

# BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN

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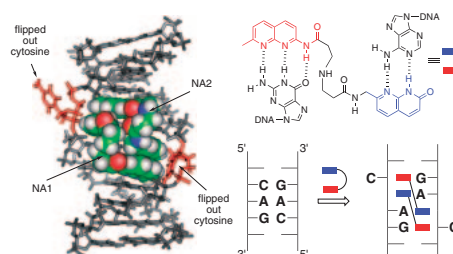
## Award Accounts

### The Chemical Society of Japan Award for Creative Work for 2007

#### Recognition of Mismatched Base Pairs in DNA

K. Nakatani

Mismatch binding ligand (MBL) selectively binds to mismatched base pairs with discrimination of the nucleotide bases. This review focuses on the inside story regarding the molecular design of MBL and its function, and potential application in genomic science.



*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
1055–1069

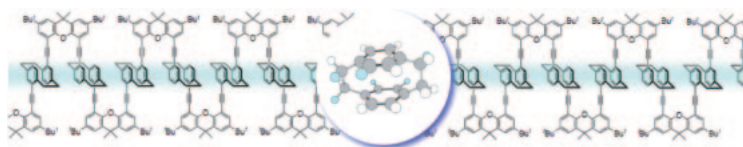
## Award Accounts

### The Chemical Society of Japan Award for Young Chemists for 2007

#### Synthesis of $\pi$ -Stacked Polymers on the Basis of [2.2]Paracyclophane

Y. Morisaki\* and Y. Chujo\*

We have synthesized  $\pi$ -stacked polymers by incorporating [2.2]paracyclophane units into the conjugated polymer backbones and developed corresponding through-space-conjugated polymers, dendrimers, polymethylenes, and aromatic-ring-layered polymers.



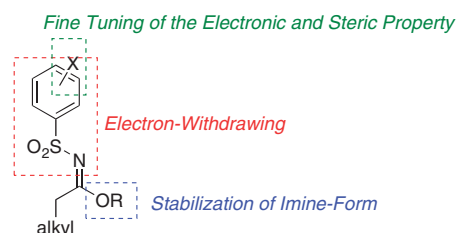
*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
1070–1082

## BCSJ Award Article

#### Catalytic Mannich-Type Reactions of Sulfonylimidates

R. Matsubara, F. Berthiol, H. V. Nguyen,  
and S. Kobayashi\*

DBU-catalyzed reactions of sulfonylimidates with protected imines in DMF provided the adducts in high yields with high anti selectivity. The reactions catalyzed by  $\text{Mg}(\text{O}^t\text{Bu})_2$  in DMF provided the adducts with high anti selectivity, while those catalyzed by  $[\text{Sr}(\text{HMDS})_2]_2$  gave syn selectivity.



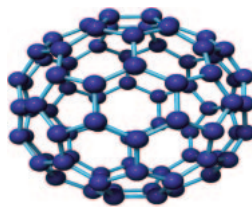
*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
1083–1102

### A New Simple Method for Maturity of Finite Groups and Application to Fullerenes and Fluxional Molecules

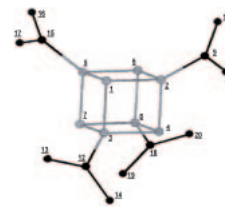
A. Moghani

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1103–1106

A simple method to specify how a given finite group is matured or unmatured is introduced via some useful examples such as a polyhex nanotorus. The  $Q$ -conjugacy character tables of the fullerene  $C_{80}$  and tetranitrocubane are then verified.



The big Fullerene  $C_{80}$



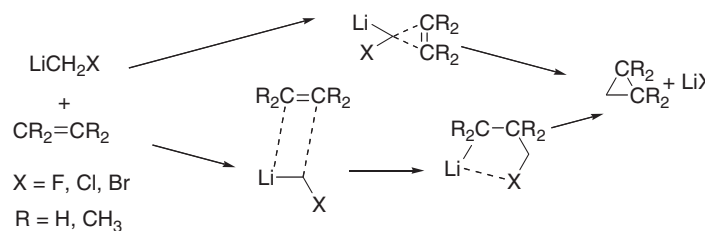
The structure of tetranitrocubane

### Cyclopropanation Reactions of Halomethyl-lithium Carbenoids: A Computational Study of the Effects of Aggregation and Solvation

L. M. Pratt,\* P. T. T. Trần, N. V. Nguyễn, and B. Ramachandran\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1107–1125

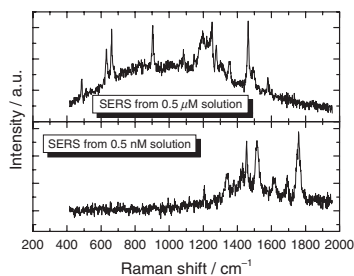
Computational results are presented to support experimental evidence that cyclopropanation reactions of halomethyl-lithium carbenoids with alkenes occur through the concerted (methylene transfer) pathway rather than the alternate stepwise (carbometalation) pathway.



