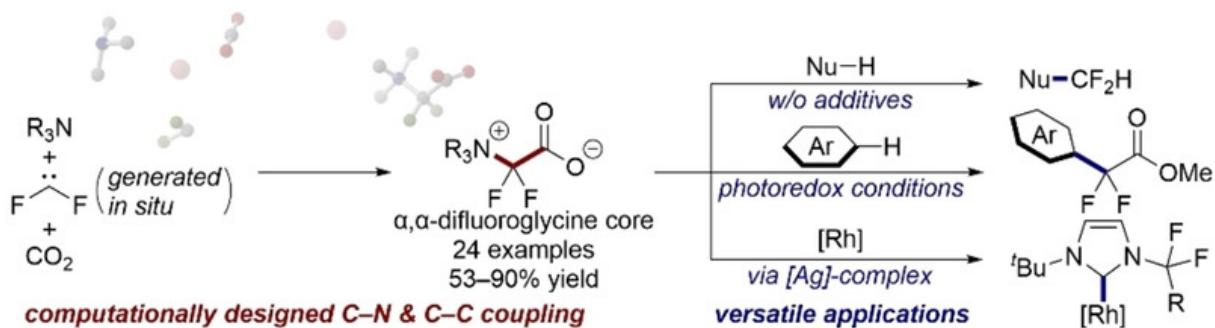
W. Kanna, Y. Harabuchi, H. Takano, H. Hayashi, S. Maeda, T. Mita



- 9). Synthesis of Difluoroglycine Derivatives from Amines, Difluorocarbene, and CO₂: Computational Design, Scope, and Applications

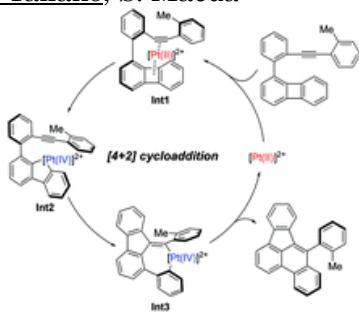
Chem. Eur. J. **2021**, *27*, 10040-10047.

H. Hayashi, H. Takano, H. Katsuyama, Y. Harabuchi, S. Maeda, T. Mita



- 10). Pt(II)-Chiral Diene-Catalyzed Enantioselective Formal [4+2] Cycloaddition Initiated by C–C Bond Cleavage and Elucidation of a Pt(II)/(IV) Cycle by DFT Calculations
Org. Chem. Front. **2021**, *8*, 6985–6991.

T. Shibata, N. Shiozawa, S. Nishibe, H. Takano, S. Maeda



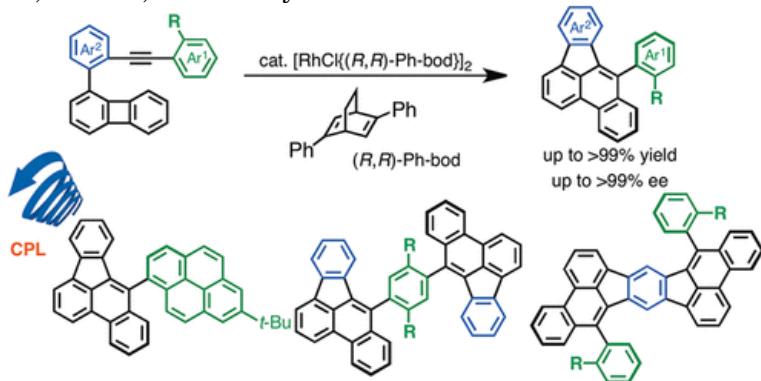
- 11). Gold-catalyzed dual C–C bond cleavage of biphenylenes bearing a pendant alkyne at ambient temperature
Org. Biomol. Chem. **2020**, *18*, 5826–5831.

