# SCIENCE BULLETIN OF JOSAI UNIVERSITY

城西大学理学部研究報告

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FACULTY OF SCIENCE

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城西大学理学部研究報告

Vol. 20 March 2012

## **Editorial Board**

Yasushi Ozaki (Chairperson) Hiroyuki Ishibashi Hiroyuki Teramae Hisanori Nagato Yoh Itoh

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# PART I ANNUAL REPORTS

## 1. Abstracts of Papers Published in Journals

#### **MATHEMATICS**

#### Minimal Polynomials and Characteristic Polynomials over Rings

H. Ishibashi

JP Journal of Algebra, Number Theory and Applications, 20(1), 49-60 (2011)

Let R be a commutative ring with 1 the identity of R and M be a free module of a finite rank over R. Further, let  $\operatorname{End}_R M$  be the endomorphism ring of M over R and  $\sigma$  be an element in  $\operatorname{End}_R M$  of which matrix is diagonalizable.

The relationship between the characteristic polynomial  $\chi_{\sigma}$  of  $\sigma$  and the minimal polynomial  $p_{\sigma}$  of  $\sigma$  will be treated. If R is an integral domain,  $p_{\sigma}$  is uniquely determined as a monic polynomial dividing  $\chi_{\sigma}$ . On the other hand if R is not an integral domain, we will construct  $\sigma$  such that  $p_{\sigma}$  is not necessarily monic nor divides  $\chi_{\sigma}$ .

#### Distributions of simple patterns in some kinds of exchangeable sequence

Kiyoshi, Inoue\*1, Shigeo, Aki\*2, Katsuomi, Hirano (\*1 Seikei University, \*2 Kansai University) Journal of Statistical Planning and Inference 141 (2011), 2532–2544

Distributions of simple patterns in some type of sequences of infinite exchangeable multistate trials are investigated. By using an extension of de Finetti's theorem, the distributions of simple patterns on exchangeable multi-state trials are studied. As an application of partially exchangeable sequences, the distributions of patterns on a Markov exchangeable sequence are also studied. A new type of partially exchangeable sequence is introduced and its properties are examined. The distribution theory in the case of the finite exchangeable sequences is also studied. Some examples are given in order to illustrate these results.

## **PHYSICS**

The forward glory effect in the differential cross sections measured below  $E_{\rm lab}$ =50 eV for the one-electron capture process in N<sup>5+</sup>—He collisions

Yoh Itoh

J. Phys. B: At. Mol. Opt. Phys. 44 175202 (pp. 1-8)

We measured the relative state-selective differential cross sections for the one-electron capture process in the N<sup>5+</sup> – He system from  $\theta_{lab}$ = – 3° to 21° at  $E_{lab}$ =27.5 and 47.5 eV using a crossed-beam apparatus. The main reaction channel was found to be N<sup>5+</sup>(1s<sup>2</sup> <sup>1</sup>S) + He  $\rightarrow$ 

 $N^{4+}(1s^23s~^2S) + He^+ + 16.8~eV$ . The differential cross section for this channel is pronounced at  $\theta_{cm} = 0$ , and it shows another peak at a certain angle that depends on the collision energy. We also measured the  $O^{5+}$  - He system for comparison at  $E_{lab} = 47.5~eV$ . The main reaction channel was determined to be  $O^{5+}(1s^22s~^2S) + He \rightarrow O^{4+}(1s^22s3p~^{1.3}P) + He^+ + 17~eV$ , and the cross section for this channel is zero at  $\theta_{cm} = 0$ , and it shows only a single peak at  $\theta_{cm} = 0.314$  rad. The stractures observed in the  $N^{5+}$  - He system were analyzed using the classical deflection function based on *ab initio* potentials. The peak observed at  $\theta_{cm} = 0$  is assigned to the forward glory effect and the second peak to the inelastic rainbow effect.