### Identification of Thiocyanine J-aggregates Adsorbed on Single Silver Nanoaggregates by Surface-Enhanced Raman Scattering and Emission Spectroscopy

Y. Kitahama,\* Y. Tanaka, T. Itoh, M. Ishikawa, and Y. Ozaki

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1126–1132



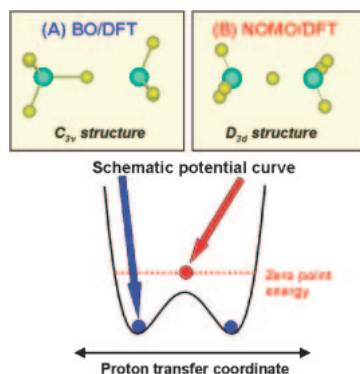
SERS spectra of single Ag nanoaggregates adsorbed by thiocyanine dyes in concentrated and diluted aqueous solutions (top and bottom, respectively). The concentration dependent SERS and background emission spectra are associated with whether J-aggregates are formed or not.

## Selected Paper

### Extension of Density Functional Theory to Nuclear Orbital plus Molecular Orbital Theory: Self-Consistent Field Calculations with the Colle–Salvetti Electron–Nucleus Correlation Functional

Y. Imamura, Y. Tsukamoto, H. Kiryu, and H. Nakai\*

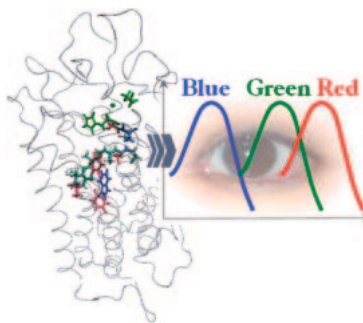
*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1133–1139



This study presents a novel methodology for non Born–Oppenheimer self-consistent field calculations including not only the electron–electron ( $e$ – $e$ ) exchange–correlation but also electron–nucleus ( $e$ – $n$ ) correlation energies, as denoted by NOMO/DFT. The NOMO/DFT method can reproduce the correct structures of “vibrational bonding” systems such as ammoniated ammonium ion ( $N_2H_7^+$ ). (A) BO/DFT and (B) NOMO/DFT refer to the structures optimized with and without nuclear quantum effects, respectively.

### Color Tuning Mechanism of Human Red, Green, and Blue Cone Pigments: SAC-CI Theoretical Study

K. Fujimoto, J. Hasegawa, and H. Nakatsuji\*

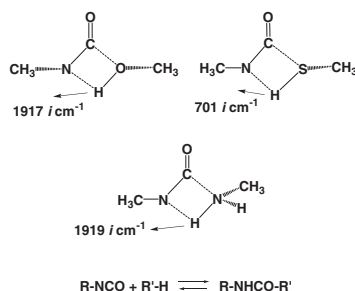


Origin of color tuning in human cone pigments has been clarified by using the SAC-CI and QM/MM methods. The absorption energies are controlled by protein-electrostatic potentials from amino acids at specific positions, suggesting some genetic origins for color tuning.

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1140–1148

### Reaction Paths toward Isocyanate Adducts

M. Hatanaka



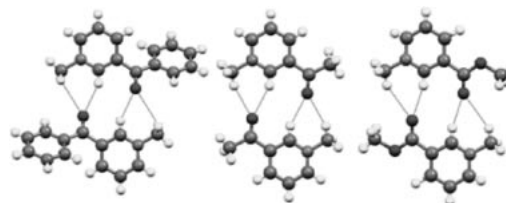
Addition reactions of isocyanates were theoretically investigated by using model compounds for urethanes, thiourethanes, and ureas. The transition states were characterized as hydrogen-transfer processes, and thermodynamic analyses were consistent with experimental results.