H. Takano, S. Okazaki, S. Nishibe, T. Ito, N. Shiozawa, N. Sugimura, K. S. Kanyiva, T. Shibata



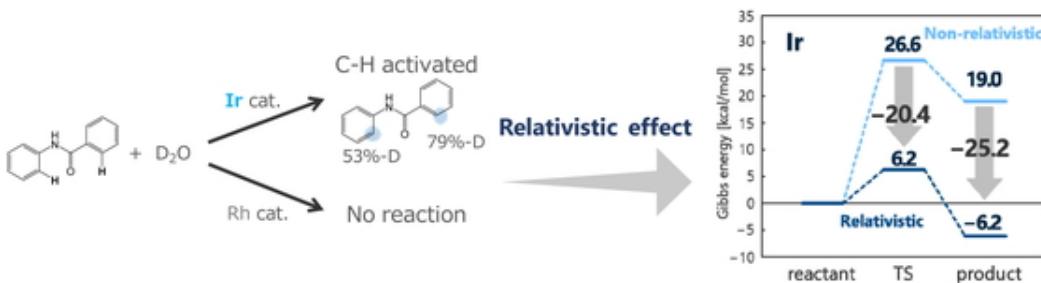
- 12). Catalytic Enantioselective Synthesis of Axially Chiral Polycyclic Aromatic Hydrocarbons (PAHs) via Regioselective C–C Bond Activation of Biphenylenes
J. Am. Chem. Soc. **2020**, *142*, 4714–4722.

H. Takano, N. Shiozawa, Y. Imai, K. S. Kanyiva and T. Shibata



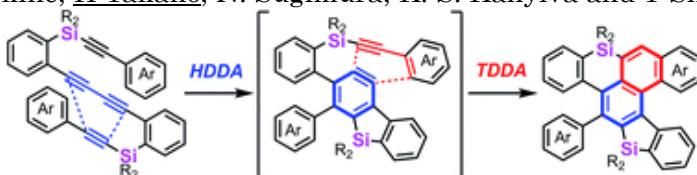
- 13). Relativistic Effect on Homogeneous Catalytic Reaction by Cationic Iridium Catalysts
J. Comput. Chem. Japan **2019**, *18*, 136–138.

C. Takashima, Y. Ikabata, H. Kurita, H. Takano, T. Shibata, H. Nakai



- 14). Consecutive HDDA and TDDA reactions of silicon-tethered tetracynes for the synthesis of dibenzosilole-fused polycyclic compounds and their unique reactivity
Chem. Sci., **2019**, *10*, 6715–6720.

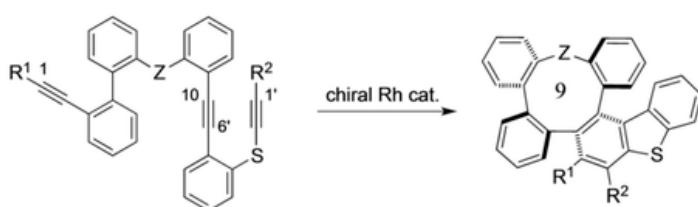
A. Mitake, R. Nagai, A. Sekine, H. Takano, N. Sugimura, K. S. Kanyiva and T. Shibata



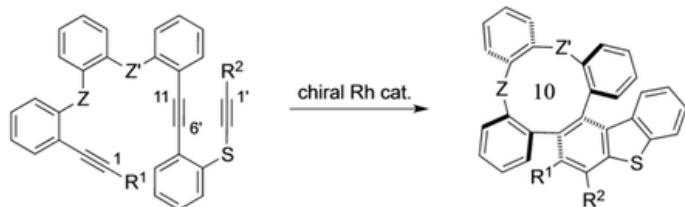
- 15). Enantioselective Synthesis of Nine- to Eleven-Membered Cyclic Polyphenylenes Containing Heteroatoms by Catalytic Intramolecular [2+2+2] Cycloaddition
Asian. J. Org. Chem. **2019**, *8*, 970–977.

