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CONTENTS

PART I　ANNUAL REPORTS

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1. Abstracts of Papers Published in Journals

MATHEMATICS

Involutions and Semiinvolutions

H. Ishibashi
Czechoslovak Mathematical Journal, **56** (131), 533–541 (2006)

As a generalization of the concept of involutions we define a new type of linear transformations called semiinvolutions, and show that any nilpotent linear endomorphism is a product of an involution and a semiinvolution. We also give a new proof for Djocovićs' theorem on a product of two involutions.

Length Problem for Automorphisms of Modules over local rings

H. Ishibashi
Linear Algebra and its Applications, **418**, 269–276 (2006)

Let R be a local ring and M a free module of a finite rank over R. We shall show that for any $\sigma \in \mathrm{Aut}_R M$ there exist a basis X for M and $\rho \in \mathrm{Aut}_R M$ such that ρ acts as a permutation on X and $\rho^{-1}\sigma$ is a product of m or less than m simple elements in $\mathrm{Aut}_R M$, where m is the order of the invariant factors of σ modulo the maximal ideal of R.

Relative invariants of 2-simple prehomogeneous vector spaces of type I

Tatsuo Kimura*[1], Takeyoshi Kogiso, Kazunari Sugiyama*[1] (*1 Institute of Mathematics, University of Tsukuba, Ibaraki 305–8571, Japan. Received 16 February 2006 Available online 30 June 2006 Communicated by Masaki Kashiwara)
Journal of Algebra, **308**, 445–483 (2007)

In the present paper, by using equivariant maps, we construct explicitly relative invariants of the 2-simple prehomogeneous vector spaces of type I, which are classified in [T. Kimura, S. Kasai, M. Inuzuka, O. Yasukura, A classification of 2-simple prehomogeneous vector spaces of type I, J. Algebra 114 (1988) 369–400]. This is a continuation of our previous work [T. Kogiso, G. Miyabe, M. Kobayashi, T. Kimura, Non-regular 2-simple prehomogeneous vector spaces of type I and their relative invariants, J. Algebra 251 (2002) 27–69; T. Kogiso, G. Miyabe, M. Kobayashi, T. Kimura, Relative invariants of some 2-simple prehomogeneous vector spaces, Math. Comp. 72 (2003) 865–889]. 2006 Elsevier Inc. All rights reserved. Keywords: 2-Simple prehomogeneous vector spaces; Relative invariants.

薄い液膜中のオストワルド熟成

安田英典，松本昌昭*（* 三菱総合研究所）
日本応用数理学会論文誌，Vol. 16, No. 4, 359-370（2006）

We study phenomena called Ostwald ripening in a thin liquid film by a numerical method. Droplets such as oil-water system in a thin film disappear or grow slowly. We simulate these phenomena by the invariant finite difference scheme of the two-phase shallow water equations. We show that difference of chemical potential between surface of droplets and outside of droplets plays an important role, and we also evaluate the speed of the flow outside droplets by the reductive perturbation method.

On the steadily rotating spirals

J.-S. Guo*[1], K.-I. Nakamura*[2], T. Ogiwara and J.-C. Tsai*[3] (*1 Department of Mathematics, National Taiwan Normal University, *2 Department of Computer Science, University of Electro Communications, *3 Department of Computer Science, National Taiwan Ocean University)
Japan Journal of Industrial and Applied Mathematics, **23**, 1-19 (2006)

We study an autonomous system of two first order ordinary differential equation. This system arises from a model for steadily rotating spiral waves in excitable media. The sharply located spiral wave fronts are modeled as planar curves. Their normal velocity is assumed to depend affine linearly on curvature. The spiral tip rotates along a circle with a constant positive rotation frequency. The tip neither grows nor retracts tangentially to the curve. With rotation frequency as a parameter, we obtain the complete classification of solutions of this system. Besides providing another approach to derive the results obtained by Fiedler-Guo-Tsai for spirals with positive curvature, we also obtain many more different solutions. In particular, we obtain spiral wave solutions with sign-changing curvature and with negative curvature.

CHEMISTRY

Infrared diode laser spectroscopy of the $\Delta\nu = 2$ band of AlF

Koui Horiai, Hiromichi Uehara
Spectrochim. Acta, **A63**, 1009-1012 (2006)

A vibrational-rotational spectrum of the $\Delta\nu = 2$ transitions of a high-temperature molecule AlF was observed between 1490 and 1586 cm^{-1} with a diode laser spectrometer. Measurements were made on the $\nu = 3-1$, $4-2$, $5-3$ and $8-6$ bands at a temperature of

900℃. Measured spectral lines were fitted to effective band constants ν_0, B_ν and D_ν for each band. Present measurements were made with only one Pb-salt laser diode. Physical significance of the effective band constants is discussed.

Infrared Spectroscopy of Ne–^{12}C^{18}O$_2$ and Xe–^{12}C^{18}O$_2$: Change in the CO$_2$ Intramolecular Potential by Formation of Rare Gas-CO$_2$ Complexes

T. Konno, S. Fukuda, Y. Ozaki
Chem. Phys. Lett., **421**, 421–426 (2006)

High-resolution infrared spectra of neon-carbon dioxide (^{12}C^{18}O$_2$) and xenon-carbon dioxide (^{12}C^{18}O$_2$) have been observed in the ν_3 band (2314 cm^{-1}) region of ^{12}C^{18}O$_2$ by diode laser absorption spectroscopy of a pulsed molecular beam. The vibrational band origins and rotational constants for these complexes are obtained and vibrationally averaged structures are derived. The observed shifts of the ν_3 band origin for Rg–CO$_2$ (Rg = Ne, Ar, Kr, Xe) with respect to that of CO$_2$ exhibit a systematic of ^{16}O–^{18}O isotope effect excepting a significant deviation for Ne–CO$_2$ from a regular trend. This apparent anormaly is interpreted in terms of a change in the intramolecular potential function of CO$_2$ caused by rare gas-carbon dioxide complex formation.