## **CHEMISTRY**

#### Mixing parameters for geometry optimization using the Hamiltonian algorithm

Hiroyuki Teramae, Takayoshi Ishimoto\*<sup>1</sup>, and Umpei Nagashima\*<sup>2</sup> (\*1 Kyushu University, \*2 National Institute of Advanced Industrial Science and Technology)

Theoret. Chem. Acc., 130, 671-678 (2011)

We study the mixing parameters for the search of an optimal geometry using the Hamiltonian algorithm (HA) combined with ab initio molecular orbital calculations. We choose the C-C-C-C dihedral angle of the butane molecule as an example. HF/3-21G level calculations are employed as the molecular orbital calculations. The distributions of the eigenvalues of mixing coefficients are fitted with the linear, quadratic, and quartic functions. Analyses of HA calculations both up to 2,000 and 60,000 iterative calculations show a possibility that the mixing process reduces the number of iterations. The low energy HF/3-21G, B3LYP/6-31G\*\*, and PCM B3LYP/aug-cc-pVDZ optimized structures of the *N*-acetyl l-histidine *N*-methyl amide and four water molecule supermolecule were also determined using the HA optimization method and compared to the recently determined thought to be global minimum energy structure.

## LiH の分子軌道エネルギー準位図 — 非経験的ハートリー・フォック法を用いて —

Amih Sagan\*<sup>1</sup>, 長嶋雲兵\*<sup>1</sup>, 寺前裕之, 長岡伸一\*<sup>2</sup> (\*1 産総研ナノシステム, \*2 愛媛大・理) *J. Comp. Chem. Jpn.*, **10**, No. 2, 75-77 (2011).

初心者向けの量子化学の教科書には異核 2 原子分子の例として LiH が取り上げられ、その分子軌道エネルギー準位図が示されている。その図では LiH の  $2\sigma$  軌道のエネルギーが H 原子の 1s 軌道よりも低い軌道エネルギーを持つとが示されているが、非経験的ハートリー・フォック 法を用いるとそれが再現できない。本ノートでは非経験的ハートリー・フォック法で描かれる LiH の軌道エネルギー準位図を示す。用いた基底関数は 6-311++G\*\*である。非経験的ハートリー・フォック計算から得られる図では、 $2\sigma$  軌道の軌道エネルギー(-8.18749eV)は Li の 2s (-5.3392eV) より低く、安定化しているが、H の 1s (-13.60eV) より高く、不安定化している。  $2\sigma$  軌道はおもに H の 1s 軌道で構成されており、H の形式電荷は約 -0.4 である。このように H 周辺に Li の 2s 電子が過剰にあるため、H の 1s 軌道から見ると相対的に電子間反発で不安定化

する。

#### HeH<sup>+</sup>の分子軌道エネルギー準位図

Amih Sagan\*<sup>1</sup>, 長岡伸一\*<sup>2</sup>, 寺前裕之, 長嶋雲兵\*<sup>1</sup> (\*1 産総研ナノシステム, \*2 愛媛大・理) *J. Comp. Chem. Jpn.*, **10**, No. 4, 147-151 (2011).

HeH<sup>+</sup> は異核 2 原子分子の最も簡単なモデルであり、その結合形成は He<sup>+</sup>+H → HeH<sup>+</sup> で表せる共有結合型とエネルギー的に安定な He+H<sup>+</sup> → HeH<sup>+</sup> の配位結合型がある。本ノートでは両者の分子軌道エネルギー準位図を示し、その違いについて説明する。用いた計算方法は HF/6-311++G\*\* である。共有結合型の分子軌道エネルギー準位図では、HeH<sup>+</sup> の  $1\sigma$  軌道の軌道エネルギー(-1.6288a.u.) は H の 1s (-0.4998a.u.) よ り低く、安定化しているが He<sup>+</sup> の 1s (-1.9983a.u.) よ り高く、不安定化している。 $1\sigma$  軌道はおもに He の 1s 軌道で構成されており、HeH<sup>+</sup> の He と H の形式電荷はそれぞれ約 0.3 および 0.7 である。このように H の電子が He<sup>+</sup> 側に寄っているため、He<sup>+</sup> の 1s 軌道から見ると相対的に電子間反発で不安定化するように見える。他方配位結合型の分子軌道エネルギー準位図では、HeH<sup>+</sup> の  $1\sigma$  軌道の軌道エネルギーは H<sup>+</sup> の 1s (-0.4998a.u.) および He の 1s (-0.9176a.u.) より低く、安定化している。He の電子が H<sup>+</sup> 側に寄るため、He の 1s 軌道の 2 つの電子の反発が緩和され安定化する。

