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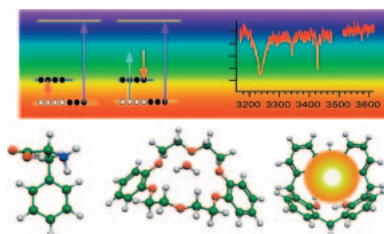
## Award Accounts

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

#### Study on the Structure and Vibrational Dynamics of Functional Molecules and Molecular Clusters by Double Resonance Vibrational Spectroscopy

T. Ebata

Development of double resonance vibrational spectroscopy and its application to molecular clusters and functional molecules are described. Conformer and size-selective vibrational spectroscopic study in frequency and time domain reveals the detailed structures as well as the dynamics of the clusters.



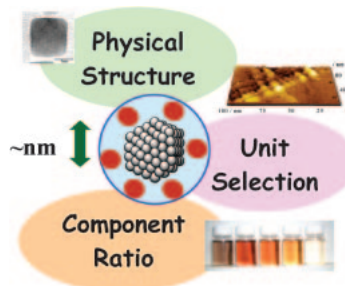
*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
127–151

## Award Accounts

### The Chemical Society of Japan Award for Young Chemists for 2006

#### Synthesis of Organic Shell–Inorganic Core Hybrid Nanoparticles by Wet Process and Investigation of Their Advanced Functions

M. Yamada



This account reviews the synthesis of inorganic nanoparticles stabilized by organic layers with electronic, optical, catalytic, and magnetic properties. The compounds are Pt nano-cube, size-selected Au nanoparticles, metal coordination nano-polymers, and metal nanoparticles functionalized with biferrocene, anthraquinone, and triphenylene derivatives.

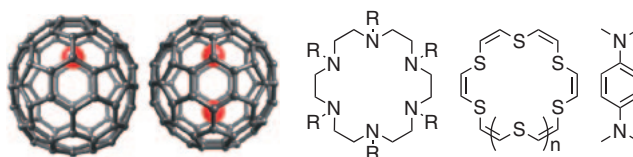
*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
152–170

## Accounts

#### Construction of Supramolecular Systems Based on Endohedral Metallofullerenes

T. Tsuchiya, T. Akasaka,\* and S. Nagase

Endohedral metallofullerenes are revealed to form an inclusion complex with azacrown ethers and unsaturated thiocrown ethers by electron transfer between them, and a stimuli-responsive reversible electron transfer system is constructed by using endohedral metallofullerenes and organic donors.



*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
171–181

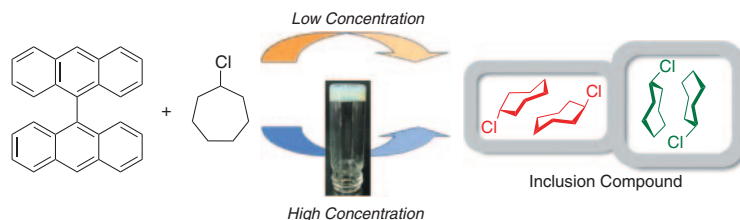
## BCSJ Award Article

### Molecular Structure of Chlorocycloheptane in Inclusion Compound with 9,9'-Bianthryl and Gelation during Crystallization

S. Toyota,\* Y. Okamoto, T. Ishikawa,  
T. Iwanaga, and M. Yamada

*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
182–186

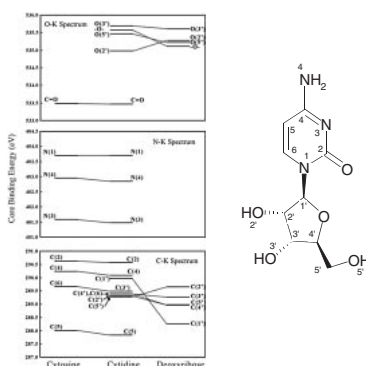
9,9'-Bianthryl formed an inclusion compound with chlorocycloheptane in a 2:1 ratio, where two guest molecules are accommodated in each cavity in either of two twist-chair forms. Under certain conditions, the gelation was followed by crystallization.