Localization of Conduction Electrons and the Magnetic Properties of the Molecular Metals β''–(BEDF–TTF)$_4$NH$_4$[M(C$_2$O$_4$)$_3$]DMF(M = Cr^{3+}, Fe^{3+})

R. B. Morgunov[*1, *2], R. P. Shibaeva[*1], E. B. Yagubskii[*2], T. Kato and Y. Tanimoto[*3] (*1 Institute of Solid state Physics, Russian Academy of Sciences, *2 Institute of Problems in Chemical Physics, Russian Academy of Sciences, *3 Hiroshima University)
J. of Ex. and Theo. Phys., **102** (1), 121–130 (2006)

The Quasi-two-dimensional organic metal β''–(BEDF–TTF)$_4$NH$_4$[M(C$_2$O$_4$)$_3$]・DMF containing the oxalate complexes of Cr^{3+} or Fe^{3+} ions between the conducting organic layers of the BEDT–TTF molecules is studied by ESR spectroscopy, and the contributions of these metallic complexes, conduction electrons, and non-equilibrium lattice defects to the magnetic susceptibility are determined. An analysis of the temperature dependence of the magnetic susceptibility and the EPR line shape has revealed partial localization of conduction electrons at $T < 20$ K in the crystals with Cr^{3+} ions.

g-Anisotropy of the S2-State Manganese Cluster in Single Crystals of Cyanobacterial Photosystem II Studied by W-Band Electron Paramagnetic Resonance Spectroscopy

H. Matsuoka[*1], K. Furukawa[*1], T. Kato, H. Mino[*2], J.-R. Shen[*3] and A. Kawamori[*4] (*1 Institute for Molecular Science, *2 Division of Material Science (Physics), Graduate School of Science, Nagoya University, *3 Department of Biology, Faculty of Science, Okayama

University, *4 School of Science and Technology, Kwansei Gakuin University)
J. Phys. Chem. B, **110**, 13242–13247 (2006)

Multiline signals from the S2-state manganese cluster in the oxygen evolving complex of photosystem II (PSII) are observed in single crystals of a thermophilic cyanobacterium *Thermosynechococcus Vulcanus* for the first time by W-band (94 GHz) electron paramagnetic resonance (EPR). At W-band, spectra are characterized by the g-anisotropy, which enabled the precise determination of the tensor. Distinct hyperfine splittings (hfs's) as seen in frozen solutions of PSII at X-band (9.5 GHz) are detected in most of the crystal orientations relative to the magnetic field. In some orientations, however, the hfs's disappear due to overlapping of a large number of EPR lines from eight crystallographic symmetry-related sites of the manganese cluster within the unit cell of the crystal. Analysis of the orientation-dependent spectral features yield the following g-tensor components: $g_x = 1.988$, $g_y = 1.981$, $g_z = 1.965$.

Triradical Cation of p-Phenylenediamine Having Two Nitroxide Radical Groups: Spin Alignment Mediated by Delocalized Spin

A. Ito*1, Y. Nakano*1, M. Urabe*1, T. Kato and K. Tanaka*1 (*1 Department of Molecular Engineering, Graduate School of Engineering, Kyoto University)
J. Am. Chem. Soc., **128**, 2948–2953 (2006)

The cationic state of a p-phenylenediamine (PDA) molecule having two nitroxide radical groups has been prepared and characterized using electrochemical, electron spin resonance (ESR) spectroscopic, and absorption spectroscopic methods. The delocalized intervalence state of the p-phenylendiamine (PDA) moiety has been detected in the cationic state. From the pulsed ESR measurements, it is confirmed that the delocalized spin induces parallel spin alignment between the localized two nitroxide groups which are magnetically weakly coupled in the neutral state. It is found that the resulting high-spin alignment does not seriously affect the delocalized intervalence state of the PDA radical cation.

High-Spin Radical Cations of a Dendritic Oligoarylamine

Y. Hirao*1, H. Ino*1, A. Ito*1, K. Tanaka*1, and T. Kato (*1 Department of Molecular Engineering, Graduate School of Engineering, Kyoto University)
J. Phys. Chem. A, **110**, 4866–4872 (2006)

A new dendritic oligoarylamine, N, N, N', N', N'', N''-hexakis [4–(di–4–anisylamino) phenyl]–1,3,5,–benzenetriamine (BTA) **2**, which contains a 1,3,5–benzenetriamine molecular unit as an potential precursor of a high-spin molecule and three oligo-arylamine moieties as spin-carrying units surrounding the core BTA, was prepared by the sequential palladium-catalyzed amination reactions. The redox property was investigated by cyclic volatmmetry, and the highly charged states up to the hexacation were accessible to **2**. The polycationic highspin species were generated by stepwise chemical oxidation, and the electronic structures were examined in detail by the continuous wave (CW) and pulsed ESR spectroscopy in comparison with the previously studied **1**. The pulsed ESR technique enable us determine the definite spin multiplicity of the generated polycationic species of **2**. It was confirmed that the dominant oxidized species observed by the two- and three-electron oxidations were assigned to the spin triplet $\mathbf{2}^{2+}$ and the spin quartet $\mathbf{2}^{3+}$, respectively.

