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Editorial Board

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1. Abstracts of Papers Published in Journals

MATHEMATICS

Fuzzy Facility Location-Allocation Problem under Hurwicz Critrion

M. Wen* and K. Iwamura (* Tsinghua University, Beijing)
European Journal of Operational Research, **184**, 627–635 (2008)

Facility location-allocation (FLA) problem has been widely studied by operational researchers due to its many practical applications. Many researchers have studied the FLA problem in a deterministic environment. However, the models they proposed cannot accommodate satisfactorily various customer demands in the real world. Thus, we consider the FLA problem with uncertainties. In this paper, a new model named α–cost model under the Hurwicz criterion is presented with fuzzy demands. In order to solve this model, the simplex algorithm, fuzzy simulations and a genetic algorithm are integrated to produce a hybrid intelligent algorithm. Finally, some numerical examples are presented to illustrate the effectiveness of the proposed algorithm.

Fuzzy Chance-Constrained Programming with Linear Combination of Possibility Measure and Necessity Measure

L. Yang* and K. Iwamura (* Beijing Jiaotong University, Beijing)
Applied Mathematical Sciences, **2**, 2271–2288 (2008)

Based on the possibility measure and necessity measure, m_λ–measure is presented and some mathematical properties of m_λ–measure are also obtained, including continuity, monotonicity, subadditivity, and so on. Critical values of fuzzy variable with respect to m_λ–measure are introduced and are employed to construct the fuzzy chance-constrained programming models. To solve the models, genetic algorithm based on fuzzy simulation is designed. Finally, two numerical examples are given to show applications of the models and algorithm.

Preparedness for the Spread of Influenza: Prohibition of Traffic, School Closure, and Vaccination of Children in the Commuter Towns of Tokyo

H. Yasuda, N. Yoshizawa*1, M. Kimura*2, M. Shigematsu*3, S. Kawaji*4, M. Oshima*3, K. Yamamoto*4, K. Suzuki*3,5 (*1 Mitsubishi Research Institute, *2 Japan Anti-Tuberculosis Association, *3 the National Institute of Infectious Disease, *4 the International Medical Center in Japan, *5 Chiba Univ.)
Journal of urban health, **85**, 619–635 (2008)

In Greater Tokyo, many people commute by train between the suburbs and downtown Tokyo for 1 to 2 h per day. The spread of influenza in the suburbs of Tokyo should be studied, including the role of commuters and the effect of government policies on the spread of disease. We analyzed the simulated spread of influenza in commuter towns along a suburban railroad, using the individual-based Monte Carlo method, and validated this analysis using surveillance data of the infection in the Tokyo suburbs. This simulation reflects the mechanism of the real spread of influenza in commuter towns. Three measures against the spread of influenza were analyzed: prohibition of traffic, school closure, and vaccination of school children. Prohibition of traffic was not effective after the introduction of influenza into the commuter towns, but, if implemented early, it was somewhat effective in delaying the epidemic. School closure delayed the epidemic and reduced the peak of the disease, but it was not as effective in decreasing the number of infected people. Vaccination of school children decreased the numbers not only of infected children but also of infected adults in the regional communities.

CHEMISTRY

Crystal Structure of PbI_2(enthylenediamine)$_2$, catena-μ-Ethylenediamine-ethylenediaminediiodolead(II) at −150°C

Hiroaki Yamanaka, Goro Hihara and Hiroshi Miyamae
Analytical Sciences, **24**, x121–x122 (2008)

The title complex is triclinic, $P\bar{1}$, $a = 7.585(3)$, $b = 7.688(4)$, $c = 12.737(6)$ Å, $\alpha = 83.22(2)$, $\beta = 73.731(19)$, $\gamma = 63.38(2)^\circ$, $V = 637.4(5)$ Å^3, and $Z = 2$ at −150℃; R is 0.0242. The structure shows a one dimensional polymer extending along $[\bar{1}11]$ with two crystallonraphically independent inversion centers lying at the middle of the C–C bond of each bridging ethylenediamine(en). The Pb atom is coordinated by two I atoms and four N atoms: the two I atoms occupy a *cis*-positoin, the two N atoms of a chelatingen lie opposed to them, and the four atoms lie in a plane containing the Pb atom; the other two N atoms of the bridging en ligands lie at both axial positions. Since the I–Pb–I angle is 144.57(1)° wide, the Pb environment geometry might be described to be a distorted pentagonal bipyramid, providing a stereochemically active lone pair of electrons of the Pb atom may occupy one coordination site.