T. Shibata, T. Fusamae, H. Takano, N. Sugimura, K. S. Kanyiva

a) Chiral nine-membered ring from 1,10-diyne moiety

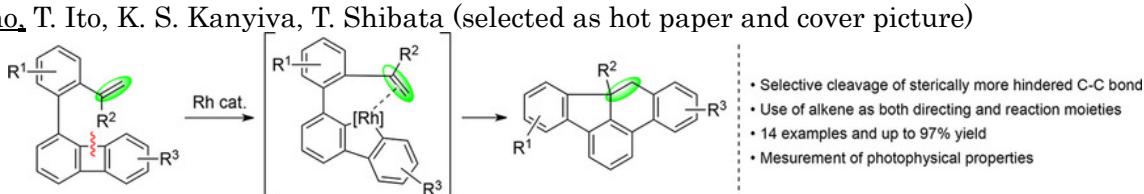


b) Chiral ten-membered ring from 1,11-diyne moiety



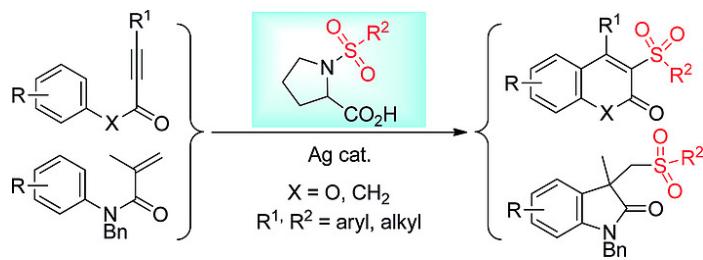
- 16). Regioselective Activation of a Sterically More Hindered C-C Bond of Biphenylenes Using an Alkene as Both a Directing Group and a Reaction Moiety
Chem. Eur. J. **2018**, *24*, 15173–15177.

H. Takano, T. Ito, K. S. Kanyiva, T. Shibata (selected as hot paper and cover picture)



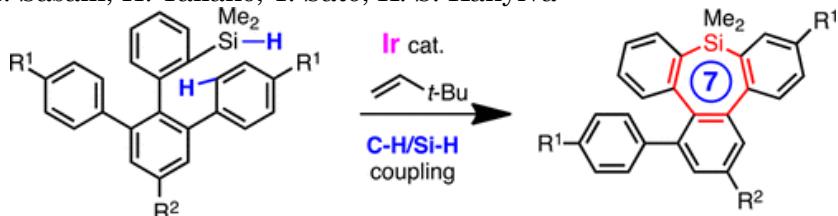
- 17). α -Amino Acid Sulfonamides as Versatile Sulfonylation Reagents: Silver-Catalyzed Synthesis of Coumarins and Oxindoles by Radical Cyclization
Eur. J. Org. Chem. **2018**, 5905–5909.

K. S. Kanyiva, D. Hamada, S. Makino, H. Takano, T. Shibata



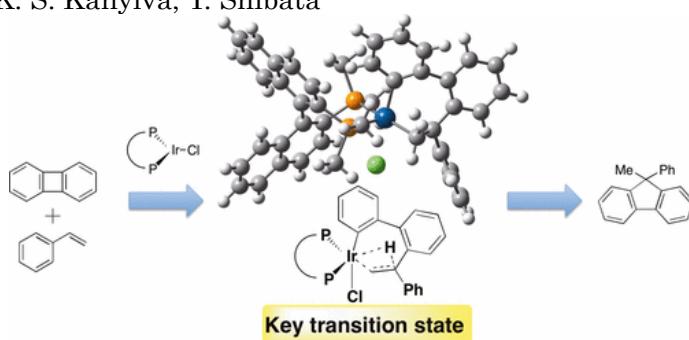
- 18). A Ir-Catalyzed Synthesis of Substituted Tribenzosilepins by Dehydrogenative C–H/Si–H Coupling
J. Org. Chem. **2018**, *83*, 3426–3432.

T. Shibata, N. Uno, T. Sasaki, H. Takano, T. Sato, K. S. Kanyiva



- 19). DFT Studies on the Mechanism of the Iridium-Catalyzed Formal [4 + 1] Cycloaddition of Biphenylene with Alkenes
ACS Omega **2017**, *2*, 5228–5234.

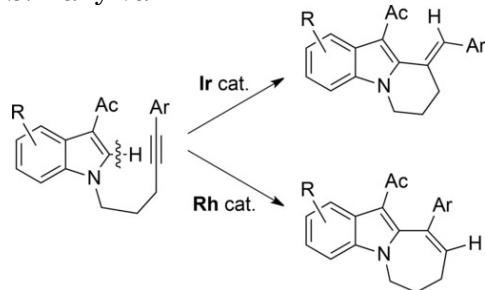
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata



- 20). Intramolecular C-H Alkenylation of *N*-Alkynylindoles: *Exo* and *Endo* Selective Cyclization by the Choice of Metal Catalysts

Adv. Synth. Catal. **2017**, *359*, 1849–1853.