The Bingel Monoadducts of La@C_{82}: Synthesis, Characterization, and Electrochemistry

L. Feng*[1], T. Wakahara*[1], T. Nakahodo*[1], T. Tsuchiya*[1], Q. Piao*[1], Y. Maeda*[2], Y. Lian*[1], T. Akasaka*[1], E. Horn*[3], K. Yoza*[4], T. Kato, N. Mizorogi*[5], and S. Nagase*[5] (*1 Center for Tsukuda Advanced Research Alliance University of Tsukuba, *2 Department of Chemistry, Tokyo Gakugei University, *3 Department of Chemistry, Rikkyo University, *4 Bruker AXS K. K., *5 Institute for Molecular Science)
Chem. Eur. J., **12**, 5578–5586 (2006)

The reaction of La@C_{82} with diethyl bromomalonate in the presence of base (the Bingel reaction) has generated five monoadducts which have been fully characterized. It is found that four of them (mono-A, -B, -C, and -D) are ESR-inactive, suggesting singly bonded regioisomers. In contrast, the fifth product (mono-E) is ESR-active, indicating that it possesses a cyclic moiety between the appended malonate group and the fullerene cage, analogous to conventional Bingel adducts. The differences in the molecular structures of mono-A, -B, -C, and -E result in varying thermal stabilities and electrochemical behavior. In particular, the singly bonded momoadducts undergo the retro-Binbel reaction either under thermal treatment of during electron transfer on the cyclic voltammetric timescale. However, mono-E shows remarkable thermal stability and perfect reversibility under the same experimental conditions.

Quantitative Structure-cytotoxicity Relationship Analysis of Coumarin and its Derivatives by Semiempirical Molecular Orbital Method

S. Ishihara*[1], Y. Yokote, and H. Sakagami*[2] (*1 Division of Basic Chemistry, Department of Oral Biology and Tissue Engineering, *2 Division of Phamacology, Department of Diagnostic and Therapeutic Sciences, Meikai University School of Dentistry, Sakado, Saitama 350–0283, Japan)
Anticancer Res., **26**, 2883–2866 (2006)

A semiempirical molecular orbital method (CAChe) was applied to delineate the relationship between cytotoxicity against the human squamous cell ca, cinoma line HSC–2 (evaluated by 50% cytotoxic concentration, CC_{50}) of 20 coumarin (2H-pyran-2-one) derivatives and twelve physical parameters (descriptors) calculated by the CONFLEX/PM3 method. There was a highly significant correlation between the CC_{50} and ionization potential, highest occupied molecular orbital (HOMO) energy, difference between electron energy of HOMO and electron energy of lowest unoccupied molecular orbital (LUMO), or absolute hardness ($r^2 = 0.756\sim0.802$). On the other hand, there was no significant correlation between the CC_{50} and heat of formation, stability of hydration, dipole moment, electron affinity, or LUMO energy ($r^2 = 0.13\sim0.36$). When the CC_{50} was plotted vs. log P, a parabolic curve was produced, with a maximum cytotoxicity (or the least CC_{50} value) at log P of 2.5. The present study demonstrated that hardness and softness, other than the electron accepting and donating properties, are important factors in estimating the cytotoxic activity of coumarin derivatives.

Studies of Photochemical Reactions of Air Pollutants. XV. Photoreactivity of Heptachlero-3′-cyclopentenyldioxy Heptachloro-2-cyclopentene Formed by Exposure of Hexaxhlorocyclopentadiene to Ultraviolet Light in Air

Kazuhiro Nojima[*1], Hiroshi Miyamae, and Yasuko Yamaahi[*1] (*1 Faculty of Pharmaceutical Science)
Chem. Pharm. Bull., **54** (3), 338-343 (2006)

Hexachlorocyclopentadiene (HCCP), one of the starting materials in the synthesis of aldrin, was found to be able to epoxidize aldrin to give dieldrin when exposed to artificial light at wavelengths longer than 290 nm. In this photochemical reaction, heptachloro-3′ cyclopentenyldioxy heptachloro-2-cyclopenten was isolated as a key intermediate, which appears to be derived from the interaction between the triplet state of photo-excited HCCP and triplet oxygen ($^3\Sigma_g^-$), but not from that between the ground state of HCCP and singlet oxygen ($^1\Delta_g$). The peroxide plays an important role in the formation of dieldrin, because it utilized oxygen atom derived from oxygen in air for the epoxidation.

Crystal Structure of cis-Dichlorobis (dimethylglyoxime) nickel (II)

Takahiro Yoshioka, Kazuki Matsushima, Goro Hihara, and Hiroshi Miyamae
Analytical Sciences, **22**, x205-x206 (2006)

The title complex crystallized in the monoclinic space group $P2_1/n$, with Z = 4, a = 7.566(3) Å, b = 11.539(4) Å, c = 16.349(7) Å, β = 97.51(2)°, V = 1415.1(9) Å^3, and R = 0.0328. The metal ion exhibits a *cis*-N_4Cl_2 distorted octahedral geometry, with the dimethylglyoxime (H_2dmg) ligands chelating through their oxime N-atom donors. The two bite angles (75.00(7)° and 74.94(8)°) are much smaller than that [Ni(Hdmg)$_2$] (80°).

