## **Chemistry Letters**

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## **Highlight Review**

780	Theoretical	Calculations	on	Electronic
	Structure and Catalytic Reaction of Orga-			
	no-f-element Complexes			

The optimized geometry structure of Cp<sub>2</sub>LnX(THF) (Cp = cyclopentadienyl, THF = tetrahydrofuran, Ln = La-Lu and X = halides. Unmarked white and gray balls represent hydrogen and carbon, respectively. The arrow indicates the direction of dipole moment.) In this article, the very recent theoretical calculations on organo-f-element complex are outlined.



Yi Luo, Parasuraman Selvam, Michihisa Koyama, Momoji Kubo, and Akira Miyamoto

The use of lanthanide complexes as catalysts in organic synthesis is currently of intense interest. In particular, organolanthanide complexes are of rapidly growing importance, and hence the understanding of the binding behavior of f orbital as well as the ionic/covalent characteristics of lanthanocene-based complexes is of significance with respect to their reactivity and their role as catalyst in organic synthesis. The purpose of this review is to give a survey of recent progress in theoretical studies on organo-f-element complexes and to highlight successful applications of density functional and quantum chemical molecular dynamics methods.

## Letter





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Atsushi Asano, Miho Shimizu, and Takuzo Kurotsu

We examined the effect of the paramagnetic  $Fe^{3+}$  ions on the <sup>1</sup>H spin-lattice relaxation time  $(T_1^{H})$  for PVA/montmorillonite-clay nanocomposites indirectly observed from the conventional <sup>13</sup>C CPMAS NMR. Rapid decrease of the  $T_1^{H}$  values with the amount of montmorillonite clay was observed for the nanocomposites, while for a PVA/saponite nanocomposite including no Fe<sup>3+</sup> ions such a decrease was not detected. This decrease relates on both amount of the paramagnetic Fe<sup>3+</sup> ions and dispersion of clay in nanocomposites. By analyzing the effect of Fe<sup>3+</sup> ions on  $T_1^{H}$  quantitatively, we found that the dispersion and amount of iron for clay are detectable in a nanocomposite nondestructively.





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838 Synthesis of Artificial Opals with Uniform Mesoporous Silica Spheres



uniform mesoporous silica spheres.

Chau-Nan Chen, Hong-Ping Lin, Chih-Pin Tsai, and Chin-Yuan Tang

840 Preparation of Water-soluble PEGylated Semiconductor Nanocrystals



Eui-Chul Kang, Atsuhiko Ogura, Kazunori Kataoka, and Yukio Nagasaki

842 Template-Directed Electrodeposition of Lamellar Platinum Nanostructures



Ji K. Zhao, Xiao Chen, Li Y. Jiao, Yong C. Chai, Guo D. Zhang, and Jie Liu

844 **Reversible Optical Rotation Change Accord**p-toly p-tolyl ing to the Enantiospecific Photochromic Reaction of [2.2]Metacyclophan-1-ene С 0 UV Me Bu Vis Bu BL. Me Bu Mè  $[\alpha]_{750} = -2050^{\circ}$  $[\alpha]_{750} = -470^{\circ}$ Michinori Takeshita and Takehiko Yamato 846 Preparation of Deuterium Labelled Organophosphonium Salts (Wittig Salts) under Hydrothermal Condition Catalyzed by D<sub>2</sub>O, Molecular Sieves **Molecular Sieves** 250 °C/ 4 MPa, 2 h Ph<sub>3</sub>PCH<sub>2</sub>R Ph<sub>3</sub>PCD<sub>2</sub>R or D<sub>2</sub>O, Molecular Sieves MW (180 °C/1.2 MPa), 0.5 h Mitsuru Yamamoto, Koichiro Oshima, and Seijiro Matsubara



Chi Yang and Wing-Tak Wong

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plane layers. The H-bonds garph set present in the zigzag ribbons are  $R_2^2(8)$ [α],  $R_2^{-1}(6)$  [β],  $R_2^{-2}(10)$  [γ],  $R_1^{-2}(6)$  [δ],  $R_2^4(12)$  [X],  $R_5^3(10)$  [ $\Omega$ ],  $R_8^6(24)$  [ $\Psi$ ] and  $R_8^4(24)$  [Φ].