Molecular Structure Optimezation and Molecular Dynamics Using Hamiltonian Algorithm: Structure of Benzodiazepine Minor Tranquilizers — Towards Non-Empirical Drug Design —

Hiroyuki Teramae, Kazushige Ohtawara[*1], Takayoshi Ishinomoto[*2, *3] and Umpei Nagashima[*2, *3]
(＊1 ART Adaptive Communication Research Laboratories, ＊2 National Institute of

Advanced Industrial Science and Technology, ＊3 CREST, Japan Science and Technology Agency）
Bull. Chem. Soc. Jpn., **81**, 1094–1102（2008）

We have studied the molecular dynamics of the benzodiazepine and thienodiazepine minor tranquilizers using a Hamiltonian Algorithm combined with ab inito molecular orbital methods. The HA utilizes classical dynamics for optimization of the complicated systems. We show that the HA gives an effective search of the potential energy surfaces and we can find an energy minimum even if we start from another energy local minimum. The conformers of these tranquilizers are calculated after computation of the molecular dynamics. Relations between electronic states and strength of tranquilizers are studied for about 17 species of benzodiazepines and thienodiazepines which are sold in the Japanese market as minor tranquilizers. The orbital energy levels of the next highest occupied molecular orbital（next-HOMO or HOMO－1）are found to be strongly related to the strength of the tranquilizers. The simple structure activity relationship is obtained by considering just one-electron properties, i.e., the molecular orbital energies.

H/D isotope effect of methyl internal rotation for acetaldehyde in ground state as calculated from a multicomponent molecular orbital method

Takayoshi Ishimoto^{*1,*2}, Yasuyuki Ishihara, Hiroyuki Teramae, Masaaki Baba^{*3} and Umpei Nagashima^{*1,*2}（＊1 National Institute of Advanced Industrial Science, ＊2 CREST, Japan Science and Technology Agency, ＊3 Kyoto University）
J. Chem. Phys., **128**, 184309（2008）

We have analyzed the differences in the methyl internal rotation induced by the H/D isotope effect for acetaldehyde（CH_3CHO）and deuterated acetaldehyde（CD_3CDO）in ground state by using the multikomponent molecular orbital（MC_MO）method, which directly accounts for the quantum effects of protons and deuterons. The rotational constant of CH_3CHO was in reasonable agreement with experimental one due to the adequate treatment of the protonic quantum effect by the MC_MO method. The C–D bond distances were about 0.007 Å shorter than the C–H distances because of the effect of anharmonicity of the potential. The Mulliken population for CD_3 in CD_3CDO is lager than that for CH_3 in CH_3CHO because the distribution of wave functions for the deuterons was more localized than that for the protons. The barrier height obtained by the MC_MO method for CH_3CHO was estimated as 401.4 cm^{-1}, which was in excellent agreement with the experimentally determined barrier height. We predicted the barrier height of CD_3CDO as 392.5 cm^{-1}. We suggest that the internal rotation of the CD_3 group was more facile than that of the CH_3 group because the C–D bond distance was observed to be shorter than the C–H distance. The localized electrons surrounding the CD_3 group in CD_3CDO caused the extent of hyperconjugation between the CD_3 and CDO groups to be smaller than that in the case of CH_3CHO, which may have also contributed to the observed differences in methyl internal rotation. The differences in bond distances and electronic populations induced by the H/D isotope effect were controlled by the difference in the distribution of wavefunctions between the protons and deuterons.

H/D isotope effect in methyl torsional interaction of acetone as calculated by a multicomponent molecular orbital method

Takayoshi Ishimoto*[1,*2] Yasuyuki Ishihara, Hiroyuki Teramae, Masaaki Baba*[3] and Umpei Nagashima*[1,*2] (*1 National Institute of Advanced Industrial Science, *2 CREST, Japan Science and Technology Agency, *3 Kyoto University)
J. Chem. Phys., **129**, 214116 (2008)