Relationship between Electronic Structure and Cytotoxic Activity of Azulenes

Teruo Kurihara, Mayumi Noguchi, Takashi Noguchi, Hidetsugu Wakabayashi, Noboru Motohashi*1 and Hiroshi Sakagami*2 (*1 Meiji Pharmaceutical University, *2 Department of Endodontics, Meikai University School of Dentistry)
International Journal of In Vivo Research, **20**, 385–390 (2006)

The structure-activity relationship of the cytotoxic activity of azulene derivatives was discussed, using theoretically calculated results. In order to clearly divide the azulenes into three groups according to their functional groups, the CC_{50}, four different dipole moments (μ_G, μ_{ESP-G}, μ_W, and μ_{ESP-W}) and heats of formation ($⊿H_f$) of the azulenes [1–24] were separately calculated in two states, gas-phase and water, by the COSMO/PM3 method. For the halogenated azulenes and isopropyl azulenes, the cytotoxic activity might follow the three quantitative structure-activity relationship (QSAR) parameters: $⊿⊿H_f$, HOMO energy and μ_w. Whereas, for the other ten compounds [3–5, 7–8, 10, 15–18], the cytotoxic actovoty might be related to the three QSAR parameters, $⊿⊿H_f$, LUMO energy and μ_G.

Relationship between Electronic Structure and Cytotoxic Activity of Tropolones

Teruo Kurihara, Hiroko Mine, Yoshimasa Satoh, Hidetsugu Wakabayashi, Noboru Motohashi*1 and Hiroshi Sakagami*2 (*1 Meiji Pharmaceutical University, *2 Department of Endodontics, Meikai University School of Dentistry)
International Journal of In Vivo Research, **20**, 391–396 (2006)

A structure-activity relationship of the cytotoxic activity of tropolone derivatives was discussed, using theoretical calculations. In order to clearly divide the tropolones into two structurally analogous groups, four different dipole moments (μ_G, μ_{ESP-G}, μ_W, and μ_{ESP-W}) and heats of formation ($⊿H_f$) of the tropolones [1–21] were calculated in the gas-phase and in water-solution by the COSMO/PM3 method. The cytotoxic activities of the tropolones and 2-methoxytropones seem to be related to the three QSAR parameters $⊿⊿H_f$, HOMO energy (E_H) and μ_w. The cytotoxic activity of the five tropone derivatives [17–21] might depend on the QSAR parameters $⊿⊿H_f$, LUMO energy (E_L) and μ_{ESP-G}. The results of the present study suggest the applicability of theoretical calculations such as frontier molecular orbital, dipole moments and $⊿⊿H_f$ in the prediction of the cytotoxic activity of tropolone derivatives

Apoptosis-inducing Activity of Trihaloacetylazulenes against Human Oral Tumor Cell Lines

Yoshiaki Akatsu, Nobuharu Oshima, Yoshie Yamagishi, Masayuki Nishishiro, Hidetsugu Wakabayashi, Teruo Kurihara, Hirotaka Kikuchi*1, Tadashi Katayama*1, Noboru Motohashi*2, Yuko Shoji*3, Hideki Nakashima*3, and Hiroshi Sakagami*1 *1 Department of

Endodontics, Meikai University School of Dentistry, ∗2 Meiji Pharmaceutical University)

Anticancer Res., **26**, 1917–1924 (2006)

We investigated twenty six trihaloacetylazulene derivatives for their tumor-specific cytotoxicity and apoptosis-inducing activity against three human normal cells (HGF, HPC, HPLF) and four human tumor cell lines (HSC–2, HSC–3, HSC–4, HL–60). The trichloroacetylazulenes generally showed higher cytotoxicity as compared with the corresponding trifluoroacetylazulenes. The trichloroacetylazulenes also showed higher tumor-specific cytotoxicity (expressed as TS value) than the corresponding trifluoroacetylazulenes. Especially, 2,3–dimethyl–1–trichloroacetylazulene and 1,3–ditrichloroacetyl–4,6,8–trimethylazulene showed the highest cytotoxicity and tumor specificity (TS$>$35.6 and $>$44.1, respectively). These compounds induced internucleosomal DNA fragmentation in HL–60 cells, but not in HSC–2 and HSC–3 cells, but activated caspase–3, –8 and –9 in all of these cells, suggesting the activation of both mitochondria-independent (extrinsic) and -dependent (intrinsic) pathways. Western blot analysis shows that 2,3–dimethyl–1–trichloroacetylazulene and 1,3–ditrichloroacetyl–4,6,8–trimethylazulene slightly increased the intracellular concentration of pro-apoptotic proteins (Bad, Bax) in HSC–2 cells. All twenty six compounds did not show anti-HIV activity. These results suggest the possible candidates of 2,3–dimethyl–1–trichloroacetylazulene and 1,3–ditrichloroacetyl–4,6,8–trimethylazulene for the future cancer chemotherapy.