# Simultaneous analysis of rotational and vibrational-rotational spectra of DF and HF to obtain irreducible molecular constants for HF

Koui Horiai and Hiromichi Uehara *Chem. Phys.*, **380**, 92-97 (2011)

Analytic expressions of corrections for the breakdown of the Born-Oppenheimer approximation to Dunham's  $Y_{ij}$  with optimal parameters, i.e., determinable clusters of expansion coefficients, are applied to a data analysis of the rotational and vibrational-rotational transitions of HF reported in the literature. All the available spectral lines of the two isotopologues, DF and HF, are simultaneously fitted to a single set of molecular parameters of HF within experimental errors. Fitting of a data set of 595 spectral transitions for DF and HF has generated only 20 minimal independent parameter values, *i.e.*, "irreducible" molecular constants of HF, that are sufficient to precisely generate 82  $Y_{ij}$  coefficients and 144 band constants in total: 41  $Y_{ij}$  and 72 band constants each for DF and HF.

# Solvent dependence of absorption intensities and frequencies of the fundamental and first overtone of NH stretching vibration of pyrrole studied by near-infrared/infrared spectroscopy and density-functional-theory calculations

Y. Futami\*<sup>1</sup>, Y. Ozaki, Y. Hamada\*<sup>2</sup>, M. J. Wojcik\*<sup>3</sup>, Y. Ozaki\*<sup>1</sup> (\*1 Department of Chemistry, School of Science and Technology, Kwansei-Gakuin University, \*2 The Open University of Japan, \*3 Faculty of Chemistry, Jagiellonian University, Poland)

J. Phys. Chem. A. 115, 1194-1198 (2011)

Near-infrared (NIR) and IR spectra were measured for pyrrole in CCl<sub>4</sub>, CHCl<sub>3</sub>, and CH<sub>2</sub>Cl<sub>2</sub> to study solvent dependence of absorption intensities and wavenumbers of the fundamental and first overtone of NH stretching vibration. It was found that the wavenumbers of the NH fundamental and its first overtone decrease in the order of CCl<sub>4</sub>, CHCl<sub>3</sub>, and CH<sub>2</sub>Cl<sub>2</sub>, which is the increasing order for of the dielectric constant of the solvents. Their absorption intensities increase in the same order, and the intensity increase is more significant for the fundamental than the overtone. These results for the solvent dependence of the wavenumbers and absorption intensities of NH stretching bands of pyrrole are quite different from those due to the formation of hydrogen bonds. Quantum chemical calculations of the wavenumbers and absorption intensities of NH stretching bands by using the 1D Schrödinger equation based on the self-consistent reaction field (SCRF)/isodensity surface polarized continuum model (IPCM) suggest that the decreases in the wavenumbers of both the fundamental and the overtone of the NH stretching mode with the increase in the dielectric constant of the solvents arise from the anharmonicity of vibrational potential and their intensity increases come from the gradual increase in the slope of the dipole moment function.

## Infrared diode laser spectroscopy of N<sub>2</sub>-<sup>12</sup>C<sup>18</sup>O<sub>2</sub>

T. Konno, S. Yamaguchi, Y. Ozaki J. Mol. Spectrosc. **270**, 66-69 (2011)

The high-resolution infrared spectrum of  $N_2^{-12}C^{18}O_2$  has been observed in the  $\nu_3$  band (2314 cm<sup>-1</sup>) region of  $^{12}C^{18}O_2$  with diode laser absorption spectroscopy of pulsed molecular beam. The geometry of  $N_2^{-12}C^{18}O_2$  is similar to  $N_2^{-12}C^{16}O_2$ , a T-shaped structure with the nitrogen molecular axis pointing towards the carbon atom. The geometrical parameters of the T-shaped ground-state structure are determined as  $R_{\rm NcmC}$ =3.7285 (5) Å and (90- $\Theta_{\rm NcmCO}$ )=6.85 (3)°. The vibrational band origin of  $N_2^{-12}C^{18}O_2$  corresponding to the  $\nu_3$  mode of  $^{12}C^{18}O_2$  shows a shift of 0.52499 (10) cm<sup>-1</sup> with respect to that of  $^{12}C^{18}O_2$ .