### Density Functional Study on Core Ionization Spectra of Cytidine and Its Fragments

A. Thompson, S. Saha, F. Wang,\*  
T. Tsuchimochi, A. Nakata,  
Y. Imamura, and H. Nakai\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
187–195

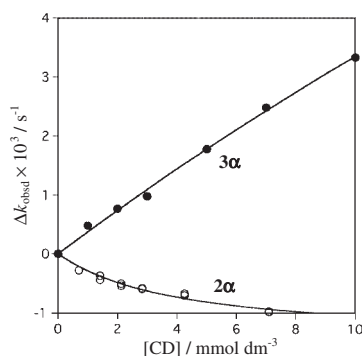


The sugar–base correlation of cytosine (base) and deoxyribose (sugar) moieties of cytidine is investigated based on their inner-shell electronic structural information using CV-B3LYP and LB94 DFT models.

### Binding and Catalytic Properties of 2-O- and 3-O-Permethyated Cyclodextrins

T. Nagata, K. Yoshikiyo,  
Y. Matsui, and T. Yamamoto\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
196–201

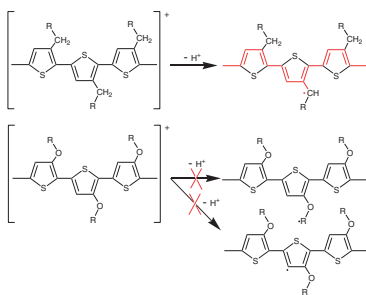


Hexakis(3-*O*-methyl)- $\alpha$ -cyclodextrin (**3 $\alpha$** ) accelerated and hexakis(2-*O*-methyl)- $\alpha$ -cyclodextrin (**2 $\alpha$** ) decelerated the cleavage of *m*-nitrophenyl acetate in an alkaline solution, suggesting that the C(2)-OH of  $\alpha$ -cyclodextrin is more catalytic than the C(3)-OH.

### Stability of a Conductive State of Poly(3-alkoxythiophene)s

K. Hatakeyama, H. Koizumi,\*  
and T. Ichikawa

*Bull. Chem. Soc. Jpn.* **2009**, *82*,  
202–205

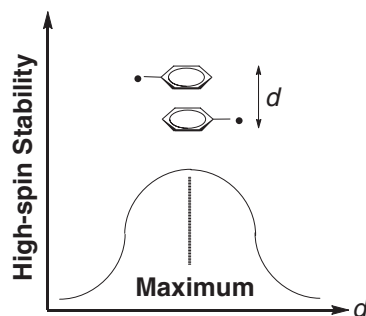


Conductive states of poly(3-alkylthiophene)s cause dedoping through deprotonation of polarons resulting in formation of stable polyenyl radicals. In contrast, the deprotonation of polarons of poly(3-alkoxythiophene)s (P3AOT) occurs with difficulty since their deprotonation gives unstable radicals. Conductive states of P3AOT are hence stable.

### Magnetic Ordering in Organic-Radical Assemblies. II

M. Hatanaka\* and R. Shiba

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 206–215



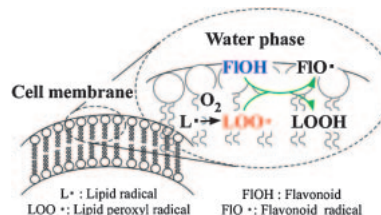
Intermolecular-distance dependence on ferromagnetic interactions in organic-radical assemblies was deduced by using localized non-bonding molecular orbitals (NBMOs). The high-spin stabilities had maxima when the magnitude of intra- and intermolecular resonance integrals was nearly equal.

### Tunneling Effect in Antioxidant Reaction of Flavonoid

T. Kakiuchi,\* K. Mukai, K. Ohara, and S. Nagaoka

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 216–218

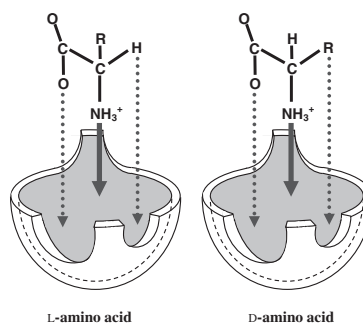
A study of the kinetics of the proton-transfer reaction of flavonoid in ethanol solution by means of stopped-flow spectroscopy indicated that proton tunneling plays an important role in the antioxidant reaction.