Inhibition of LPS-stimulated NO Production in Mouse Macrophage-like Cells by Trihaloacetylazulenes

Nobuharu Oshima, Yoshiaki Akatsu, Masayuki Nishishiro, Hidetsugu Wakabayashi, Teruo Kurihara, Kazue Satoh*[1], Noboru Motohashi*[2], and Hiroshi Sakagami*[3] (∗1 Analysis Center, School of Pharmaceutical Sciences, Showa University, ∗2 Meiji Pharmaceutical University, ∗3 Department of Endodontics, Meikai University School of Dentistry)

Anticancer Res., **26**, 2921–2928 (2006)

We investigated the effect of twenty six trihaloacetylazulene derivatives on nitric oxide (NO) production by mouse macrophage-like cells Raw 264.7. Trichloroacetylazulenes generally showed higher cytotoxicity as compared with the corresponding trifluoroacetylazulenes. All compounds inhibited the NO production by lipopolysaccharide (LPS)-activated Raw 264.7 cells to various extents. 3–Trifluoroacetylguaiazulene, 1–trifluoroacetyl–1,6,8–trimethylazulene, 3–methyl–1–trichloroacetylazulene and 3–ethyl–1–trichloroacetylazulene showed lower cytotoxic activity and most effectively inhibited the NO production. Western blot shows that 3–trifluoroacetylauaiazulene and 1–trifluoroacetyl–4,6,8–trimethylazulene dose-dependently reduced the intracellular concentration of inducible NO synthase (iNOS), whereas 3–methyl–1–trichloroacetylazulene and 3–ethyl–1–trichloroacetylazulene only marginally affected the iNOS protein expression. RT-PCR analysis showed that 3–trifluoroacetylguaiazulene and 3–methyl–1–trichloroacetylazulene reduced the iNOS mRNA expression approximately by 50%. These compunds affected cyclooxygenase-2 protein and mRNA expression in biphasic fashions, depending on the concentrations. ESR spectroscopy shows that 3-Trifluoroacetylguaiazulene, 1-trifluoroacetyl-4,6,8-trimethylazulene, 3-methyl-1-trichloroacetylazulene and 3-ethyl-1-trichloroacetylazulene neither produced radical, nor scavenged NO, superoxide anion and diphenyl-2-picrylhydrazyl radicals. The present study suggests that the inhibitory effects of trifluoroacetylazulenes and trichloroacetylazulenes on NO production by activated macrophages might be derived from different mechanisms.

2. Books, Reviews and Other Printings

MATHEMATICS

Endomorphisms of a Module over a Local Ring

H. Ishibashi
京都大学数理解析研究所講究録 **1503**, 92–94, 2006

Lambda Credibility

Kakuzo Iwamura and Makoto Horiike*[1] (*1 Faculty of Economics, Teikyo University)
Proceedings of the Fifth International Conference on Information and Management Sciences, July 1–8, 2006, Chengdu, China, pp. 508–513

The Shortest Path Problem Considering Angles

Makoto Horiike*[1] and Kakuzo Iwamura (*1 Faculty of Economics, Teikyo University)
Proceedings of the Fourth International Conference on Information and the Fourth Irish Conference on the Mathematical Foundations of Computer Science and Information Technology '06, Information-MFCSIT '06, August 1–5, 2006, Cork, Ireland, pp. 126–129

Mathematics in Our Daily Life

Takeyoshi Kogiso
Josai Information Sciences Researches vol. 16 No. 1 (2006. 3), 63–75

Multiplicity one property and the decomposition of *b*-functions

Sato, Fumihiro; Sugiyama, Kazunari
Internat. J. Math. 17 (2006), no. 2, 195–229
by T. Kogiso in Math. Sci. net of American Math. Soc. (2006) (On line)

***b*-function of a prehomogeneous vector space with no regular component**

Sugiyama, Kazunari, Comment. Math. Univ. St. Pauli 54 (2005), No. 2, 99–119
by T. Kogiso in Math. Sci. net of American Math. Soc. (2006) (On line)

CHEMISTRY

総説：「高磁場–高周波数電子スピン共鳴測定（多周波数 ESR 測定）」

加藤立久，分光研究，第55巻，第6号，pp. 369-378（2006）

21世紀の化学 シリーズ1「基礎有機化学」

小林啓二
朝倉書店（2006）

BIOLOGY

ヒトの性成熟年齢における親子相関
小須田和彦
城西大学研究年報（自然科学編）28: 1-9（2005）

3. Oral Presentations

MATHEMATICS

Representation of Endomorphisms of a module over local rings

H. Ishibashi
ICNAAM 2006, Hotel Belvedere Imperal, Hersonissos，クレタ，ギリシャ，2006年9月15日-19日

Spread of Influenza in Tokyo

H. Yasuda, K. Suzuki* (* NIID)
2nd symposium on emerging and reemerging infectious disease (Tokyo), 2007年2月27日

薄膜相分離のパターン形成

安田英典，松本昌昭*（* 三菱総合研究所）
仮想実験と大規模シミュレーションが拓く先端科学2007（大阪），2007年2月2日

Simulation Based Risk Assessment and Public Risk Perception of Pandemic Influenza

H. Yasuda, N. Yoshizawa*1, M. Matsumoto*1, S. Kawaji*2, K. Suzuki*3 (*1 MRI, *2 IMCJ, *3 NIID)
The Third International Symposium on Transmission Models for Infectious Disease (Kyoto), 2007年1月9-10日