# The stabilities and formation kinetics of some macrocycles with copper (II): crystal structures of some pendant arm macrocycles

Hava Ozay\*<sup>1</sup>, Yakup Baran\*<sup>1</sup> and Hiroshi Miyamae (\*1 Department of Chemistry, Art and Science Faculty, Onsekiz Mart University, Turkey)

J. Coord. Chem., 64(8), 1469-1480 (2011).

Kinetics of complex formation and stability constants of tetra-(2-hydroxpropyl) substituted cyclam  $(L^3)$  and cyclen  $(L^4)$  with copper (II) have been studied in aqueous solution at room temperature. These data are compared to the corresponding parent compounds (cyclam  $L^1$  and cyclen  $L^2$ ) in an attempt to define the effect of pendant arm upon kinetics and stability

constants of the complexes. The kinetics were observed by stopped-flow measurements followed at multiwavelengths. These ligands were chosen to furnish information concerning effect of pendant groups and cavity size on the kinetics and stability of the complexes. Stopped-flow and spectrophotometric titration techniques were used for evaluation of the kinetics and stability constants, respectively. The apparent rate constants increase as  $CuL^3 > CuL^4 > CuL^1 > CuL^2$ . Activation parameters and stability constants of the complexes were estimated. The effect of cavity size on the rate of reaction can be observed in  $CuL^3 > CuL^4$  and  $CuL^1 > CuL^2$  and the effect of pendant groups in  $CuL^3 > CuL^1$  and  $CuL^4 > CuL^2$ . Mechanism of the complex formation reaction is proposed. The enhanced stability of the copper (II) complexes formed with  $L^1$  and  $L^2$  macrocyclic ligands is compared to those formed with analogous pendant arm species.

#### Photorearrangements in Spiro-Conjoined Cyclohexa-2,5-dien-1-one

M. Suzuki, K. Imai, H. Wakabayashi, A. Arita\*<sup>1</sup>, K. Johmoto\*<sup>1</sup>, H. Uekusa\*<sup>1</sup>, and K. Kobayashi (\*1 Department of Chemistry and Material Science, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo)

Tetrahedron, 67, 5500-5506 (2011).

The unexpected formation of cyclohexa-2,5-dien-1-one (6) spiro-conjoined with a dihydrobenzofuran framework, and the photochemical behavior of this compound in solution as well as in the solid state are described. The photoreaction of 6 in solution affords two rearranged products, one (7) accompanied by the enlargement of the oxygen heterocyclic ring and the other (8) accompanied by cyclopentadienone fragmentation. In the solid state, the former is the sole photoproduct of both solvated and desolvated crystals. The latter product was obtained as polycrystalline solids by thermal release of solvent molecules, and its structure was elucidated by ab initio determination from X-ray powder diffraction data followed by the Rietveld refinement.

# Supramolecular Networks in Crystalline Inclusion Complexes Formed from a New Host: 2, 2-Bis(4-hydroxy-3-phenylphenyl)-1*H*-indene-1,3(2*H*)-dione

Kenta Kasugai, Suzumi Hashimoto, Kazunori Imai, Aya Sakon\*<sup>1</sup>, Kotaro Fujii\*<sup>1</sup>, Hidehiro Uekusa\*<sup>1</sup>, Naoto, Hayashi\*<sup>2</sup>, and Keiji Kobayashi (\*1 Department of Chemistry and Material Science, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo \*2 Department of Chemistry, Faculty of Science, Toyama University, Gofuku, Toyama)

Cryst. Growth Des. 11, 4044-4052 (2011).