We analyzed the H/D isotope effect in the methyl torsional interactions accompanying two methyl internal rotations for acetone (CH_3COCH_3) and deuterated acetone (CD_3COCD_3 and CH_3COCD_3) in the ground state by using the multicomponent molecular orbital (MC_MO) method, which directly accounts for the quantum effects of protons and deuterons. Our estimated rotational constants and moments of inertia for CH_3COCH_3 and CD_3COCD_3 agreed well with the experimental results because of the adequate treatment of protonic and deuteronic quantum effects afforded by the MC_MO method. Because the C–D bond distance in the CD_3 group was shorter than the C–H distance in CH_3 owing to the anharmonicity of the potential, the difference in potential energy surfaces of CH_3COCH_3, CD_3COCD_3, and CH_3COCD_3 was strongly related to the differences induced in geometrical parameters by the H/D isotope effect. The potential energy obtained by the MC_MO method was estimated as 290.88 cm^{-1} for CH_3COCH_3, which is well agreed with the experimental results. For CH_3COCD_3, two potential energies were obtained for CH_3 and CD_3 internal rotations. The MC_MO method successfully elucidated the H/D isotope effect for methyl-methyl repulsive interactions by allowing the adequate treatment of protonic and deuteronic wave functions. The potential energies and bond distances associated with methyl internal rotation induced by the HID isotope effect were also controlled by the distribution ol wave functions of protons and deuterons.

Study on Raffenetti's P File Format in Conventional *Ab Initio* Self-Consistent-Field Molecular Orbital Calculations in Parallel Computational Environment

Hiroyuki Teramae and Kazushige Ohtawara* (* ATR Adaptive Communication Research Laboratories)
J. Comp. Chem. Japan., **7**, 179–184 (2008)

We compare the CPU time and the wall clock time of the Raffenetti's P file algorithm with the usual algorithm on the two electron integrals storing with four suffixes of the *ab initio* Hartree-Fock calculations. The calculations are performed with the flutoprazepam, triazolam, clotiazepam, etizolam, and flutazolam molecules. These molecules are all minor-tranquilizers with the benzodiazepine or thienodiazepine backbone. The 3-21 G basis sets are employed. Almost in all cases, P file algorithm gave slower speed than the usual algorithm. The number of two electron integrals increases almost two times larger than the usual algorithms. In a large molecule, the matrix of the two electron integrals becomes very sparse and the recombination of the integrals just increases the total number of the integrals. It is concluded that the P method sometimes calculates faster but sometimes does not. In large scale calculations, it should be suggested to perform a test calculation to confirm which method is faster prior to the real calculations.

Novel push-pull π-conjugated compounds suffering steric hindrance between donor and acceptor subunits

D. Masuda, H. Wakabayashi, H. Miyamae, H. Teramae, K. Kobayashi
Tetrahedron Lett., **49**, 4342–4345 (2008)

A novel push-pull compound with a 1,3-bis(dicyanomethylene)indan-2-ylidene moiety as an acceptor subunit has been prepared along with its two derivatives. These molecules are severely distorted from its planar structure and in solution undergo dynamic interconversion between bent structures. The structural features and UV-vis spectroscopic results suggest that the zwitter-ionic nature of the molecule is enhanced in the ground state, which is also supported theoretically by density functional calculations.

Dynamic Behavior of Cyclic Hemiacetals of 2-Hydroxy-2-(2-hydroxyphenyl)-1,3-indandione Derivatives

Suzumi Hashimoto, Natsumi Sakuma, Hidetsugu Wakabayashi, Hiroshi Miyamae and Keiji Kobayashi
Chemistry Letters, **37**, 696–697 (2008)

The crystalline product obtained by the reaction of ninhydrin with phenol has been confirmed by X-ray analysis to take an intramolecular hemiacetal structure of the title compound. In solution, however, its structure was revealed to be in dynamic internal conversion between the enantiomeric pairs of the hemiacetal form, resulting in a time-averaged structure of *Cs* symmetry. These results were deduced from the variable-temperature ^{1}H-NMR spectra, which showed the splitting of the two broad signals due to the indan-1,3-dione moiety into four signals at about −45℃. The activation free energy was estimated by the coalescence temperature method.