T. Shibata, T. Baba, H. Takano, K. S. Kanyiva



- 21). Iridium-Catalyzed Formal [4+1] Cycloaddition of Biphenylenes with Alkenes Initiated by C–C Bond Cleavage for the Synthesis of 9,9-Disubstituted Fluorenes

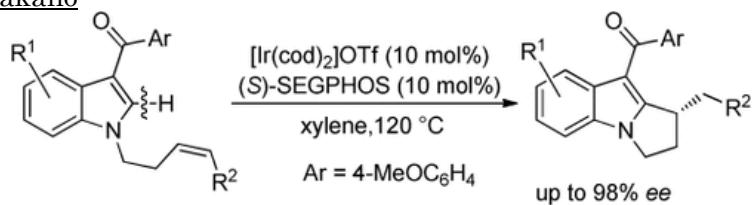
Org. Lett. **2016**, *18*, 1860–1863.

H. Takano, K. S. Kanyiva, T. Shibata



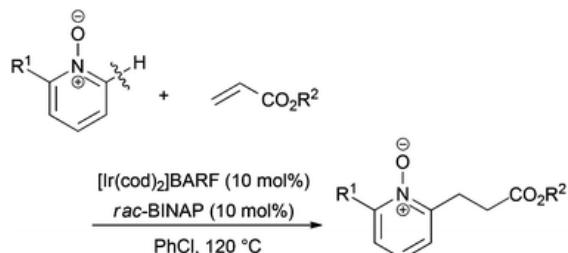
22). Iridium-Catalyzed Intramolecular Enantioselective C-H Alkylation at the C-2 Position of *N*-Alkenylindoles
Adv. Synth. Catal. **2015**, *357*, 1131-1135.

T. Shibata, N. Ryu, H. Takano



23). Cationic iridium-catalyzed C–H alkylation of 2-substituted pyridine *N*-oxides with acrylates
Org. Chem. Front. **2015**, *2*, 383-387.

T. Shibata, H. Takano,

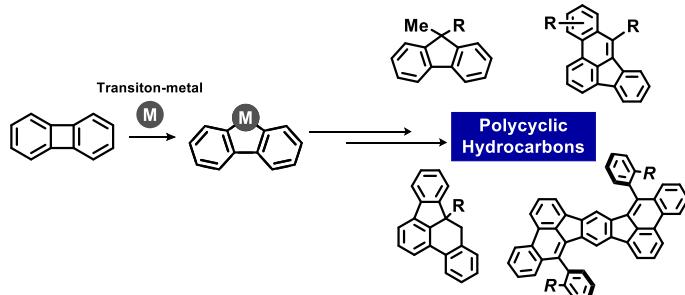


5. Review

1). Versatile Transformations of Biphenylenes by Transition-Metal Catalysts and Application for the Synthesis of Polycyclic Hydrocarbons

J. Synth. Org. Chem. Jpn. **2021**, *79*, 849-858.

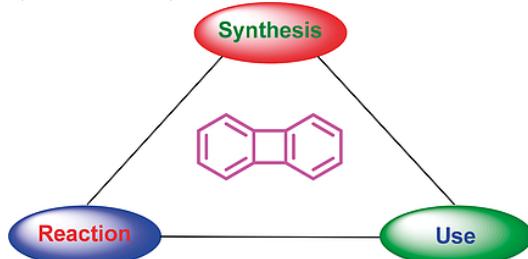
H. Takano, T. Shibata



2). Recent Advances of Biphenylene: Synthesis, Reactions and Uses

Eur. J. Org. Chem. **2019**, 2871–2883.

