Organic Materials Chemistry

Shuichi Suzuki(Lecturer)

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1. Current Research and Principal Research Interests

Organic molecules with pi-conjugated open-shell electronic systems play an important role as components of functional molecular materials with conducting, magnetic, and novel electronic properties. Incorporation of heteroatoms, as a part of substituents or by replacing carbon atoms, is a promising way to control their electronic properties and intermolecular interactions. Synthesis is an initial key step for such new molecular materials. I am particularly interested in design and synthesis of the new heteroatom-incorporated open-shell molecules with extremely pi-conjugated system.

Herein, research topics related to my Ph.D thesis are described.
Title of my Ph.D thesis: Heteroatomic Effects on an Odd-Alternant pi-Electronic System: Syntheses and Properties of Nitrogen-Incorporated Phenalenyl Derivatives
Phenalenyl is a well-known odd-alternant hydrocarbon with high symmetry. It has a unique character to form three stable redox species, cation, neutral radical and anion, because of its non-bonding molecular orbital (NBMO). For this reason, phenalenyl derivatives have attracted a great deal of attention as good models to realize spin-mediated molecular functionality such as multi-stage amphoteric redox ability, high conductivity, and unique magnetic properties. Recent progress in phenalenyl chemistry has been especially noted since the first isolation of phenalenyl radical in the crystalline state by the preparation of 2,5,8-tri-tert-butylphenalenyl radical (TBPLY). We have designed and synthesized the tert-butylated 1,3-diazaphenalenyl (TBDAP) as the first stable heteroatom-incorporated phenalenyl radical, and clarified its electronic spin structure, and crystal structure. Furthermore, we have synthesized other nitrogen-incorporated phenalenyl derivatives.

2. Selected Publications

1. Shuichi Suzuki, Yasushi Morita, Kozo Fukui, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji, “Aromaticity on the Pancake-Bonded Dimer of Neutral Phenalenyl Radical as Studied by MS and NMR Spectroscopies and NICS Analysis”, J. Am. Chem. Soc., 128, 2530-2531 (2006).

2. Shuichi Suzuki, Yasushi Morita, Kozo Fukui, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji, “Hexaazaphenalenyl Anion Revisited: A Highly-Symmetric Planar π-System with Multiple-Networking Ability for Self-Assembled Metal Complexation”, *Inorg. Chem.*, **44**, 8197-8199 (2005).

3. Shuichi Suzuki, Yasushi Morita, Kozo Fukui, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji, “Effect of Methoxy Groups in a 1,3-Diazaphenalenyl π-System: Electronic-Spin Structure of 4,9-Dimethoxy-1,3-diazaphenalenyl”, *Polyhedron*, **24**, 2618-2624 (2005).

4. Yasushi Morita, Shuichi Suzuki, Shigeaki Nakazawa, Kozo Fukui, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji, “A Synthetic Study of Metal Complexes of Coordinated Neutral Radicals Based on an Azaphenalenyl System”, *Polyhedron*, **22**, 2215-2218 (2003).

5. Yasushi Morita, Kozo Fukui, Shuichi Suzuki, Takashi Aoki, Shigeaki Nakazawa, Koichi Tamaki, Akira Fuyuhiro, Kagetoshi Yamamoto, Kazunobu Sato, Daisuke Shiomi, Akira Naito, Takeji Takui, Kazuhiro Nakasuji, “Electronic-Spin and Columnar Crystal Structures of Stable 2,5,8-Tri-tert-butyl-1,3-diazaphenalenyl Radical”, *Polyhedron*, **22**, 2199-2204 (2003).

6. Yasushi Morita, Shuichi Suzuki, Junya Kawai, Shinsuke Nishida, Kozo Fukui, Kazunobu Sato, Daisuke Shiomi, Takeji Takui, Kazuhiro Nakasuji, “Generation and Properties of 2,5,8-Tri-tert-butyl-6-oxo-7,9-diazaphenalenyl”, *Synth. Met.* **137**, 1209-1210 (2003).

7. Yasushi Morita, Takashi Aoki, Kozo Fukui, Shigeaki Nakazawa, Koichi Tamaki, Shuichi Suzuki, Akira Fuyuhiro, Kagetoshi Yamamoto, Kazunobu Sato, Daisuke Shiomi, Akira Naito, Takeji Takui, Kazuhiro Nakasuji, “A New Trend in Phenalenyl Chemistry: A Persistent Neutral Radical, 2,5,8-Tri-tert-butyl-1,3-diazaphenalenyl, and the Excited Triplet State of the Gable syn-Dimer in the Crystal of Column Motif”, *Angew. Chem., Int. Ed.*, **41**, 1793-1796 (2002).