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

Juri Takahashi, Takashi Sekine, Masayuki Nishishiro, Atsuhiro Arai, Hidetsugu

Wakabayashi, Teruo Kurihara, Ken Hashimoto*[1], Kazue Satoh*[2], Noboru Motohashi*[3] and Hiroshi Sakagami*[1] (*1 Department of Endodontics, Meikai University School of Dentistry, *2 Analysis Center, School of Pharmaceutical Sciences, Showa University, *3 Meiji Pharmaceutical University)
Anticancer Res., **28**, 171–178 (2008)

The effect of twenty trihaloacetylazulene derivatives with one halogen atom, on nitric oxide (NO) production by mouse macrophage-like cells Raw 264.7 was investigated. 2-Methoxyazulenes and 2-ethoxyazulenes exhibited comparable cytotoxicity. Trichloroacetylazulenes generally exhibited higher cytotoxicity, as compared with the corresponding trifluoroacetylazulenes. Substitution of chloride, bromide or iodine at the C-3 position further enhanced their cytotoxicity. All of these compounds failed to stimulate the Raw 264.7 cells to produce detectable amounts of NO, but did inhibit NO production by LPS-activated Raw 264.7 cells to different extents. Compounds 1-trichloroacetyl-2-methoxyazulene and 1-trichloroacetyl-2-ethoxyazulene, with less compared to cytotoxic activity, inhibited NO production to the greatest extent, producing the highest selectivity index (SI) of >24.7 and >28.7, respectively. This was accompanied by the efficient inhibition of inducible NO synthase (iNOS) mRNA expression, but not of iNOS protein abundance. The present study suggests that the inhibitory effects of trifluoroacetylazulenes and trichloroacetylazulenes on NO production by activated macrophages might be derived from the perturbation of NO anabolism (inhibition of iNOS mRNA expression and possibly the inactivation of iNOS protein) rather than NO catabolism (NO scavenging).

Tumor-specific Cytotoxicity and Type of Cell Death Induced by Benzocycloheptoxazines in Human Tumor Cell Lines

Hiromi Murayama, Kaori Miyahara, Hidetsugu Wakabayashi, Teruo Kurihara, Ken Hashimoto*[1], Osamu Amano*[1], Hirotaka Kikuchi*[1], Yukio Nakamura*[1], Yumiko Kanda*[1], Shiro Kunii*[1], Noboru Motohashi*[2] and Hiroshi Sakagami*[1] (*1 Department of Endodontics, Meikai University School of Dentistry, *2 Meiji Pharmaceutical University)
Anticancer Res., **28**, 1069–1078 (2008)

Twenty-six benzocycloheptoxazine derivatives were investigated for their tumor-specific cytotoxicity and apoptosis-inducing activity against three human normal cell and four human tumor cell lines. Benzo[*b*]cyclohepta[*e*][1,4]thiazine exhibited very weak cytotoxicity, whereas its 6,8,10-tribromo derivative exhibited higher cytotoxicity and tumor specificity (TS=5.6). 6*H*-Benzo[*b*]cyclohepta[*e*][1,4]diazine and its cation exhibited no tumor specificity. Among eighteen benzo[*b*]cyclohepta[*e*][1,4]oxazine derivatives, 6,8,10-tribromo, 6-bromo-2-methyl, and 6-bromo-2-chloro derivatives showed the highest tumor-specific cytotoxicity (TS=12.5, 9.1 and 11.5, respectively). 14*H*-[1,4]Benzoxazino[3',2': 3,4]cyclohepta[1,2-*b*][1,4]benzoxazine and its 7-bromo and 7-isopropyl derivatives had much lower cytotoxicity and tumor-specificity. 6,8,10-tribromo, 6-bromo-2-methyl, and

6-bromo-2-chloro derivatives at 50% cytotoxic concentration (CC_{50}) induced internucleosomal DNA fragmentation and caspase activation in HL-60 cells. On the other hand, these compounds induced apoptosis only at concentrations higher than CC_{50} in HSC-2 cells and failed to induce apoptosis in FISC-4 cells. 6,8,10-tribromo, 6-bromo-2-methyl, and 6-bromo-2-chloro derivatives induced the formation of acidic organelles as. Transmission electron microscopy demonstrated the induction of moderate enlargement of mitochondria, the endoplasmic reticulum and nuclear membrane, and the vacuolation of the endoplasmic reticulum and the presence of a number of lamellar body-like organelles. These results indicate the diversity of the type of cell death induced by benzocycloheptoxazine derivatives in human tumor cell lines.