### Structural Requirement for Chiral Recognition of Amino Acid by (18-Crown-6)-tetracarboxylic Acid: Binding Analysis in Solution and Solid States

H. Nagata,\* Y. Machida, H. Nishi, M. Kamiguchi, K. Minoura, and T. Ishida

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 219–229



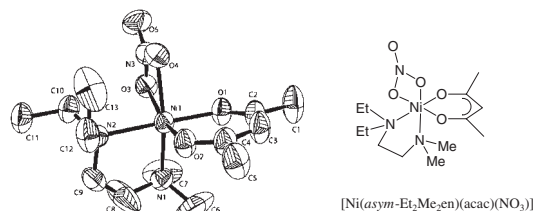
We discuss in this report the mechanism of chiral separation of amino acids by (+)-18C6H<sub>4</sub> based on the results of molecular conformation of (+)-18C6H<sub>4</sub> and its interaction mode with amino acids in solid and solution states.

### Alkyl-Substitution Effect of the Diamine on Coordination Geometry and Ligand-Field Strength of Nickel(II) Mixed-Ligand Complexes Containing N-Alkylethylenediamine, Acetylacetonate, and Nitrate Ligands

H. Shirase, M. Saito, M. Arakawa-Itoh, and Y. Fukuda\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 230–235

In mixed-ligand nickel(II) complexes, [Ni(Et<sub>x</sub>Me<sub>4-x</sub>en)(acac)(NO<sub>3</sub>)], where acac = acetylacetonate, x = 0–4, the increase of ethyl groups decreases the ligand-field stabilization energy and enhances the ionic dissociation of NO<sub>3</sub><sup>-</sup> in nitromethane solution due to the increase in inter-ligand repulsion.



### Tropolone-Terminated Oligomeric Fluorophores with Responsive Properties to External Environment

K. Takagi,\* K. Saiki, H. Hayashi, H. Ohsawa, S. Matsuoka, and M. Suzuki

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 236–241

Three tropolone-terminated oligomeric fluorophores were prepared by palladium-catalyzed coupling reaction to investigate their optical properties and coordination ability to metal ions. For example, Tp2OP showed positive solvatochromic behavior due to charge transfer of the emitting state.

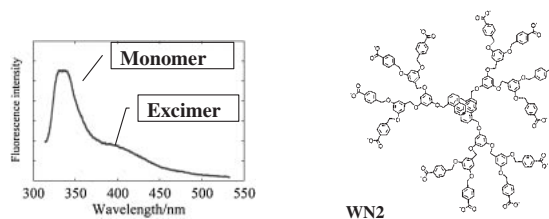


### Fluorescence Characteristics of Naphthalene Dendrimers at Low Concentration in Aqueous Solution

R. Akatsuka, Y. Shinohara, T. Sato, Y. Nishimura, and T. Arai\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 242–248

The first excimer fluorescence of naphthalene moiety was observed at very low concentration ( $5.0 \times 10^{-6}$  M) by introducing dendritic structure.

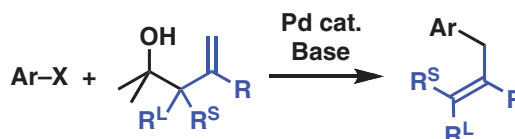


### Synthesis of Prenylarenes and Related (Multisubstituted Allyl)arenes from Aryl Halides and Homoallyl Alcohols via Palladium-Catalyzed Retro-Allylation

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

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 249–253

The reactions of aryl halides with 2,3,3-trimethyl-4-penten-2-ol in the presence of a palladium catalyst result in prenyl transfer from the alcohol to aryl halides via retro-allylation, yielding prenylarenes.