A scissors-shaped compound, 2, 2-bis (4-hydroxy-3-phenylphenyl)-1H-indene-1,3 (2H) -dione (1), has been prepared as a new host species for crystalline host-guest complexes. Compound 1 afforded complexes of 1:1 host-to-guest ratio with acetone, EtOH, and CH<sub>2</sub>Cl<sub>2</sub>, and a 2:3 complex with benzene. The crystal structures of these complexes were elucidated. In

all four crystals, a side-by-side dimer linked by head-to-tail > C=O---HO- hydrogen bonds is formed and functions as the building unit of supramolecular networks. Except for  $(1)_2$  (benzene)<sub>3</sub>, the complexes featured intermolecular carbonyl-carbonyl interactions resulting in all-planar antiparallel alignment with markedly short C---O distances (< 3.15 Å). In (1) (EtOH), the four-centered interaction including two hydroxyl and two carbonyl groups was observed and designated as a quasi-bifurcated hydrogen bonding motif. Such a four-molecular interaction has been observed to occur widely in crystal structures as proved by database searches from the Cambridge Structural Database (CSD). In all the crystals, the host molecules formed a channel type void occupied by guest molecules. The crystal structure of the desolvated crystals of 1 has been elucidated for its polycrystalline solids by ab initio structure determination from powder X-ray diffraction data followed by the Rietveld refinement.

#### Polymorphism in Solvate Crystals of Indantrione 1,2-Dioxime

Mitsuaki Suzuki and Keiji Kobayashi *Cryst. Growth Des.* **11**, 1814-1820 (2011)

Indantrione 1,2-dioxime (1) afforded crystals solvated by different species of alcohols and in different stoichiometries. Among those, three pairs of polymorphic forms, which are of the same solvent and stoichiometry, were obtained. The crystal structures of those polymorphs, formulated as  $\alpha$ - and  $\beta$ -(1) (MeOH),  $\alpha$ - and  $\beta$ -(1) (MeOH)<sub>1/2</sub>, and  $\alpha$ - and  $\beta$ -(1) (EtOH), were elucidated along with that of (1) (i-PrOH). The common building block in the crystal structures is a centrosymmetric planar dimer linked by bifurcated hydrogen bonding. The dimer is further assembled through alcohol molecules to form a tapelike linear chains. The difference in crystal structure between all pairs of the polymorphs is principally attributed to a distinct hydrogen bonding motif between the dimer and solvated alcohol molecules. Carbonyl-carbonyl interaction is also recognized to play a role in molecular alignment in most cases; the carbonyl groups of neighboring molecules are in close contact and have an all-planar antiparal-lel arrangement.

#### Crystal Structure of Benzene-Solvate of Bis (benzophenone) Azine. A Color Polymorph

Kazunori Imai, Mai Takahashi, Rie Ishii, and Keiji Kobayashi *X-ray Structure Analysis Online*, **27**, 75–76 (2011)

A crystalline complex of bis (benzophenone) azine (BBA), solvated by benzene in BBA: benznene=1:1 ratio, was isolated as yellow crystals, and its crystal structure was determined by single crystal X-ray diffraction analysis at 223 K. The complex crystallizes in the triclinic crystal system in the space group of P-1 (#2) with the cell parameters a=8.646(6) Å, b=9.096 (5) Å, c=9.217(6) Å, a=78.01(2)°,  $\beta$ =64.23(2)°,  $\gamma$ =67.39(2)°, Z=1, and V=601.9(6) A³. Benzene is embedded in a channel running along the c-axis. The yellow color of the complex, in contrast to the colorless solvent-free crystals, is attributed to the planar geometry of the C=N-

#### Hormetic and UV-Protective Effects of Azulene-related Compounds

Jun-ichi Ueki, Aki Shimada, Hiroshi Sakagami<sup>\*1</sup>, and Hidetsugu Wakabayashi (\*1 Department of Endodontics, Meikai University School of Dentistry)

International Journal of In Vivo Research, 25, 41-48 (2011)