大都市近郊のインフルエンザ流行伝播シミュレーション

安田英典，鈴木和男*（* 国立感染症研究所）
第3回生物数学の理論とその応用，京大数理解析研究所（京都），2006年12月4-7日

Simulation of New Type Influenza Outbreak

H. Yasuda, K. Suzuki* (* NIID)
The 15th Symposium on the International Medical Cooperation (Tokyo), 2006年11月17日

大都市郊外のインフルエンザ流行伝播シミュレーション

安田英典
第2回京都算楽会，関西セミナーハウス（京都），2006年10月15日

$Sp(2,\mathbb{R})$の一般主系列表現の行列要素の Harish-Chandra 展開

飯田正敏
研究集会「代数群上の球関数（あるいはもっと一般の特殊関数を含む）と，多変数保型形式論へのその応用」（東京大学），2006 年 12 月

クリスプ・クラスタリング問題を解くアルゴリズムの一改良

岩村覚三，堀池真琴[*1]（*1 帝京大学経済学部）
日本オペレーションズ・リサーチ学会「不確実性理論の経営科学への応用」研究部会，2006 年 6 月 3 日，千葉大学理学系総合研究棟 1 階 105 室

IMS 2006 Chendu 6/30–7/9 に参加して

岩村覚三
日本オペレーションズ・リサーチ学会「不確実性理論の経営科学への応用」研究部会，2006 年 7 月 29 日，千葉大学理学系総合研究棟 1 階 105 室

Existence proof of finitely many independent fuzzy variables

岩村覚三，景山正幸[*1]，堀池真琴[*2]，北久保　茂[*3]（*1 千葉大学理学部大学院，*2 帝京大学経済学部，*3 日本工業大学工学部）
日本オペレーションズ・リサーチ学会「不確実性理論の経営科学への応用」研究部会，日本工大シンポジウム，2006 年 12 月 25 日–26 日，日本工大学友会館

Traveling Waves for a Reaction-diffusion Equation with Periodic Nonlinearity

Toshiko Ogiwara
AIMS' 6th International Conference on Dynamical Systems and Differential Equations and Applications, Poitier University (France), June, 2006

結晶成長モデルに関連した反応拡散方程式の解の挙動について

荻原俊子
研究会「NSC 12 周年：非線形数理の現状と発展」，北海道大学，2006 年 10 月

周期関数を非線形項に持つ反応拡散方程式の解の漸近挙動

田中実鈴[*1]，荻原俊子，大出真理[*2]（*1 城西大学大学院理学研究科数学専攻，*2 栃木県佐野市立佐野南中学校）
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CHEMISTRY

高温分子 GaF の赤外分光

堀合公威，野口剛範，上原博通
分子構造総合討論会（静岡），2006 年 9 月，4P098

HF の回転・振動回転スペクトルとその fit

野口剛範，堀合公威，上原博通
分子構造総合討論会（静岡），2006 年 9 月，4P099

Synthesis of Methyl dithioanthranilate and Formation of Dihydro-3,1(4*H*)-benzooxazine-4-thiones and -benzothiazine-4-thiones

Motomu Muraoka and Tatsuo Yamamoto
22nd International Symposium on the Organic Chemistry of Sulfur (Saitama, Japan) Aug. 20-25, 2006
Abstracts p. 144

希ガス-N_2O 錯体の赤外スペクトルの量子化学計算

齋藤　豊，紺野東一，尾崎　裕
日本化学会第 86 回春季年会（船橋），2006 年 3 月

希ガス-CO_2 van der Waals 錯体の構造の同位体効果

山口槙也，紺野東一，尾崎　裕
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金属クラスターを内包するフラーレンの分子磁性

加藤立久，川崎裕貴，山田道夫[*1]，飯塚裕子[*1]，赤阪　健[*1]（*1 筑波大学学際領域研究センター）
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配位結合ケージに包摂された銅ポルフィリン二量体のスピン結合状態

渡辺健太郎，加藤立久，小野公輔[*1]，吉沢道人[*1]，藤田　誠[*1]（東京大学大学院工学研究科）
第 45 回電子スピンサイエンス学会（京都），2006 年 11 月，講演要旨集，pp. 104-105

ニンヒドリンとヒドラジン類との反応生成物における互変異性構造

石井理恵，武鹿野陽子，若林英嗣，宮前　博，小林啓二
日本化学会第86回春季年会（東京），2006年3月，講演要旨集，2PA090

三個のスピロ炭素原子からなるシクロプロパン誘導体 ── その意外な生成と性質

清原彩子，若林英嗣，小林啓二，山本　学，真崎康博
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ニンヒドリンとフェノール類との反応生成物における環状ヘミアセタール構造

橋本　涼，若林英嗣，小林啓二
日本化学会第86回春季年会（東京），2006年3月，講演要旨集，3PA001

ニンヒドリンとチオフェン類との反応により生成する着色化合物の構造

鈴江暢野，若林英嗣，小林啓二
日本化学会第86回春季年会（東京），2006年3月，講演要旨集，3PA002

トリハロアセチルアズレン類の合成とその薬理活性

若林英嗣，西代正志，赤津孔明，大島伸晴，山岸淑恵，栗原照夫，本橋　登[*1]，坂上　宏[*2]（*1 明治薬科大学，*2 明海大学）
日本化学会第86回春季年会（東京），2006年3月，講演要旨集，3PB083

グアイアズレンと*N*-クロルコハク酸イミドとの反応

若林英嗣，佐藤　剛，郡司妙子，小山知美，青木一洋，本橋力哉，栗原照夫
日本化学会第86回春季年会（東京），2006年3月，講演要旨集，3PB084

The Reaction of Thiophenes with Ninhidorin

Nono Suzue, Hidetsugu Wakabayashi, and Keiji Kobayashi
22nd International Symposium on the Organic Chemistry of Sulfur（ISOCS-22）P-67
August 20-25, 2006, Saitama, Japan