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1149–1151

### Substituent Effects on Formation of Cation Dimers by Weak Hydrogen Bonds in Crystals of Carbonyl Pyridinium Salts of Ni(dmit)<sub>2</sub>

K. Tomono,\* A. Koyano, T. Morita, and K. Miyamura

Ability to form dimers by weak C–H...O hydrogen bonds was found to depend on the electronic properties of the substituents in the crystal of metal complex salt.



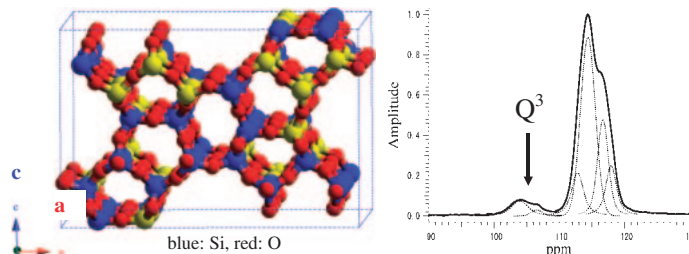
Three dimers constructed by C–H...O hydrogen bonds

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1152–1159

### Quantitative Analysis of Structural Defect in Silicalite by Rietveld Refinements Using X-ray Powder Diffraction and <sup>29</sup>Si MAS NMR

M. Inui, T. Ikeda,\* T. Suzuki, K. Sugita, and F. Mizukami

The distribution of Si atom defects in a silicalite optimized for the vapor-phase Beckmann rearrangement process was investigated by using PXRD and <sup>29</sup>Si MAS NMR techniques. The defect atoms (yellow balls) were observed as Q<sup>3</sup> resonances in the <sup>29</sup>Si MAS NMR spectrum.



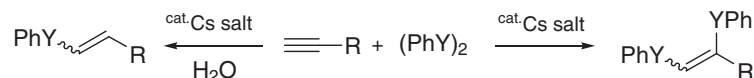
*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1160–1169

### Cesium Salt-Catalyzed Addition of Diphenyl Dichalcogenides to Alkynes: Selective Synthesis of Bis- and Mono(phenylchalcogeno)alkenes

Y. Nishiyama,\* H. Ohnishi, and Y. Koguma

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1170–1174

A cesium salt has a unique catalytic ability for the reaction of bis(alkynes with diphenyl dichalcogenides to give the corresponding *vic*-bis(phenylchalcogeno)alkenes in moderate to good yields. When H<sub>2</sub>O was added to the reaction medium, the monophenylchalcogenation of the alkynes occurred giving phenylchalcogenoalkenes in moderate yields.

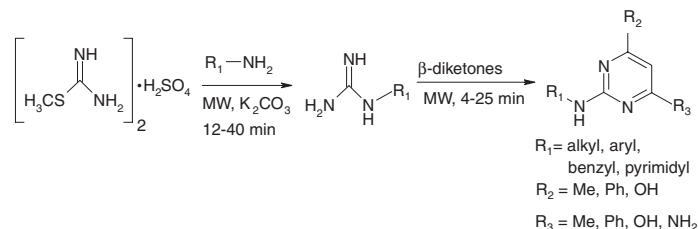


### One-Pot Two-Step Solvent-Free Rapid and Clean Synthesis of 2-(Substituted Amino)-pyrimidines by Microwave Irradiation

S. Goswami,\* A. Hazra, and S. Jana

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1175–1181

A series of various 2-(substituted amino)pyrimidines has been synthesized in a one-pot two-step microwave procedure, initially by the reaction of (*S*)-methylisothiurea sulphate with different amines followed by condensation with various  $\beta$ -diketones under solid-phase and catalyst-free conditions.

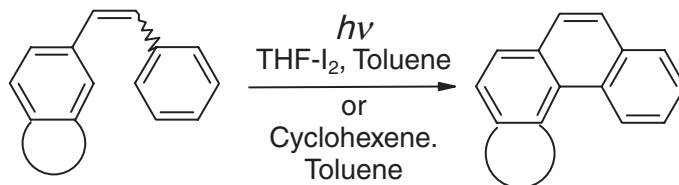


### Synthesis of Derivatives of Phenanthrene and Helicene by Improved Procedures of Photocyclization of Stilbenes

H. R. Talele, M. J. Gohil, and A. V. Bedekar\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1182–1186

Photocyclization of stilbenes is carried out with I<sub>2</sub>-THF in place of propylene oxide or with cyclohexene as an oxidant.