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

Kaori Miyahara, Hiromi Murayama, Hidetsugu Wakabayashi, Teruo Kurihara, Ken Hashimoto*[1], Kazue Satoh*[2], Noboru Motohashi*[3] and Hiroshi Sakagami*[1] (*1 Department of Endodontics, Meikai University School of Dentistry, *2 Analysis Center, School of Pharmaceutical Sciences, Showa University, *3 Meiji Pharmaceutical University)
Anticancer Res., **28**, 2657-2662 (2008)

Twenty-six benzocycloheptoxazine derivatives were investigated for their effect on nitric oxide (NO) production by lipopolysaccharide (LPS)-stimulated mouse macrophage-like RAW264.7 cells. Benzo[*b*]cyclohepta[*e*][1,4]thiazine most effectively inhibited the LPS-stimulated NO production at noncytotoxic concentrations. 6*H*-Benzo[*b*]cyclohepta[*e*][1,4]diazine cation, and benzo[*b*]cyclohepta[*e*][1,4]oxazine and its 6-bromo derivative also efficiently inhibited the LPS-stimulated NO production. Another sixteen benzo[*b*]cyclohepta[*e*][1,4]oxazine derivatives, 14*H*-[1,4]benzoxazino[3,2': 3,4]cyclohepta[1,2-*b*][1,4]benzoxazine and its 7-bromo- and 7-isopropyl- derivatives were slightly less active (selectivity index (SI)=8.3-66). Bromination of benzo[*b*]cyclohepta[*e*][1,4]thiazine, benzo[*b*]cyclohepta[*e*][1,4]oxazine and 2-methylbenzo[*b*]cyclohepta[*e*][1,4]oxazine at C-6, C-8 or C-10 positions resulted in the significant reduction of the inhibitory activity. The observed inhibitory activity of benzo[*b*]cyclohepta[*e*][1,4]thiazine and its 6,8-dibromo derivatives were not due to the reduction of the intracellular level of inducible NO synthase protein (based on Western blot analysis), nor to NO scavenging activity. These results suggest the possible anti-inflammatory action of benzocycloheptoxazine derivatives via inhibition of LPS-activated macrophages.

Synthesis of 1,2-Azulenequinone Derivatives by Bromine-Oxidation

Hidetsugu Wakabayashi, Osamu Irinamihira, Satoshi Shibata, Teruo Kurihara, Yuzuru Uchiyama*[1], Akira Ohta*[1] and Kunihide Fujimori*[1] (*1 Department of Chemistry, Faculty of Science, Shinshu University)

Heterocycles, **76**, No.2, 1133–1140 (2008)

Treatment of 2–hydroxyazulene with 3 equiv. of $C_5H_5N \cdot HBr_3$ in aqueous THF-AcOH at 0℃ for 1 h afforded 1,1,3–tribromoazulene–2–one. 3–Bromo–1,2–azulenequinone was obtained by the hydrolysis of 1,1,3–tribromoazulene–2–one in the presence of Ag_2O. Annulated 6–bromoazuleno[1,2–*b*]quinoxaline was readily obtained by the reaction of 3–bromo–1,2–azulenequinone with *o*–phenylenediamme.

Nanorods of Endohedral Metallofullerene Derivative

T. Tsuchiya[*1], R. Kumashiro[*2], K. Tanigaki[*2], Y. Matsunaga[*1], M. O. Ishitsuka[*1], T. Wakahara[*1], Y. Maeda[*1], Y. Takano[*1], M. Aoyagi[*1], T. Akasaka[*1], M. T. H. Liu[*3], T. Kato, K. Suenaga[*4], J. S. Jeong[*4], S. Iijima[*4], F. Kimura[*5], T. Kimura[*5] and S. Nagase[*6] (*1 Center for Tsukuba Advanced Research Alliance University of Tsukuba, *2 Department of Physics, Graduate School of Science, Tohoku University, *3 Department of Chemistry, University of Prince Edward Island, *4 National Institute of Advanced Industrial Science and Technology (AIST), *5 Division of Forest and Biomaterials Science, Graduate School of Agriculture, Kyoto University, *6 Institute for Molecular Science)
J. Am. Chem. Soc., **130**, 450–51 (2008)

Formation of crystalline fibers of C_{60} with a diameter of submicrometers by a liquid-liquid interfacial precipitation method was reported. The formation of crystals of endohedral metallofullerene, however, remains difficult. We have successfully obtained the columnar crystals of endohedral metallofullerene derivative La@ C_{82} (Ad: adamantylidene) by slow evaporation and clarified its packing structure. Chemical derivatization is one of the efficient step for accomplishing the orderly alignment of endohedral metallofullerenes.