Preparation of Hemithioindigos by Oxidation of Benzo[*b*]thiophene Compounds

Hiroyuki Endo, Suzumi Hashimoto, Hidetsugu Wakabayashi, and Keiji Kobayashi
22nd International Symposium on the Organic Chemistry of Sulfur（ISOCS-22）P-69
August 20-25, 2006, Saitama, Japan

3 個のスピロ接合炭素からなるシクロプロパンの合成と性質

清原彩子，金住　誠，若林英嗣，宮前　博，加藤立久，小林啓二
第 18 回基礎有機化学連合討論会（福岡），2006 年 10 月，講演要旨集，2PB52

1,3−ジイミノインダン誘導体におけるプロトトロピーのキャラクタリゼーション

武鹿野陽子，若林英嗣，宮前　博，小林啓二
第 18 回基礎有機化学連合討論会（福岡），2006 年 10 月，講演要旨集，2PB53

無溶媒・摩砕混合による，ジメチルグリオキシムとニッケル塩との錯体の合成

日原五郎，松島一樹，吉岡孝広，宮前　博
第 56 回錯体化学討論会（広島），2006 年 9 月，講演要旨集，p. 60

$K[Fe(bpy)_3][Co(ox)_3]ClO_4$ の合成と性質（bpy＝2,2'−ビピリジン，H_2ox：＝シュウ酸）

吉岡孝広，立屋敷　哲*，加藤立久，日原五郎，宮前　博（* 女子栄養大学）
第 56 回錯体化学討論会（広島），2006 年 9 月，講演要旨集，p. 61

$[OsL_2(en)]^{2+}$（L=phen, bpy）の光配位子酸化反応

立屋敷　哲*，加藤太朗，大崎　愛，宮前　博，日原五郎（* 女子栄養大学）
第 56 回錯体化学討論会（広島），2006 年 9 月，講演要旨集，p. 204

Molecular Cloning and Characterization of Feather Barbs Keratin Genes of Pigeon

Riko Takahashi and Kiso Akahane
20th IUBMB International Congress of Biochemistry and Molecular Biology and 11th FAOBMB Congress (Kyoto), Jun. 18-23, 2006 Abstracts, p. 308

半経験的分子軌道法による Coumarin 誘導体の構造と細胞傷害活性の予測

石原真理子，横手よし子，坂上　宏
第 80 回日本薬理学会（2007），p. 144

高次元アルゴリズムを用いた Enkephalin の構造解析

土屋恭平，寺前裕之，渡邊寿雄，石元孝佳，長嶋雲兵
日本コンピューター化学会 2006 春期年会（東京），2006 年 5 月，講演要旨集，1P22

高次元アルゴリズムにおける混合性パラメーターに関する研究

寺前裕之，土屋恭平，石原康行，小山晃弘，佐藤　麗，清野　巧，坪　寛之，石元孝佳，長嶋雲兵
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高次元アルゴリズムを用いた Enkephalin の構造解析（Ⅱ）

土屋恭平，寺前裕之，渡邊寿雄，石元孝佳，長嶋雲兵
日本コンピューター化学会 2006 秋期年会（函館），2006 年 10 月，講演要旨集，2P13

PHYSICS

古典軌道計算に基づく電荷移行反応微分断面積の解析

伊藤　陽，大槻一雅[*]（* 電通大工）
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BIOLOGY

ヒト集団における夫婦相関
小須田和彦
日本動物行動学会第 25 回大会（岡山），2006 年 10 月，講演要旨集，p. 38

PHYSICAL EDUCATION

女子長距離ランナーの月経異常が唾液分泌型免疫グロブリン A に与える影響

清水和弘[*1]，相澤勝治[*1]，鈴木なつ未[*1]，木村文律[*1]，中尾喜美子[*2]，鈴木尚人，村井文江[*1]，河野一郎[*1]，目崎　登[*1]（*1 筑波大学，*2 千葉大学）
日本体力医学会（神戸国際会議場），2006 年 9 月

4. Abstract of Doctoral Dissertation

$^{12}C^{18}O_2$ ファン・デル・ワールス錯体の赤外スペクトルに関する研究（英文）

紺野東一
提出先：東京農工大学（平成18年3月24日）

本論文は主に，$C^{16}O_2$ の同位体種である $C^{18}O_2$ と希ガス原子，Ne, Ar, Kr, Xe とのファン・デル・ワールス錯体および（$C^{18}O_2$）$_2$ の高分解能赤外分光について記述したものである。これまでに，$C^{16}O_2$ と希ガス原子との錯体や（$C^{16}O_2$）$_2$ の高分解能分光は幾つかなされているが，$C^{18}O_2$ を含む錯体の報告は未だ無い。これらの錯体の振動回数スペクトルを $C^{18}O_2$ の ν_3 バンド（反対称伸縮，2314 cm^{-1}）領域で，パルスジェットダイオードレーザー分光装置を用いて観測した。解析の結果，得られた分子定数から構造パラメーターを決定し，錯体を形成することによる分子内ポテンシャルの変化と分子間構造の ^{16}O–^{18}O 同位体効果について論じている。