858 Copolymerization of Aziridines and Carbon Monoxide Catalyzed by a Heterodinuclear Organopalladinum–Cobalt Complex

Heterodinuclear organopalladium-cobalt complex having a 2,2'-bipyridine ligand (bpy)AcPd–Co(CO)<sub>4</sub> catalyzes copolymeriztion of unsubstituted and both *C*- and *N*-monosubstituted aziridines, such as aziridine, 2-methylaziridine, and *N*-ethylaziridine, and CO (3–6 MPa) in THF at 100 °C for 6 h.

(bpy)AcPd-Co(CO)<sub>4</sub> (3 mol%)

THF, 100 °C, 6 h

со

5 MPa



860 Templated Assembly of a Monolayer Consisting of a Coordination Nanobox at Air-Water Interface



81%

Masaru Aoyagi, Hiroyuki Minamikawa, and Toshimi Shimizu

862 Solvatochromic Shift of Phthalocyanine Q-band Governed by a Single Solvent Parameter

Solvatochromic shift of Q-band for some octahedral phthalocyanine complexes is governed only by refractive index of the solvent, indicating that interaction of phthalocyanine transition dipole moment and induced dipole moment generated in the surrounding solvent molecules is predominant.



Hiroaki Isago, Yutaka Kagaya, and Akiyuki Matsushita

864 S<sub>N</sub>2 Type Hydrolysis of Secondary Alkyl Halides and Sulfonates in Hydrothermal Water



Yuki Yamasaki, Takaharu Hirayama, Koichiro Oshima, and Seijiro Matsubara

866 Soluble Polymer-supported Synthesis of trans  $\beta$ -Lactams with High Diastereoselectivity

High diastereoselective synthesis of *trans*  $\beta$ -lactams on PEG was accomplished by introducing an auxiliary.



Shan-Zhong Jian and Yan-Guang Wang



Insertion into a Carbon-Carbon Single Bond

Eight-membered ring ketones can be synthesized in a single chemical operation through a fivemembered acylrodium intermediate generated from 2-(o-styryl)cyclobutanones.

Takanori Matsuda, Atsushi Fujimoto, Mitsuru Ishibashi, and Masahiro Murakami

C-103







- 892 Synthesis of Novel Spiro-condensed Dithienosiloles and the Application to Organic FET
  - Joji Ohshita, Kwang-Hoi Lee, Daisuke Hamamoto, Yoshihito Kunugi, Junnai Ikadai, Young-Woo Kwak, and Atsutaka Kunai

Xianhong Wen, Ming Guo, Ziyang Liu, and Fei

Tan

894 Nanotube Formation in Solution between  $\beta$ -Cyclodextrin and Cinchonine



Me<sub>2</sub>Si

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888 Solid Phase Synthesis of Hydroxy Benzothiazepinones through Cyclative Release under Thermolysis



-SiMe<sub>3</sub>

doped-S

۱u u

Gelation

i<sub>d</sub>/µA

0

=-100 V

80V

60V

222888888<sup>-40V</sup>

-20 -40 -60 -80 -100

 $V_{\rm d}$  / V

H. M. Sampath Kumar, P. Pawan Chakravarthy, M. Shesha Rao, Sipak Joyasawal, and J. S. Yadav

890 Complex Formation and Gelation between Copolymers Containing Pendant Azobenzene Groups and Cyclodextrin Polymers



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OMe



Tomoki Yamasaki, Nobutaka Ozaki, Yasunari Saika, Kozo Ohta, Kenji Goboh, Fumiko Nakamura, Masato Hashimoto, and Seichi Okeya

930

934

936

First transition metal complexes of 1,8-bis(dimethylamino)naphthalene (protone sponge) were synthesized.



932

