

平成23年度 研究業績

久保 孝史 (大阪大学大学院理学研究科、A03班 計画班員)

1. 発表論文等 (査読付き論文, 著書, 総説等の発表状況)

- (1) Synthesis, Crystal Structure, and Physical Properties of Sterically Unprotected Hydrocarbon Radicals
Kubo, T.*; Katada, Y.; Shimizu, A.; Hirao, Y.*; Sato, K.; Takui, T.; Uruichi, M.; Yakushi, K.; Haddon, R. C.* *J. Am. Chem. Soc.* **2011**, *133*(36), 14240-14243.
- (2) Experimental consideration of covalent bonding interactions in stacks of singlet biradicals having Kekulé structures
Shimizu, A.; Hirao, Y.; Nakano, M.; Kubo, T.*; *J. Phys. Org. Chem.* **2011**, *24*(10), 876-882.
- (3) “Marking” the Nitrogen Atoms of Phenyl-(2-pyridyl)-(3-pyridyl)-(4-pyridyl)methane. Synthesis and Absolute Configuration of the Corresponding Tris(pyridine *N*-oxide)
Matsumoto, K.*; Miki, K.; Inagaki, T.; Nehira, T.; Pescitelli, G.; Hirao, Y.; Kurata, H.; Kawase, T.; Kubo, T.* *Chirality* **2011**, *23*(7), 543–548.
- (4) Triarylamines on [3]Radialene Scaffold: Novel [3]Radialene-based, Multi-step, Wide-range Redox Systems with Remarkably Low Oxidation Potentials
Matsumoto, K.*; Yamada, N.; Enomoto, T.; Kurata, H.; Kawase, T.; Oda, M. *Chem. Lett.* **2011**, *40*(9), 1033–1035.
- (5) Size dependences of the diradical character and the second hyperpolarizabilities in dicyclopenta-fused acenes: relationships with their aromaticity/antiaromaticity
Motomura, S.; Nakano, M.*; Fukui, F.; Yoneda, K.; Kubo, T.; Carion, R.; Champagne, B. *Phys. Chem. Chem. Phys.* **2011**, *13*, 20575–20583.
- (6) 17,17-Dialkyltetra benzo[a,c,g,i]fluorenes with Extremely High Solid-state Fluorescent Quantum Yields: Relationship between Crystal Structure and Fluorescent Properties
Kitamura, C.*; Tanigawa, Y.; Kobayashi, T.; Naito, H.; Kurata, H.; Kawase, T.* *Tetrahedron* **2012**, *68*(6), 1688-1694.
- (7) Synthesis, Electronic and Morphological Properties of Tetrahedral Oligothiophenes with *n*-Hexyl Terminal Groups
Matsumoto, K.*; Kugo, S.; Takajo, D.; Inaba, A.; Hirao, Y.; Kurata, H.; Kawase, T. Kubo, T.* *Chem. Asian J.* **2012**, *7*(1), 225–232.

2. 学会発表等 (国内外の招待講演および国際会議での発表状況)

- (1) Singlet Open-Shell Character of Conjugated Kekulé Molecules.

- Kubo, T.; Nakano, M.; Kamada, K. 9th International Conference of Computational Methods in Sciences and Engineering (ICCMSE2011), Halkidiki, Greece, 2011.10.2-7 (基調講演) .
- (2) Singlet biradical character of Kekulé PAHs.
Konishi, A.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Nakano, M.; Kubo, T. 5th Pacific Symposium on Radical Chemistry (PSRC-5), Shirahama, Wakayama, Japan, 2011.9.25-28 (招待講演) .
- (3) Synthesis and open-shell character of anthenes.
Kubo, T. India–Japan symposium on graphene, Tokyo, Japan, 2012.2.29-3.2 (招待講演) .
- (4) The singlet open-shell character of anthenes: synthesis and characterization of quarteranthene.
Konishi, A.; Shimizu, A.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Kubo, T.; Nakano, M.; Champagne B. 14th International Symposium on Novel Aromatic Compounds, Eugene, Oregon, USA, 2011.7.24-29 (ポスター発表) .
- (5) Development of Novel Soft Porous Material Based on 3-fold Interpenetrated Quartz Type Hydrogen-Bonded Network.
Inokuchi, D.; Hirao, Y.; Takahashi, K.; Matsumoto, K.; Kurata, H.; Mori, H.; Kubo, T. 14th International Symposium on Novel Aromatic Compounds (ISNA-14), Eugene, Oregon, USA, 2011.7.24-29 (ポスター発表) .
- (6) Studies on the Synthesis and Properties of Dendrimer Molecule Based on Tetrakis(2-thienyl)methane Framework.
Kugo S.; Matsumoto, K.; Takajo, D.; Hirao, Y.; Kurata, H.; Kubo, T. 14th International Symposium on Novel Aromatic Compounds (ISNA-14), Eugene, Oregon, USA, 2011.7.24-29 (ポスター発表) .
- (7) Mechanochromism of 2,2'-Bis(spirodienone)-Bridged-3,3'-Bithiophene Derivatives.
Kurata, H.; Atsuji, Y.; Hirao, Y.; Matsumoto, K.; Amimoto, K.; Kubo, T. 14th International Symposium on Novel Aromatic Compounds, Eugene, Oregon, USA, 2011.7.24-29 (ポスター発表) .
- (8) Synthetic Study of Cage-Shaped Oligothiophenes.
Adachi, K.; Kurata, H.; Hirao, Y.; Matsumoto, K.; Kubo, T. 14th International Symposium on Novel Aromatic Compounds, Eugene, Oregon, USA, 2011.7.24-29 (ポスター発表) .
- (9) Highly delocalized polycyclic aromatic hydrocarbon (PAH) radical.
Kubo, T.; Katada, Y.; Shimizu, A.; Hirao, Y.; Matsumoto, K.; Kurata, H.; Haddon, R. C. 14th International Symposium on Novel Aromatic Compounds, Eugene, Oregon, USA, 2011.7.24-29 (ポスター発表) .

3. 特許

4. 学会・シンポジウム等の開催状況

5. 受賞等

(1) 小西 彬仁 (博士 2 年)

ポスター賞 第 22 回基礎有機化学討論会、2011.9.21-23

6. 新聞報道等

(1) **Selected by the Editorial Board of SYNFACTS** (*Synfacts* **2011**, *12*, 1304)

Synthesis, Crystal Structure, and Physical Properties of Sterically Unprotected Hydrocarbon Radicals

Kubo, T.*; Katada, Y.; Shimizu, A.; Hirao, Y.*; Sato, K.; Takui, T.; Uruichi, M.; Yakushi, K.; Haddon, R. C.* *J. Am. Chem. Soc.* **2011**, *133*, 14240-14243.

7. 国民との科学・技術対話

- (1) 一般市民 15 名を対象とした授業 (サイエンスカフェ) を 2012 年 3 月 3 日に大阪大学総合博物館で行った。講師は久保孝史。講義時間は 90 分。アンケート有で評価点 (良 5 点~悪 1 点) は、5 点が 9 名、4 点が 6 名。

8. 領域内の共同研究の準備・実施状況とその成果

- (1) 共同研究先：物質・材料研究機構ナノ有機センター，三木一司グループ (A01 班，公募班員)

派遣人員 (派遣)：小西 彬仁 (博士 2 年)

派遣期間 (派遣)：2011.10.16-29

共同研究内容：フロー系二光子吸収を用いた芳香族縮環反応の開発

共同研究成果：種々の条件検討をおこなったが、縮環反応に適した条件を見つけることができなかった。