第1章「緒論」では，$C^{18}O_2$ ファン・デル・ワールス錯体の赤外分光研究を行うに当たって，クラスター，ファン・デル・ワールス錯体，高分解能分光について簡単に述べ，また，CO_2 錯体に関しては，歴史的背景も踏まえて記述してある。GeSe は本主題の弱く結合した系とは反対の強く結合した系に属するけれども，高分解能赤外分光の対象となる豊富な自然同位体種を持つ分子の一つとして，GeSe を採り上げたことについても記述してある。

第2章「実験と解析」では，Rg–$C^{18}O_2$(Rg ＝ Ne, Ar, Kr, Xe）と（$C^{18}O_2$）$_2$ に対する実験と解析方法について装置の概略図を加えて記述してある。

第3章「Ar–$^{12}C^{18}O_2$ の赤外吸収分光：錯体を形成する上での分子内ポテンシャルにおける変化」では，Ar–$^{12}C^{18}O_2$ ファン・デル・ワールス錯体の赤外吸収スペクトルが 2312–2314 cm^{-1} 領域で観測され，解析の結果得られたその構造はファン・デル・ワールス振動の振幅に及ぼす同位体効果に基づいて Ar–$^{12}C^{16}O_2$ の構造から見積もった構造と本質的に一致する。Ar–$^{12}C^{18}O_2$ の ν_4 モードのバンドオリジンは $^{12}C^{18}O_2$ の ν_3 モードのバンドオリジンから 0.4567 cm^{-1}のレッドシフトを示す。Ar 原子と錯体を形成する上での CO_2 の分子内ポテンシャルにおける変化はバンドオリジンのシフトにおよぼす同位体効果から決定される。

第4章「Kr–$^{12}C^{18}O_2$ の赤外分光：錯体の形成による CO_2 分子内ポテンシャルにおける変化と分子間振動平均構造におよぼす同位体効果」では，Kr–$^{12}C^{18}O_2$ の高分解能赤外スペクトルがモノマー $^{12}C^{18}O_2$ の ν_3 バンド領域で観測され，解析の結果，$^{12}C^{18}O_2$ の ν_3 モードに対応する Kr–$^{12}C^{18}O_2$ の振動のバンドオリジンは $^{12}C^{18}O_2$ のそれから 0.86510(30)cm^{-1} のレッドシフトを示す。T 型構造に対する基底状態における振動平均構造パラメーターは $R_{\mathrm{KrC}} = 3.6204(11)$Å，$\Theta_{\mathrm{KrCO}} = 83.51(10)^{\circ}$ と決定される。錯体を形成する上での CO_2 の分子内ポテンシャルにおける変化は観測したレッドシフトから誘導され，R_{KrC} と Θ_{KrCO} におよぼす同位対効果は ab initio 計算により再現される。

第5章「Ne–$^{12}C^{18}O_2$ と Xe–$^{12}C^{18}O_2$ の赤外分光：希ガス–CO_2 錯体を形成する上での CO_2 の分子内ポテンシャルにおける変化」では，Ne–$^{12}C^{18}O_2$ と Xe–$^{12}C^{18}O_2$ の高分解能赤外スペクトルが $^{12}C^{18}O_2$ の ν_3 バンド領域で観測された。これらの錯体に対する錯体形成上の分子内ポテンシャルにおける変化はこれまでと同様に，バンドオリジンのシフトから導かれる。その変化は，Xe–CO_2 ではほとんど調和となり，Xe→Kr→Ar→Ne の順に非調和性が増す。

第6章「（$^{12}C^{18}O_2$）$_2$ の赤外分光と（CO_2）$_2$ の振動平均構造におよぼす同位体効果」では，ダイ

マー $(^{12}\mathrm{C}^{18}\mathrm{O}_2)_2$ の高分解能赤外スペクトルが $^{12}\mathrm{C}^{18}\mathrm{O}_2$ の ν_3 バンド領域で観測され，$^{12}\mathrm{C}^{18}\mathrm{O}_2$ の ν_3 モードに対応する $(^{12}\mathrm{C}^{18}\mathrm{O}_2)_2$ の振動バンドオリジンは，$^{12}\mathrm{C}^{18}\mathrm{O}_2$ の ν_3 バンドオリジンから 1.62362(19)cm^{-1} のブルーシフトを示す。スリップドパラレル構造に対する基底状態における構造パラメーターは $R_{\mathrm{OC}} = 3.5947(11)$Å，$\Theta_{\mathrm{CCO}} = 57.97(7)^\circ$ と決定される。4つの分子間自由度に対して，ab initio ポテンシャル上で振動波動関数を計算することにより，R_{OC} におよぼす同位体効果は主として面内の tilt から生じていることが分かる。

第7章「高温分子 GeSe の赤外ダイオードレーザー分光」では，GeSe の振動回転スペクトルがヒートパイプ高温セルを備えたダイオードレーザー分光器を用いて観測され，771本のスペクトル線が6つの GeSe 同位体種の $\Delta v=1$ band に帰属された。これらのデータに138本のマイクロ波のデータを加えて2つの異なったポテンシャル関数（Dunham potential function, radial function）へそれぞれ最小二乗フィットすることにより分子定数が得られた。フィットの性質はほとんど変わらない。自然存在比が最も高い $^{74}\mathrm{Ge}^{80}\mathrm{Se}$ の ω_{e} の値は 402.66129(70)cm^{-1} と決定される。

第8章では，「まとめ」を記述してある。

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