Three-metal-center spin interactions trough the intercalation of metal azapophines and pophines into an organic pillared coordination box

K. Ono*, M. Yoshizawa*, T. Kato and M. Fujita* (* Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo)
Chem. Commun., 2328–30 (2008)

We report a unique approach to form linear Cu(II)–M–Cu(II) arrays (M=Cu(II), Pd(II), and Co(II)) through the intercalation of metal azaporphines and porphines into an organic pillared coordination box. The box self-assembles from two panels, three pillars and six Pd(II) hinges. In this strategy, the metal porphine/azaporphine is a cartridge of metal ions and, in principle, any metals can be arrayed in the box by selecting the cartridge. When three Cu(II)–azaporphine cartridges are intercalated, a quartet state of the interacting three Cu(II) centers is observed.

Trimacrocyclic arylamine and its polycationic states

A. Ito[*1], Y. Yamagishi[*1], K. Fukui[*1], S. Inoue[*1], Y. Hirao[*1], K. Furukawa[*2], T. Kato and K. Tanaka[*1] (*1 Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, *2 Institute for Molecular Science)
Chem. Commun., 6573–75 (2008)

Alternating meta-phenylene- and para-phenylene-linked oligoarylamines are considered as promising molecular parts for the molecule-based electronics due to their intriguing magnetic and electronic properties. We can employ them as the component pieces to prepare the two- and/or three-dimensionally structured oligoarylamines. Expectedly, these molecules were oxidized into di(radical cation) with parallel spin-alignment.

An N-substituted azal[1_4]metacyclophane tetracation: a spin-quintet tetraradical with four para-phenylenediamine-based semi-quinone moieties

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Chem. Commun., 3242–44 (2008)

We focused on nitrogen-bridged metacyclophanes (aza[1n]metacyclophanes), and reported the preparation and properties of a series of these compounds. When nitrogen atoms are incorporated as bridging units into aromatic compounds, they afford multi-redox activity. In particular, polyarylamines, in which meta-phenylenes are connected by nitrogen bridging units, can be expected to become high-spin materials. After an exhaustive oxidation procedure, the poly(radical cation)s of several oligoarylamines are found to be in high spin states.

Does Gd@C_{82} Have an Anomalous Endohedral Structure? Synthesis and Single Crystal X-ray Structure of the Carbene Adduct

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J. Am. Chem. Soc., **130**, 12840–41 (2008)

We have carried out the single crystal X-ray crystallographic analysis of the Gd@C_{82} carbene adduct (Gd@C_{82}((Ad: adamantylidene)) together with theoretical calculations.

These results do not support the anomalous structure of Gd@C_{82}.

Metal-oxide photoassisted degradation of binary systems of cationic/anionic surfactants and their components in aqueous dispersions

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J. Adv. Oxid. Technol., **11**, pp.222–230 (2008)

The TiO_2 photo-assisted degrdns. of a series of anionic (dodecylbenzenesulfonate DBS; dodecylsulfonate, DoS) and cationic (hexadecyltrimemylammonium, HTAB; benzyldodecyldimethyl- ammonium BDDAB; and dodecylpyridinium, C12–PC) surfactants were examd. in aq. media along with their cationic/anionic 1: 1 binary complexes: (i) HTAB/DBS, (ii) BDDAB[DoS and (iii) C12–PC/DoS. The processes were monitored by surface tension measurements, by total org. carbon (TOC) assays and carbon dioxide evolution. Some hydroxylated intermediates of the BDDAB system were identified by TOF–MS techniques. The degrdn. of the anionic surfactants was significant involving prior adsorption of the species on the pos. charged metal-oxide particle surface. By contrast, the degrdn. of the cationic surfactants was rather limited owing to lack of adsorption on the TiO_2 surface under the same conditions. The biodegrdn. of the DBS, HTAB, BDDAB and C12–PC surfactants was also examd. using municipal sludge bacteria. Only the anionic DBS surfactant biodegraded to ca. 65% within 14 days of incubation; the others failed to biodegrade even after 28 days of incubation. An adsorption model is proposed for the binary complexes on the metal-oxide surface.