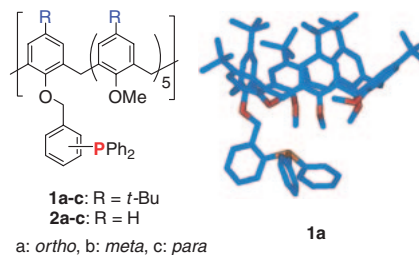


### Synthesis and Structural Characterization of a Series of Mono-*O*-(diphenylphosphinobenzyl)-calix[6]arenes with and without *tert*-Butyl Moieties at the Upper Rim

T. Fujihara, S. Kubouchi, Y. Obora, M. Tokunaga, K. Takenaka, and Y. Tsuji\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1187–1193

A series of mono-*O*-(diphenylphosphinobenzyl)calix[6]arene ligands with the *tert*-butyl groups at the upper rim (**1**) and without the *tert*-butyl moieties (**2**) were synthesized, characterized, and used in rhodium-catalyzed hydroformylation.

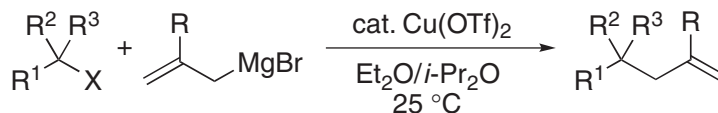


**Copper-Catalyzed Allylation of Alkyl Halides with Allylic Grignard Reagents**

M. Sai, H. Yorimitsu,\* and K. Oshima\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1194–1196

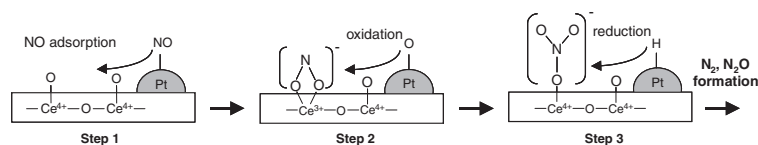
Treatment of alkyl halides, including secondary and tertiary alkyl bromides, with allylic Grignard reagents in the presence of a catalytic amount of copper(II) triflate in diisopropyl ether at 25 °C yielded the corresponding allylated products in high yields.

**Lean NO<sub>x</sub> Reduction by Hydrogen over Pt-Supported Rare Earth Oxide Catalysts and Their In Situ DRIFTS Study**

M. Itoh, K. Motoki, M. Saito, J. Iwamoto, and K. Machida\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1197–1202

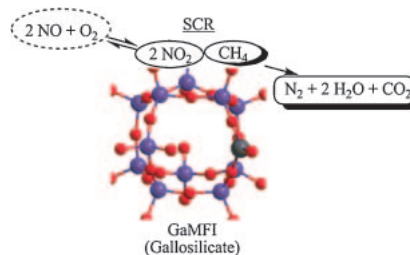
Only Pt/CeO<sub>2</sub> possessed good activity for H<sub>2</sub>-SCR of NO<sub>x</sub> in a series of rare earth oxide used as a support. NO<sub>x</sub> reduction could proceed through hydrogen attack to the adsorbed nitrate species as suggested from DRIFTS study.

**Gallosilicate-Based Catalysts for NO<sub>x</sub>-SCR with CH<sub>4</sub>**

K. Nagashima, S. Nakamura, K. Okada, A. Nakahira, and H. Aritani\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1203–1208

Ga-incorporated H-MFI (GaMFI) metallosilicate catalysts show robust activity for selective catalytic reduction of NO<sub>x</sub> (NO<sub>x</sub>-SCR) with CH<sub>4</sub>. Local structure around Ga in GaMFI is very stable, but distorted Si-O<sub>4</sub> local structure is formed after the NO<sub>x</sub>-SCR with CH<sub>4</sub>.

**A Comparative Study on the Formation and Spectral Properties of the Polypseudo-rotaxanes of β-Cyclodextrin and Poly(propylene glycol) under Different Conditions**

X. Q. Guo, L. X. Song,\* Z. Dang, and F. Y. Du

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 1209–1213

The different preparation methods result in different host-guest stoichiometries, molecular stacking forms, and thermal stabilities of polypseudo-rotaxanes.