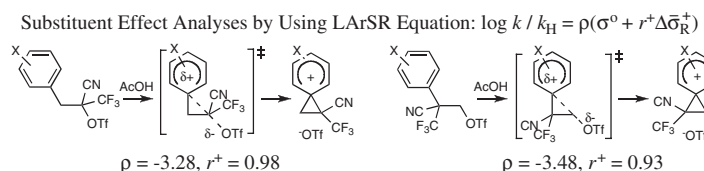


### Exalted Resonance Demands in the Substituent Effects on the Acetolyses of 2-Arylethyl Trifluoromethanesulfonates Destabilized by CN and CF<sub>3</sub> Groups

S. Usui,\* S. Tsuboya, Y. Umezawa, K. Hazama, and M. Okamura

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 254–260

Extremely large  $r^+$  values of 0.98 and 0.93 were obtained in the substituent effect on the acetolyses of 2-aryl-1-cyano-1-(trifluoromethyl)ethyl trifluoromethanesulfonates and 2-aryl-2-cyano-2-(trifluoromethyl)ethyl trifluoromethanesulfonates, respectively. These  $r^+$  values suggest strong participation of the  $\beta$ -aryl group in deactivated aryl-assisted solvolyses.

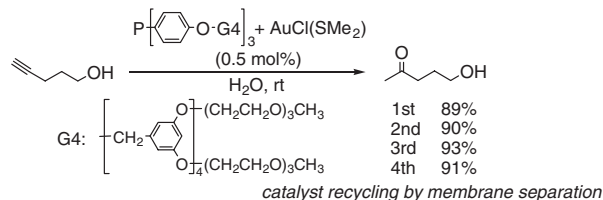


### Synthesis of Water-Soluble Dendritic Phosphine Ligands and Their Application to Hydration of Alkynes in Aqueous Media

K. Fujita,\* M. Kujime, and T. Muraki

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 261–266

By employing the water-soluble phosphine–gold(I) dendrimers as a catalyst, hydration of alkynes proceeded smoothly. Furthermore, by membrane separation based on the nano-order size of the dendritic catalyst, the gold(I) catalyst was recycled without deactivation.

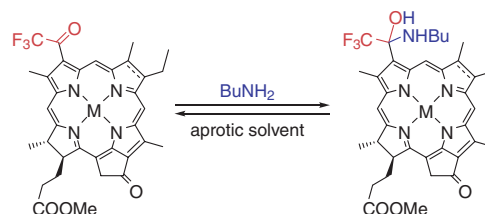


### Chlorophyll- and Bacteriochlorophyll-Derived Colorimetric Chemosensors for Amine Detection

S. Sasaki, Y. Kotegawa, and H. Tamiaki\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 267–271

A trifluoroacetyl group was introduced on a chlorin or bacteriochlorin skeleton to develop new chromoreceptors for amine detection. The chemosensors showed visual color changes by the formation of  $\alpha$ -amino alcohol adducts.

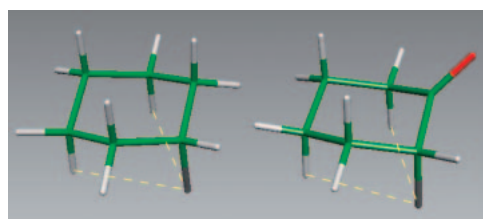


### The Origin of the Relative Stability of Axial Conformers of Cyclohexane and Cyclohexanone Derivatives: Importance of the CH/n and CH/ $\pi$ Hydrogen Bonds

O. Takahashi,\* K. Yamasaki, Y. Kohno,\*  
K. Ueda, H. Suezawa, and M. Nishio\*

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 272–276

MO calculations were carried out to investigate the Gibbs energy of conformational isomers of substituted cyclohexanes and cyclohexanones. The conformer bearing an oxygen or halogen atom at the axial orientation is relatively stable as compared to corresponding alkyl cyclohexanes.



### Photochemical Removal of NO, NO<sub>2</sub>, and N<sub>2</sub>O by 146 nm Kr<sub>2</sub> Excimer Lamp in N<sub>2</sub> at Atmospheric Pressure

M. Tsuji,\* N. Kamo, T. Kawahara,  
M. Kawahara, M. Senda,  
and N. Hishinuma

*Bull. Chem. Soc. Jpn.* **2009**, *82*, 277–284