Successful Scission of a Recalcitrant Triazinic Ring. The photoassisted total breakup of cynuric acid in ozonized TiO_2 aqueous dispersions in the presence of an electron acceptor (H_2O_2)

I. Yanagisawa*[1], T. Oyama, N. Serpone*[2] and H. Hidaka*[1] (*1 Frontier Reserch Center for the Global Environment Science, Meisei University, *2 Dipartimento di Chimica Organica, Università di Pavia, Via Taramelli 10, Pavia 27100, Ita1y)

J. Phys. Chem., C, **112**, pp.18125–18133 (2008)

The oxidative breakup of the highly recalcitrant cyanuric acid ring was examd. in UV-irradiated oxygen- and ozone-satd. TiO_2 suspensions at pH 12.0 and natural pH 5.6. The breakup and mineralization of cyanuric acid were assayed by total org. carbon (TOC) detns. (loss of TOC in soln. being equiv. to CO_2 formation); intermediates and other final products were detd. by HPLC ion chromatog. (IC). Final reaction products were thus CO_2 gas and NO_{3-} and NH_{4+} ions. The quantity of the ring nitrogens converted to nitrate and ammonium ions in soln. quantified the degree of mineralization of the substrate, as did the level of TOC loss. Complete mineralization of this recalcitrant substrate occurred in the presence of H_2O_2 (optimal concn., 0.016M) in alk. media under UV irradn. that normally cannot be degraded by the typical TiO_2–photoassisted procedures, even in alk. media. In particular, the enhanced effect of O_3/H_2O_2 on the breakup of the triazinic ring and its ultimate mineralization was of greater significance than any adsorption of the substrate under alk. conditions. Possible orientations of cyanuric acid toward the TiO_2 particle surface have been inferred from theor. calcns. of point charges, whereas the positions of possible attack of the substrate by surface-bound or free OH radicals have been inferred from frontier electron d. calcns.

Photoassisted dehalogenation and mineralization of chloro/fluoro-benzoic acid derivatives in aqueous media

H. Hidaka*[1], H. Honjou*[1], T. Koike*[1], Y, Mitsutsuka*[1], T. Oyama and N. Serpone*[2] (*1 Frontier Reserch Center for the Global Environment Science, Meisei University, *2 Dipartimento di Chimica Organica, Università di Pavia, Via Taramelli 10, Pavia 27100, Italy)
J. Photochem. Photobiol. A: Chem., **197**, pp.115–123 (2008)

The photoassisted dehalogenation and mineralization of chloro/fluoro-benzoic acid derivs. occurring at the TiO_2/H_2O interface under oxygen-satd. and UV-light exposure were examd. by UV absorption spectroscopy, ion chromatog. and time-of-flight (TOF) mass spectrometry to identify intermediate products. Contrary to defluorination, dechlorination occurred readily, presumably because of the weaker C–Cl bond relative to the C–F bond. Photodegrdn. through arom. ring cleavage also occurred fairly rapidly followed by the ultimate evolution of CO_2 gas through prior formation of formate and bicarbonate species. When neg. inductive effect groups, such as the chloro and fluoro groups, are positioned ortho and para to the carboxylic acid group, as in the 2Cl–4F–BA, 2Cl–6F–BA, and 4Cl–2F–BA derivs., dechlorination was faster than when the chioro group was meta to the carboxylic acid group. Theor. calcd. frontier election densities and point charges of all the atoms in the Cl/F–BA derivs. are given. Plausible steps in the photo-degrdn./-mineralization of these substrates are discussed.

2. Books, Reviews and Other Printings

MATHEMATICS

インフルエンザ伝播の数理モデル

安田英典，鈴木和男*（* 千葉大学）
医学のあゆみ，**224**, No. 11863-864（2008）

CHEMISTRY

Theoretical Studies of Phenothiazines, Benzo[*a*]phenothiazines and Benz[*c*]acridines

Teruo Kurihara, Kazumi Shinohara, Makoto Inabe, Hidetsugu Wakabayashi, Noboru Motohashi[*1], Hiroshi Sakagami[*2]and Joseph Molnar[*3]（*1 Meiji Pharmaceutical University, *2 Division of Pharmacology, Department of Diagnostic and Therapeutic Sciences, Meikai University School of Dentistry, *3 University of Szeged, Institute of Microbiology and Immunobiology, Albert Szent-Gyorgyi Medical Center）
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EARTH SCIENCE

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バレーボール国際試合における医事活動について

田中喜久美*[1]，川之上　豊*[2]，明石正和（*1 甲府看護専門学校，*2 大妻女子大学）
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3. Oral Presentations