H. Takano, T. Ito, K. S. Kanyiva, T. Shibata,



6. Patent

1). T. Mita, S. Maeda, H. Takano, PCT patent application, Aug 10th, 2022 (PCT/JP2022/ 30598)

2). エチレンを原料に用いた 1,2-ビス（ジフェニルホスフィノ）エタン（DPPE）誘導体の合成法
 美多 剛, 前田 理, 高野 秀明

特願 2021-131481 出願(2021 年 8 月 11 日)

7. Conference

- 1). AFIR 法に基づくエチレンの二官能基化反応による対称及び非対称 DPPE 誘導体の合成と配位子への展開 (Oral)
The 8th Hokkaido University Cross-Departmental Symposium, Online meeting, Oct 2022
H. Takano, H. Katsuyama, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda, T. Mita
- 2). Facile Synthesis of Symmetric/Unsymmetric DPPE Derivatives from Gaseous Ethylene and Application for Transition-Metal Complexes (Oral)
68th Symposium on Organometallic Chemistry, O3-13, Online meeting, Sep 2022
H. Takano, H. Katsuyama, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda, T. Mita
- 3). 電解還元法を用いたヘテロ芳香環の脱芳香族ジカルボキシル化反応 (Oral)
第 20 回次世代を担う有機化学シンポジウム, 金沢, May 2022
高野 秀明, You Yong, 神名 航, 林 裕樹, 前田 理, 美多 剛
- 4). AFIR 法を用いた立体特異的なペリ環状反応の自動経路探索:天然物の自動探索を目指して (Oral)
第 24 回理論化学討論会, 金沢, May 2022
H. Takano, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda, T. Mita
- 5). Development of New Reactions by Quantum Chemical Calculations: the Synthesis of Unsymmetric DPPE via Difunctionalization of Ethylene (Oral)
The 102nd CSJ Annual Meeting, Online meeting, K4-2pm-03, Mar 2022
H. Takano, H. Katsuyama, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda, T. Mita
- 6). Photochemical Radical Double Functionalization of Ethylene Gas Guided by Quantum Chemical Calculations (Poster)
The 4th ICReDD International Symposium, Online meeting, Mar 2022.
H. Takano, H. Katsuyama, H. Hayashi, W. Kanna, Y. Harabuchi, S. Maeda, T. Mita
- 7). Light-driven radical double functionalization of ethylene gas guided by quantum chemical calculations (Poster)
Pacificchem2021, Online meeting, Dec 2021
H. Takano, Y. Harabuchi, S. Maeda, T. Mita
- 8). エチレンガスのラジカルダブル官能基化反応を指向した AFIR 法に基づく新規反応開発 (Oral)
119th Symposium on Organic Synthesis, O-13, Online meeting, Nov 2021
高野秀明、美多剛、原渕祐、前田理
- 9). AFIR 法に基づくエチレンガスの光触媒を用いたラジカルダブル官能基化反応の開発 (Oral)
第 47 回反応と合成の進歩シンポジウム, 2O-16, Online meeting, Oct 2021
高野秀明、美多剛、原渕祐、前田理
- 10). Development of Radical Difunctionalization of Ethylene Gas Predicted by Quantum Chemical Calculations (Oral)
The 101st CSJ Annual Meeting, Online meeting, A21-3am-02, Mar 2021
H. Takano, T. Mita, Y. Harabuchi, S. Maeda
- 11). Highly enantioselective synthesis of axially chiral polyaromatic hydrocarbons by transition-metal catalysts (Oral)
第 11 回大津会議, Online, Feb 2021
高野秀明
- 12). Development of Catalytic Transformation via Regioselective Cleavage of Sterically Hindered C-C Bond Promoted by Unsaturated Bonds as Both Directing Group and Reaction Site (Oral)
66th Symposium on Organometallic Chemistry, O1-01, Tokyo Metropolitan University (Japan), Sep 2019
H. Takano, T. Ito, N. Shiozawa, K. S. Kanyiva, T. Shibata
- 13). Rhodium-catalyzed regioselective activation of sterically hindered C-C bond of Biphenylene" (Poster)
ESOC2019 - 21st European Symposium on Organic Chemistry, PO-149, Vienna (Austria), Jul 2019
H. Takano, T. Ito, N. Shiozawa, K. S. Kanyiva, T. Shibata
- 14). ロジウム触媒を用いた立体的に混み合った C-C 結合開裂を伴う分子内環化反応の開発 (Poster)
52nd Summer School of Organometallic Chemistry, 1P-7, Okayama (Japan), Jun 2019
Hideaki Takano
- 15). Computational Study of Iridium Complexes as Transition States in Formal [4+1] Cycloaddition of Biphenylene with Alkenes: Rational Explanation of [4+1] Prior to [4+2] Cycloaddition (Poster)
The 24th International SPACC Symposium -Metal Complexes for Green and Sustainable Development-, P-13, University of Auckland (New Zealand), Nov 2017