We have previously reported a possible anti-inflammatory activity of azulene-, tropolone- and azulenequinone-related compounds. To further pursue the newly discoverd biological activity of these compounds, five compounds that inhibited nitric oxide production by activated macrophages were investigated for their possible hormetic and anti-radiation effects. Materials and Methods. Viable cell numbers of human oral normal cells and three oral squamous cell carcinoma cell lines on treatment with various concentrations of each azulene-related compound was evaluated by MTT method. Apoptosis induction was monitored by caspase-3 activation and DNA fragmentation. Among five compounds, only benzo[b]cyclohepta[e][1,4]thiazine slightly stimulated the growth of all three normal cell types, but not tumor cell lines, at concentrations slightly higher than cytotoxic concentrations. Using a newly established evaluation system for UV-induced cellular damage, we found that this compound slightly but significantly protected the cells from UV-induced cellular injury, and its effect was synergistically enhanced by sodium ascorbate. These data suggest the possible application of benzo[b]cyclohepta[e][1,4]thiazine in UV protection therapy.

#### Quest for Anti-inflammatory Substances Using IL-1b-stimulated Gingival Fibroblasts

Manami Ono, Kaori Kantoh, Jun-ichi Ueki, Aki Shimada, Hidetsugu Wakabayashi, Tomohiko Matsuda\*<sup>1</sup>, Hiroshi Sakagami\*<sup>1</sup>, Hidefumi Kumada\*<sup>2</sup>, Nobushiro Hamada\*<sup>2</sup>, Madoka Kitajima\*<sup>3</sup>, Hiroshi Oizumi\*<sup>3</sup>, and Takaaki Oizumi\*<sup>3</sup> (\*1 Meikai University School of Dentistry, \*2 Department of Oral Microbiology, Kanagawa Dental College, \*3 Daiwa Biological Research Institute Co., Ltd.,)

International Journal of In Vivo Research, 25, 763-768 (2011)

We have previously reported that azulene-related compounds, and alkaline extract of Sasa senanensis Rehder potently inhibited nitric oxide (NO) production by lipopolysaccharide (LPS)-stimulated mouse macrophages. We investigated here whether they can inhibit proinflammatory cytokine production by activated human gingival fibroblast (HGF). HGF was established from the periodontal tissues of extracted tooth. Viable cell number was determined by MTT method. Production of Prostaglandin  $E_2$  (PGE<sub>2</sub>) and cytokines was determined by enzyme immunoassay, and enzyme-linked immunosorbent assay, respectively. Interleukin (IL)-1 $\beta$  did not inhibit, but rather slightly stimulated the growth of HGF cells. IL-1 $\beta$  stimulated the production of PGE<sub>2</sub>, IL-6, IL-8 and monocyte chemotactic protein-1 very potently, but not that of nitric oxide and tumor necrosis factor- $\alpha$ . Native LPS and synthetic lipid A from

E coli and P gingivalis was much less stimulatory. Dexamethasone, not indomethacin, was an efficient inhibitor of IL-8 production. Among five azulene-related compounds, benzo[b]cyclohepta[e][1,4]thiazine most potently inhibited the IL-8 production by HGF cells, as well as NO production by activated RAW264.7 cells. The alkaline extract of Sasa senanensis Rehder significantly inhibited IL-8 production, without affecting the cell viability. The present system may be applicable for use in the search for anti-gingivitis substances.

## **BIOLOGY**

A recessive lethal gene, l-Cy, found in a natural population of Drosophila melanogaster.

K. Kosuda

Drosophila Information Service 94: 157-158 (2011)

The In(2LR) Cy chromosome has been used to make the second chromosomes of Drosophila ila melanogaster homozygous as a most useful balancer for the study of deleterious gene in natural populations. The Cy balancer is lethal in the homozygous condition and has a complicated inversion both in left and right arms. Lots of second chromosomes were extracted from several natural populations and they were tested whether they carry recessive lethal mutations. Their lethality was also examined in the heterozygous condition with the Cy balancer. A recessive lethal allele that kills the heterozygotes with In(2LR) Cy balancer was detected from a natural population in Szentendre near Budapest. This lethal gene is tentatively named l-Cy. It is highly probable that l-Cy is a small deletion in the second chromosome. The discovery of l-Cy strongly supports for the idea that the Cy balancer chromosome caries a recessive lethal gene.