MATHEMATICS

Product Credibility Space with Credibilistically Independent fuzzy variables

K. Iwamura and M. Kageyama* (* The Institute of Statistical Mathematics)
日本オペレーションズ・リサーチ学会「不確実環境下での柔構造最適化モデリングゲ」研究部会
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Possibility Measure, Product Possibility Space and the Notion of Independence

K. Iwamura, M. Kageyama*[1] and Y. Qin*[2] (*1 The Institute of Statistical Mathematics, *2 Graduate School of Science, Chiba University)
Seventh International Conference on Information and Management Sciences, August 12–19, 2008, Urumuchi, China, pp.337–340

Product Possibility Space with Finitely Many Independent Fuzzy Vectors

岩村覚三，安田正實*[1]，景山正幸*[2]，蔵野正美*[3]（*1 千葉大学理学部，*2 統計数理研究所，*3 千葉大学名誉教授）
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Preparedness of Influenza in the commuter towns of Tokyo; Analysis of model cities and a metaphor model

H. Yasuda, K. Suzuki* (* Chiba Univ.)
The NIMS 2008 Conference & The 4th East Asia SIAM Conference, 2008/10/10–12, Daejeon, Korea

多安定型反応拡散方程式におけるフロントの挙動

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Front dynamics in reaction-diffusion equation with multiple stable nonlinearity

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Porous structure of bis（trisbipyridineruthenium(II)）trisoxalatocobaltate(III)chloride

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CSの高分解能スペクトルのnon-Born-Oppenheimer解析

廣瀬　隆，野口剛範，堀合公威，上原博通
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^{13}CS振動回転スペクトルの観測とnon-Born-Oppenheimer解析

廣瀬　隆，堀合公威，上原博通
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配座変換を伴なう1,5-プロトン移動ダイナミクス

百地　舞，若林英嗣，小林啓二
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分子内ヘミアセタール構造を剛直部分とするホスト化合物の設計

橋本　涼，若林英嗣，宮前　博，小林啓二
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α-ケトヒドラゾノ化合物の互変異性構造

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5-(2-ベンゾ[*b*]チエニル)ジベンゾスベレノールの光反応

小野塚達也，毛利真也，若林英嗣，小林啓二
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寺前裕之，橋詰大志郎，長岡伸一[*1]，長嶋雲兵[*2]（*1 愛媛大理，*2 産業技術総合研究所計算科学研究部門・JST-CREST）
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石原康行，寺前裕之，石元孝佳[*]，長嶋雲兵[*]（* 産業技術総合研究所計算科学研究部門・JST-CREST）
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高次元アルゴリズムによる向精神薬の理論的研究

寺前裕之，太田原一成[*1]，石元孝佳[*2]，長嶋雲兵[*2]（*1 ATR 適応コミュニケーション研，*2 産業技術総合研究所計算科学研究部門・JST-CREST）
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寺前裕之，藤田若菜，長岡伸一[*1]，長嶋雲兵[*2]（*1 愛媛大理，*2 産業技術総合研究所計算科学研究部門・JST-CREST）
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佐藤　悟[*1]，前田　優[*1]，稲田浩司[*1]，山田道夫[*1]，土屋敬広[*1]，石塚みどり[*1]，長谷川　正[*1]，赤

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加藤立久，長田良一，枝松　徹，Michael Scheloske[*1]，Wolfgang Harneit[*1]，若原孝次[*2]，宮澤薫一[*2]（*1 Free University Berlin, *2 物材研）
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ポリイン・ヨウ素混合溶液における禁制吸収帯の強度増強効果

和田資子[*]，若林知成[*]，長田良一, 加藤立久（* 近畿大理工）
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C_2H_4–$C^{16}O_2$とC_2H_4–$C^{18}O_2$の高分解能赤外スペクトル

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van der Waals錯体，R_2O–CO_2とR_2O–OCS（R=CH_3, CH_3CH_2）の量子化学計算

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大型太陽光反応装置による水質汚染物質の光触媒分解反応

柳澤一平*，竹内　雅*，岡崎篤志*，小池崇喜*，大山俊之，日高久夫*（* 明星大地球環境科学センター）
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Complete mineralization of the recalcitrant cyanuric acid substrate by ozonation in aqueous TiO_2 suspensions

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State-selected differential cross section measurements for the one-electron capture processes in the F^{4+}–He, Ne Ar systems at $E_{\mathrm{lab}} = 45\mathrm{eV}$

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