- H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 16). Computational Mechanistic Study for the Iridium-Catalyzed Formal [4+1] Cycloaddition of Biphenylene with Alkenes (Oral)
The 97th CSJ Annual Meeting, Keio University, Tokyo, 3E2-28, Mar 2017
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 17). Iridium-Catalyzed Formal [4+1] Cycloaddition for the Synthesis of 9,9'-Disubstituted Fluorenes and DFT Studies of the Reaction Mechanism (Poster)
66th Symposium on Organometallic Chemistry, P2-37, Waseda (Japan), Sep 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 18). Synthesis of 9,9'-Disubstituted Fluorene Derivatives by Iridium Catalyst Initiated by C-C Bond Cleavage of Biphenylenes (Invited lecture)
ISPAC 2016, ORS12, Kuching (Malaysia), Aug 2016
H. Takano
- 19). Iridium-catalyzed reaction of biphenylenes with alkenes initiated by C-C bond cleavage (Poster)
International Conference on Organometallic Chemistry 2016, 186, Melbourne (Australia), Jul 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 20). イリジウム触媒を用いた C-C 結合開裂を経る[4+1]付加環化反応の開発 (Poster)
49th Summer School of Organometallic Chemistry, Gunma (Japan), Jul 2016
Hideaki Takano
- 21). Iridium-Catalyzed Formal [4+1] Cycloaddition Initiated by C-C Bond Cleavage of Biphenylenes (Poster)
109th Symposium on Organic Synthesis, P-22, Tokyo Institute of Technology (Japan), Jun 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 22). Synthesis of 9,9'-Disubstituted Fluorene Derivatives by Iridium Catalyst via C-C Bond Activation of Biphenylenes (Oral)
The 96th CSJ Annual Meeting, 2H7-18, Doshisha University (Japan), Mar 2016
H. Takano, N. Sugimura, K. S. Kanyiva, T. Shibata
- 23). C-H alkylation for 2-substituted pyridine N-oxide by a cationic iridium(I) catalyst" (Poster)
Pacificchem2015, ORGN2539, Hawaii (America), Dec 2015
H. Takano, T. Shibata
- 24). Chiral Cationic Iridium-Catalyzed Enantioselective Intramolecular C-H Alkylation at the C-2 Position of Indoles (Poster)
62nd Symposium on Organometallic Chemistry, P2-47, Kansai University (Japan), Sep 2015
H. Takano, N. Ryu, T. Shibata
- 25). Enantioselective intramolecular C-H alkylation at the C-2 position of indole by a chiral cationic iridium(I) catalyst (Poster)
OMCOS18, P-429, Barcelona (Spain), Jun 2015
H. Takano, N. Ryu, T. Shibata
- 26). Cationic Iridium-Catalyzed Enantioselective Intramolecular C-H alkylation at the C-2 Position of Indoles (Poster)
Symposium on Molecular Chirality 2015, PP-20D, Waseda University (Japan), Jun 2015
H. Takano, N. Ryu, T. Shibata
- 27). Ir(I)-Catalyzed C2-Selective C-H Alkylation of Pyridine N-Oxides (Oral)
The 95th CSJ Annual Meeting, 2E5-11, Nihon University (Japan), Mar 2015
H. Takano, T. Shibata

8. Award

- 2022 Best Presentation Award, The 8th Hokkaido University Cross-Departmental Symposium
- 2021 Otsu Conference Award Fellow
- 2020 博士学位賞
- 2017 Yoshiro Sekine Award (Top grade award for M.S. in my major)
- 2016 27th International Conference on Organometallic Chemistry(ICOMC) Student Award and Travel Bursary (<http://icomc2016.com/student-award-travel-bursary/>)
- 2015 Top grade award for undergraduate school in my department

9. Membership

- The Chemical Society of Japan

- The Society of Synthetic Organic Chemistry, Japan
- Kinka Chemical Society