## 2. Books, Reviews and Other Printings

## **BIOLOGY**

キイロショウジョウバエ第2染色体のバランサーに隠されている劣性致死遺伝子, *L-Cy* 

小須田和彦

城西大学研究年報(自然科学編), 34, 1-8 (2011)

ヒト集団における選択交配 I. 性的成熟年令

小須田和彦

城西大学研究年報(自然科学編), 33, 1-8 (2010)

## **EARTH SCIENCE**

三浦半島における水中堆積物 ――三浦層群三崎層下部の標準地質柱状図 ――

谷口英嗣

城西大学研究年報(自然科学編), 34, 61-68 (2011)

## 3. Oral Presentations

#### **MATHEMATICS**

#### Factorizations of Automorphisms of a Module over a Local Ring

H. Ishibashi

International Conference on Mathematics of Date, 2010-2011, Allahabad, India, December 31, 2010-January 4, 2011

#### 順序保存力学系と生物分子モーターモデルへの応用

荻原俊子

NSC セミナー, 北海道大学, 2011年2月

# Existence and asymptotic stability of periodic fronts to some quasilinear parabolic equations

Toshiko Ogiwara

Mathematics and Biology: a READILAB Seminar Day, University of Paris Diderot-Paris 7 (France), 2011年9月

# Convergence results in order-preserving dynamical systems and applications to a molecular motor system

Toshiko Ogiwara

Reaction-Diffusion Systems in Mathematics and Life Sciences, University of Montpellier 2 (France),  $2011 \pm 9 \, \text{F}$ 

#### Hopf mappings and functional equitions of the Fourier transforms of polynomials

小木曽岳義

Workshop of Teichmueller Spaces and related topics (Sakado), 2011年1月

#### 広義 Hurwitz 問題と慨均質ベクトル空間

小木曽岳義

研究集会「慨均質ベクトル空間の分類とその応用」(つくば), 2011年2月

#### Fourier transforms of polynomials and Prehomogeneous vector spaces

Takeyoshi Kogiso

Pukyong National University, Pusan Korea, 2nd Nonlinear Analysis and Convex Analysis International Conference. 2011年8月

#### Representation of Clifford algebras and local functional equation

小木曽岳義

鳥取市ふれあい県民会館講義室、表現論ワークショップ、2011年12月

#### A Sufficient and Necessary Condition of Uncertain Distribution

Z. Peng and K. Iwamura

日本 OR 学会「DP 部会合同シンポジウム 2011」(千葉), 2011 年 10 月

#### **PHYSICS**

#### Ne<sup>4+</sup>-He 衝突における一電子移行反応の二重微分断面積測定

伊藤 陽

日本物理学会第 66 回年次大会. 新潟大学 (中止: Web 発表). 2011 年 3 月. 25aRA-5

#### **CHEMISTRY**

#### TD DFT 法による分子内プロトン移動反応に関する研究

寺前裕之,長岡伸一\*<sup>1</sup>,長嶋雲兵\*<sup>2</sup> (\*1 愛媛大院理, \*2 産総研) 第 14 回理論化学討論会(岡山), 2011 年 5 月,講演要旨集 2P01

#### LiH の分子軌道エネルギー準位図 — 非経験的ハートリー・フォック法を用いて —

Amih Sagan\*<sup>1</sup>, 長嶋雲兵\*<sup>1</sup>, 寺前裕之, 長岡伸一\*<sup>2</sup> (\*1 産総研, \*2 愛媛大) 日本コンピュータ化学会 2011 年春季年会(東京), 2011 年 6 月, 講演要旨集 3P01

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寺前裕之, 丸尾容子\*<sup>1</sup>, 中村二朗\*<sup>1</sup> (\*1 NTT 環境エネルギー研) 日本コンピュータ化学会 2011 年春季年会(東京), 2011 年 6 月, 講演要旨集 3P06

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Hiroyuki Teramae, Yasuko Y. Maruo\*¹, Jiro Nakamura\*¹ (\*1 NTT Energy & Environmental Laboratories)

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